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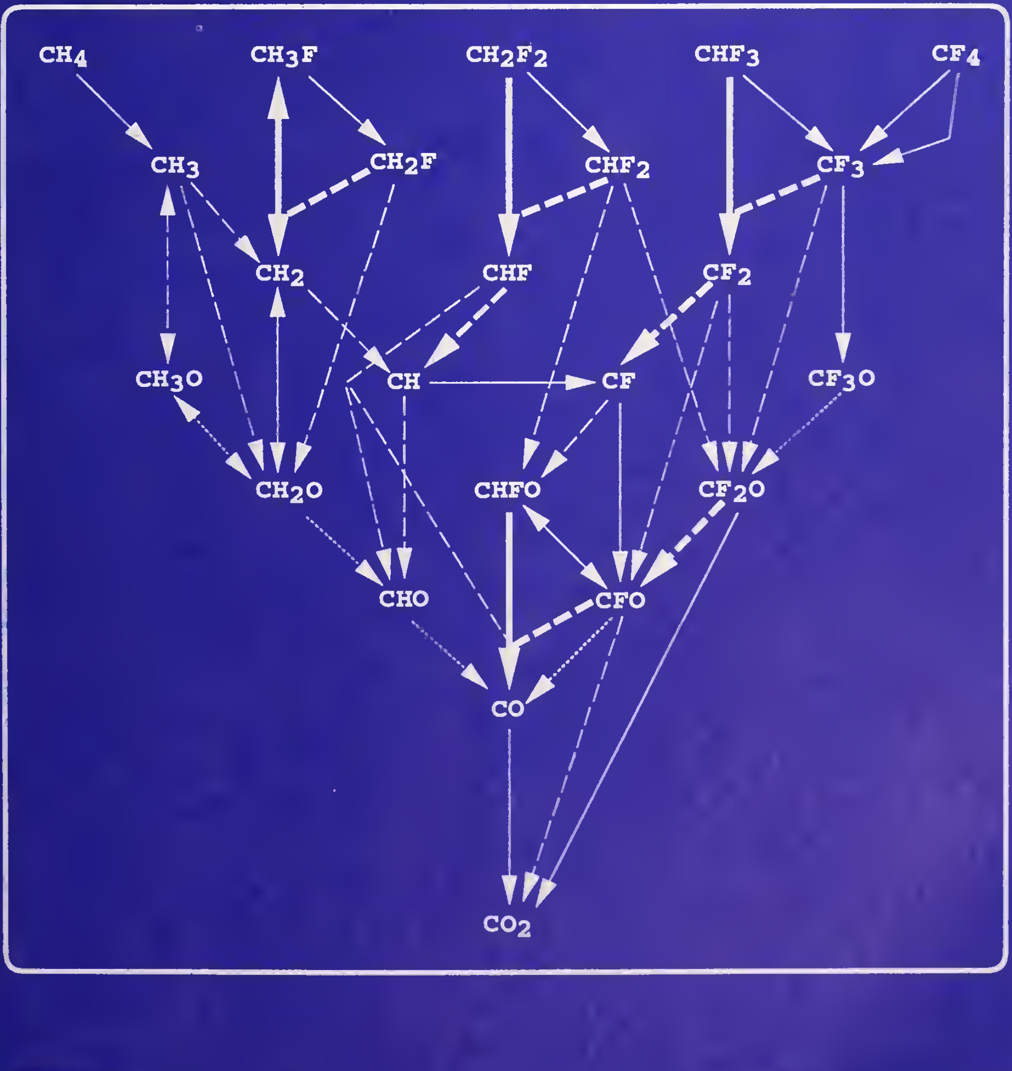
Thermochemical and Chemical Kinetic Data for Fluorinated Hydrocarbons

D. R. F. Burgess, Jr., M. R. Zachariah, W. Tsang, and P. R. Westmoreland



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[1] At Boulder, CO 80303.

[2] Some elements at Boulder, CO 80303.

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EXECUTIVE SUMMARY

A comprehensive, detailed chemical kinetic mechanism was developed and is presented for C_1 and C_2 fluorinated hydrocarbon destruction and flame suppression. Existing fluorinated hydrocarbon thermochemistry and kinetics were compiled from the literature and evaluated. For species where no or incomplete thermochemistry was available, these data were calculated through application of *ab initio* molecular orbital theory. Group additivity values were determined consistent with experimental and *ab initio* data. For reactions where no or limited kinetics was available, these data were estimated by analogy to hydrocarbon reactions, by using empirical relationships from other fluorinated hydrocarbon reactions, by *ab initio* transition state calculations, and by application of RRKM and QRRK methods. The chemistry was modeled considering different transport conditions (plug flow, premixed flame, opposed flow diffusion flame) and using different fuels (methane, ethylene), equivalence ratios, agents (fluoromethanes, fluoroethanes) and agent concentrations. This report provides a compilation and analysis of the thermochemical and chemical kinetic data used in this work.

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1. Introduction

1.1. Overview

The thermochemical and chemical kinetic data presented here were compiled as a part of flame-inhibition modeling that was part of a large, short-term, intensive effort at NIST that evaluated (for the U.S. Air Force, Navy, Army and Federal Aviation Administration) potential fluorinated hydrocarbons and other agents as replacements for Halon 1301 (CF_3Br). The modeling effort complemented the many experimental measurements in the overall NIST program, which characterized the effectiveness of various potential replacements. Our work focused on agent chemistry. This report is to provide documentation of the thermochemical and chemical kinetic data used in the modeling work. Further details of the evaluation of the thermochemical and chemical kinetic data and the *ab initio* calculations will be provided elsewhere, as will the results of the simulations of flame inhibition.

Halon 1301 is very effective as a chemical extinguisher. However, it is also extremely effective for depleting stratospheric ozone. Consequently, its production and use are restricted. The major objective of the modeling part of the overall work was to provide a chemical basis for rationalizing the relative degree of effectiveness of each candidate agent. A fundamental understanding of the chemistry of these agents in hydrocarbon flames should facilitate identification of desired characteristics of effective agents. That is, utilization of simple chemical concepts should enable screening and selection of potential agents with minimal time and human resources.

In order to accomplish this goal, it was necessary to develop a chemical mechanism based on elementary reaction steps for their destruction, their participation in and influence on hydrocarbon flame chemistry, as well as for prediction of potential by-products of incomplete combustion. However, neither a comprehensive mechanism nor a general review of the relevant the relevant chemistry existed prior to this study. Consequently, a significant effort was required in order simply to construct such a comprehensive mechanism prior to its use in any simulations. Further refinement of the mechanism requires experimental validation by flame measurements.

The focus of the mechanism development work was restricted to the chemistry involving only fluoromethanes and fluoroethanes. This includes both four of the candidate agents specifically being considered as replacements (i.e., CH_2F_2, CF_3-CH_2F, CF_3-CHF_2, CF_3-CF_3), as well as all of the other possible fluoromethanes and fluoroethanes. Larger fluorinated hydrocarbon agents (e.g., C_3F_8) and chlorine-substituted agents (e.g., CHF_2Cl) were not explicitly considered in our study, because these additions significantly increase the complexity of the chemistry that must be considered. However, the effectiveness of each can be estimated to some degree by analogy to the other agents that were studied. This can be done by using the qualitative trends observed and the fundamental understanding of the chemistry developed by this and future work.

The complete set of fluoromethanes and fluoroethanes were studied for two basic reasons. These are discussed below.

First, when the four specific candidate agents being considered decompose in the flame, they generate a pool of fluorinated hydrocarbon stable species and radicals, which results in the formation of many of the other fluoromethanes and fluoroethanes. Consequently, in order to describe the decomposition of the four specific agents (and resultant chemistry) adequately, it is necessary to describe the chemistry of all of the many intermediates and products that are created, including most of the other fluoromethanes and fluoroethanes. For example, the lowest energy and primary decomposition pathway for one of the candidate agents, CF_3-CF_3, involves dissociation of the C-C bond to form (two) •CF_3 radicals. These •CF_3 radicals will then react with methyl radicals, •CH_3, which are present in significant concentrations in hydrocarbon flames. This radical-radical combination reaction has two decomposition channels whose relative importance is dependent upon temperature and pressure. One channel results in the formation of a fluoroethylene, $CH_2{=}CF_2$ (and HF by-product). The other channel results in the formation of another fluoroethane, CH_3-CF_3. It is important that the mechanism adequately predicts the combustion products, the magnitude and rate of heat release in the flame, and ultimately the effectiveness of the added agent. Consequently, this requires that the mechanism also be able to describe correctly the decomposition of these two additional stable fluorinated hydrocarbon species (CH_3-CF_3, $CH_2{=}CF_2$). When one considers all decomposition channels for both the candidate agents and their decomposition products, one essentially must include all chemistry describing almost all of the fluoromethanes and fluoroethanes.

Second, given that there are to date few experimental data with which to make comparisons, it is imperative to provide a level of self-consistency to this purely modeling work by considering a range of modeling parameters, including different reactor/flame geometries, different fuels, different (potential) agents, and many other conditions. In doing so, it allowed us to develop confidence in the validity of the qualitative trends that we observed. Quantitative prediction of the absolute or even relative effectiveness of the specific agents will require successful comparison of the simulations with experimental measurements.

1.2. Background

There has been a significant amount of work over many years that has investigated the effectiveness of halogenated fire suppressants, as well as other types of fire suppressants (see Bibliography section). We will not review this body of work, but refer the reader to these and other relevant sources. A large part of our work is based on the pioneering work in this area by Biordi and coworkers (*e.g.*, Biordi *et al.*, 1973), Dixon-Lewis (*e.g.*, Dixon-Lewis, 1977), Fristrom (*e.g.*, Fristrom and Van Tiggelen, 1979) and Westbrook (1983). In earlier experiments on a range of candidates, CF_3Br was identified as being very effective for extinguishing flames. However, the mechanism for inhibition by CF_3Br was not understood. Biordi and coworkers measured both stable and radical species in methane flames doped with CF_3Br using a flame-sampling molecular beam mass spectrometer. Many of the relevant elementary reactions that describe the decomposition of CF_3Br, its chemistry, and its influence on hydrocarbon flames were determined in this work. Westbrook developed the first comprehensive chemical mechanism to describe in detail the chemistry of CF_3Br and modeled inhibition in hydrocarbon flames. As a result of this work, it is generally agreed that flame suppression by bromine-containing compounds is a result of catalytic destruction of H atom species by Br atoms. The ability of bromine to recycle in the chemical system in the flame is directly related to the weak molecular bonds formed by bromine. Thus, bromine when complexed in molecules such as CF_3Br, CH_3Br, HBr, and Br_2, can through a number of reactions regenerate Br atoms. It was also determined in these studies that •CF_3, formed by decomposition of CF_3Br, also removes H atoms by competition with radicals important to combustion (*e.g.*, H, O, OH, HO_2).

There are a variety of ways in which fire suppressants act in inhibiting hydrocarbon flames. Most of these effects are intimately related. For example, a heat loss means a temperature decrease, which causes the chemistry to slow, which means fewer radicals leading to product formation, which means less heat generated, which results in a further temperature decrease and so on. One can separate suppression effects into two general categories: physical and chemical (although there is overlap). Chemical effects are directly related to the characteristics of the specific molecule (*e.g.*, H, F, or Cl substitution), while physical effects, in general, are not. For example, the heat capacity of a molecule is a physical effect, since to a first approximation it is largely a function of the number of atoms in the molecule and their connectivity but not the identity of the molecule (*i.e.*, its chemical composition).

There are a number of physical effects that relate to fluid mechanics, mass transport, and heat transport processes that were not specifically studied as a part of this modeling work. Physical effects that should be taken into account are, for example, PVT properties (pressure-volume-temperature), discharge dynamics, dispersion mechanics, as well as more complex flow reactor geometries than could be considered in this work. We will not discuss these physical effects in any detail here. However, it is necessary to understand the impact of these effects as they relate to our results in order to provide a framework for transfer of the results of our simulations to more realistic conditions. Some of the fluid mechanics and mass transport effects include dilution, turbulent mixing, diffusive mixing, thermal diffusion, and buoyancy. Heat related effects, which cannot directly be addressed in the simulations, include the latent heat of vaporization and non-adiabatic effects, such as radiative cooling or heat losses for flames attached to a cold surface.

There are a number of different types of chemical effects. Most of these involve different competing factors. First, all of the fluorinated hydrocarbons will eventually decompose and then burn (forming CO_2, H_2O, and HF). This liberates heat and increases flame temperatures (this speeds flame chemistry). On the other hand, the agents considered as replacements are large molecules with many atoms. Consequently, their high heat capacities may result in a decrease in flame temperature prior to complete combustion (this slows flame chemistry). The competition between these two factors is strongly dependent upon conditions; most important of which is the mechanics of mixing of the fuel and the oxidizer. Another set of competing effects involves fluorinated radicals produced by agent decomposition. These radicals are slower to burn than their pure hydrocarbon analogues, because the C-F bond is significantly stronger than the C-H bond. Consequently, reactions involving these radicals may effectively compete with analogous pure hydrocarbon chemistry by creating less "flammable" intermediates, thereby inhibiting combustion of the hydrocarbon fuel. For example, since the agents are added to the air stream, their immediate decomposition products (radicals) are formed in oxygen-rich, relatively cold regions of the flame. Consequently, these radicals may be involved in termination steps, such as $\bullet CF_3 + HO_2\bullet \rightarrow CHF_3 + O_2$, slowing radical chain reactions and inhibiting the flame. These radicals also compete with hydrocarbon radicals for important H, O, and OH radicals. On the other hand, these radicals also react with stable molecules in the colder air stream (*e.g.*, O_2), generating more radicals, such as O atoms, and thereby initiating chemistry or promoting combustion of the fuel.

1.3. Mechanism Development

We constructed a large comprehensive reaction set or "mechanism" for fluorinated hydrocarbon chemistry involving C_1 and C_2 stable and radical hydrocarbon species, including partially oxidized fluorinated hydrocarbons. The mechanism should be considered only a framework for future model development, rather than a finished product. Future refinements will require experimental validation by high-temperature flow reactor, premixed flame, and diffusion flame measurements, as well as measurements of important, yet currently uncertain rate constants.

1.4. Acknowledgments

The authors wish to acknowledge support of the project "Agent Screening for Halon 1301 Aviation Replacement" by the U.S. Naval Air Systems Command, the U.S. Army Aviation and Troop Command, the Federal Aviation Administration Technical Center, and the U.S. Air Force. This program at NIST was under the direction of Mr. Michael Bennett at the Wright

Patterson AFB Flight Dynamics Laboratory, Vehicle Subsystems Division, Survivability Enhancement Branch. The authors also wish to express their gratitude to Dr. Carl F. Melius of Sandia National Laboratories for use of the BAC (Bond Additivity Corrections) code.

2. Thermochemistry

2.1. Overview

Existing thermochemical data were compiled and evaluated. Where few or no data existed for potential species of interest (most of the radicals), we estimated that thermochemistry using both empirical methods, such as group additivity (Benson, 1976), and also through application of *ab initio* molecular orbital calculations (Melius, 1990; Curtiss *et al.*, 1991; Frisch *et al.*, 1992). In all cases (experimental, empirical, and *ab initio*), significant effort was made to utilize thermochemical data for each species that was consistent with data for all other species.

There are a number of general sources of relevant compiled and evaluated thermochemical data. These include *The Chemical Thermodynamics of Organic Compounds* (Stull *et al.*, 1969), *JANAF Thermochemical Tables* (Stull and Prophet, 1971; Chase *et al.*, 1985), *Thermochemical Data of Organic Compounds* (Pedley *et al.*, 1986), *TRC Thermodynamic Tables* (Rodgers, 1989), *Physical and Thermodynamic Properties of Pure Chemicals* (Daubert and Danner, 1985), and *NIST Structures and Properties Database and Estimation Program* (Stein *et al.*, 1991). There are two compilations/evaluations of fluorinated hydrocarbons in the *Journal of Physical and Chemical Reference Data*: "Ideal Gas Thermodynamic Properties of Six Fluoroethanes" (Chen *et al.*, 1975) and "Ideal Gas Thermodynamic Properties of Halomethanes" (Kudchadker and Kudchadker, 1978). There are two compilations/evaluations of fluorinated hydrocarbons in the *Russian Chemical Reviews*: "Thermochemistry of Halogenomethanes" (Kolesov, 1978) and "Thermochemistry of Haloethanes" (Kolesov and Papina, 1983). There are a few individual sources of more recent data for thermochemistry that are relevant. These include "Thermochemistry of Fluorocarbon Radicals" (Rodgers, 1978), "Hydrocarbon Bond Dissociation Energies" (McMillen and Golden, 1982), "A Kinetic Study of the Reactions of OH Radicals with Fluoroethanes. Estimates of C-H Bond Strengths in Fluoroalkanes" (Martin and Paraskevopoulos, 1983), and "Halomethylenes: Effects of Halogen Substitution on Absolute Heats of Formation" (Lias *et al.*, 1985). There are numerous other references with thermodynamic data for fluorinated hydrocarbons that we have compiled as part of this work. These are included in the Bibliography section and some of them will be cited and, possibly, be discussed in more detail in the relevant sections.

It should be noted that for some of the stable species and for many of the radicals, we have relied upon recent *ab initio* calculations of thermochemical data. This includes both *ab initio* calculations done as part of work and those done previously by other workers. Tschuikow-Roux and coworkers have calculated thermochemistry for the fluoroethyl radicals (Chen *et al.*, 1990a, 1990b; Chen *et al.*, 1991a, 1991b). Nyden (1993) has used *ab initio* calculations to obtain thermochemical data for a number of the fluoroethanes and fluoroethyl radicals. Details of our *ab initio* calculations can be found elsewhere (Burgess *et al.*, 1994; Zachariah *et al.*, 1995).

The thermochemical data that was used is given Tables 1-3 for hydrogen/oxygen and hydrocarbon species (Table 1), H/F species and C_1 fluorinated hydrocarbons (Table 2), and C_2 fluorinated hydrocarbons (Table 3). These tables include enthalpies of formation, entropies (at standard state), and temperature-dependent heat capacities. Comparisons between our calculated values (Zachariah *et al.*, 1995) and different literature values (experimental and estimated) for heats of formation are given in Table 4. Reported uncertainties in the literature values are also given in Table 4.

A discussion of the uncertainties in the thermochemical data is given in the text with each class of species. The literature values include those which have been calculated using *ab initio* methods. A critical evaluation of the *ab initio* values in comparison with experimentally derived values will be given in a future publication. In each case where the uncertainty in the data from the literature was not assigned, we have provided a value based on our limited evaluation of the data and typical uncertainties for that type of data.

The literature values for heats of formation consist of a number of different types of data. Many are good quality, experimentally derived values based on heat of combustion or heat of reaction data, where the other reactants and products have well-established heats of formation. The uncertainty in these data are typically less than 4 kJ/mol. Some of the data, although experimentally derived, have somewhat higher uncertainties due to side reactions or where the other reactants and products have somewhat uncertain heats of formation. Typically, these values have heats of formation with uncertainties of about 4-8 kJ/mol.

In some cases, the literature values are based, in whole or in part, on bond additivity, group additivity, or other trends in heats of formation of related species. Typically, these values have heats of formation with uncertainties of about 8-12 kJ/mol. Many of the radicals have literature values for their heats of formation that were determined using the heats of formation of the parent species and bond dissociation energies that were either indirectly measured or were reasonable estimates based on trends in other molecules. For example, Martin and Paraskevopoulos (1983) have estimated C-H bond strengths in fluoromethanes and fluoroethanes (and, consequently, heats of formations for the fluoromethyl and fluoroethyl radicals) through correlations between the rates of H atom abstraction by OH radicals, C-H vibrational frequencies, and known C-H bond strengths. We have supplemented these data with our own estimates in order to provide heats of formation for the other fluoroethyl radicals in the absence of other literature values.

2.2. H/O/F and Hydrocarbon Species

We used standard hydrogen/oxygen and hydrocarbon thermochemistry, most of which can be found in the JANAF tables (Stull and Prophet, 1971; Chase *et al.*, 1985) or in a Sandia compilation (Kee *et al.*, 1987), as can data for F and HF. There is a more recent value for the heat of formation of HF (Johnson *et al.*, 1973). However, we used the JANAF value for consistency, because many thermochemical and rate data for fluorinated species are based on the JANAF recommendation. More recent data on thermochemistry for C_2H_3 and HCO have been utilized. Future mechanism refinements should include re-adjustment of any other thermochemistry (or rate constants) that are based upon older values for the heat of formation of these species.

Other simple species (*e.g.*, F_2, FO•, HOF, FOF, FOO•, HOOF) were initially considered in the mechanism but were later excluded because they did not contribute to the overall chemistry.

2.3. C_1 Fluorinated Hydrocarbons

2.3.1. Fluoromethanes

We have chosen to employ heats of formation for the fluoromethanes recommended by Kolesov (1978) with the entropy and heat capacity data found in a review article (Rodgers *et al.*, 1974) in the Journal of Physical and Chemical Reference Data (JPCRD). We note that heats of formation for the fluoromethanes from our *ab initio* calculations (Zachariah *et al.*, 1995) using the BAC-MP4 method (Melius, 1990) are within about 2 kJ/mol of these recommended values.

There are a number of sources of compiled or evaluated thermochemical data for the fluoromethanes (CH_3F, CH_2F_2, CHF_3, and CF_4). Thermochemical data for the fluoromethanes has been reviewed by Lacher and Skinner (1968), by Stull *et al.* (1969), and by Cox and Pilcher (1970). Thermochemical data can also be found in the JANAF tables (Stull and Prophet, 1971), has been re-examined subsequently in JPCRD (Rodgers *et al.*, 1974), by Pedley *et al.* (1986), and mostly recently, by Gurvich, Veyts, and Alcock (1991). The most recent edition of the JANAF tables (Chase *et al.*, 1985) did not re-examine thermochemical data for the fluoromethanes. Recommendations for the heats of formation of the fluoromethanes have been also been made by Kolesov (1968). Gelles and Pitzer (1953) have tabulated entropy at standard state and heat capacity as a function of temperature for the fluoromethanes (and other halogenated methanes).

Heats of formation for CH_2F_2 and CF_4 are the best known, with uncertainties of less than 1.5 kJ/mol, and are derived from their heats of combustion. The JPCRD recommended value for the heat of formation of CH_2F_2 is based on a measurement by Neugebauer and Margrave (1958) of the heat of combustion of CH_2F_2. The heat of formation of CF_4 is based on measurements of a number of different heats of reactions involving CF_4 by Scott *et al.* (1955), Good *et al.* (1956), Neugebauer and Margrave (1956), Cox *et al.* (1965), Wood *et al.* (1967), Domalski and Armstrong (1967), and Greenberg and Hubbard (1968).

The heat of formation of CHF_3 has a slightly higher uncertainty (than for CH_2F_2 and CF_4) of about 4 kJ/mol due to side reactions (producing CF_4) in its combustion. The JPCRD recommended value for the heat of formation of CHF_3 is based on a heat of combustion measurement by Neugebauer and Margrave (1958). The heat of formation of CHF_3 has also been calculated using equilibrium data with CF_3Br and CF_3I as measured by Corbett *et al.* (1963), Goy *et al.* (1967), Coomber and Whittle (1967). The heat of formation of CHF_3 can also be calculated assuming a heat of formation for $\bullet CF_3$ and kinetic data (forward and reverse reactions) involving HCl, HBr, and HI as measured by Coomber and Whittle (1966), Amphlett and Whittle (1968), and Goy *et al.* (1967), respectively.

The heat of formation of CH_3F has been estimated (with an uncertainty of about 10 kJ/mol) employing empirical trends in heats of formation of the other fluoromethanes, since there are no experimentally derived values (other than from appearance potential measurements). Although CH_3F is unlikely to be a key species in fluorinated hydrocarbon-inhibited hydrocarbon flames, as the simplest fluorinated hydrocarbon, its heat of formation is significant for benchmarking heats of formation of other fluorinated hydrocarbons. Empirical estimates for the heat of formation of CH_3F have also been made by Zahn (1934), Allen (1959), Bernstein (1965), Rodgers (1967), and Lacher and Skinner (1968). The recommended value in the JANAF tables (Stull and Prophet, 1971) is based on appearance potentials for CH_3^+ from CH_3F measured by Lossing *et al.* (1954). Dibeler and Reese (1955) and Tsuda *et al.* (1964) have also measured roughly the same appearance potential.

2.3.2. Fluoromethyl Radicals

We have chosen to employ the heats of formation recommended by McMillen and Golden (1982). For entropies at standard state and heat capacity data, we used values for $\bullet CF_3$ from the JANAF tables. Since (to our knowledge) no experimentally derived entropy and heat capacity data exist for $\bullet CH_2F$ and $\bullet CHF_2$, we used that derived from our BAC-MP4 *ab initio* calculations. We note that the calculated heats of formation for the fluoromethyl radicals are within about 4 kJ/mol of the recommended experimental values.

There are a few sources of compiled or evaluated thermochemical data for the fluoromethyl radicals. Thermochemical data for the perfluoromethyl radical ($\bullet CF_3$) can be found in the JANAF tables (Stull and Prophet, 1971) and have been re-examined subsequently by Rodgers (1978). The heat of formation of $\bullet CF_3$ has an uncertainty of about 5 kJ/mol. Experimentally derived heats of formation (from bond dissociation energies and heat of reactions) for all of the fluoromethyl radicals (•CH_2F, •CHF_2, •CF_3) can be found in evaluations by McMillen and Golden (1982) and Pickard and Rodgers (1983) with uncertainties of less than 10 kJ/mol.

The evaluated thermochemical data for •CH_2F and •CHF_2 are based on a number of different experimental measurements. Okafo and Whittle (1974) have used heat of reaction data to determine the bond dissociation energy for CHF_2-Br, from which the heat of formation of •CHF_2 can be calculated. Martin and Paraskevopoulos (1983) have measured the rates of reaction of OH with some fluoromethanes and fluoroethanes and developed correlation between C-H bond dissociation energies, C-H stretching frequencies, and rates of abstraction of H atoms by OH radicals from fluoroalkanes. From heats of formation of the parent fluoromethanes and estimated C-H bond dissociation energies, one can determine values for the heats of formation of •CH_2F, •CHF_2, and •CF_3. Whittle and coworkers have used heat of reaction data to determine the bond dissociation energies of CHF_2-H and CHF_2-Br (Okafo and Whittle, 1974), from which the heat of formation of •CHF_2 can be calculated. Using kinetic data, bond dissociation energies for CH_2F-H have obtained by Pritchard and Perona (1969) and for CHF_2-H by Kerr and Timlin (1971), from which one can calculate the heats of formation of the corresponding radicals.

The evaluated thermochemical data for •CF_3 are based on a number of different experimental measurements. The heat of formation of •CF_3 has been calculated assuming a heat of formation for CHF_3 and kinetic data (forward and reverse reactions) involving HCl, HBr, and HI, as measured by Coomber and Whittle (1966), Amphlett and Whittle (1968), and Goy *et al.* (196 7), respectively. It can also be calculated assuming a heat of formation of CF_3I and kinetic data for its reaction with I_2, as determined by Coomber and Whittle (1966). Pritchard and Thommarson (1964) used kinetic data from competing reactions to determine the CF_3-H bond dissociation energy and, consequently, the heat of formation of •CF_3 can be calculated assuming a heat of formation for CHF_3. Whittle and coworkers have used heat of reaction data to determine the bond dissociation energies for CF_3-CF_3 (Coomber and Whittle, 1967), CF_3-Br (Ferguson and Whittle, 1972), and CF_3-I (Okafo and Whittle, 1975), from which the heat of formation of •CF_3 can be calculated. Tsang (1986) has determined a value for the heat of formation of •CF_3 based on the bond dissociation energy of CF_3-Br from shock tube decomposition studies.

2.3.3. Fluoromethylenes and Fluoromethylidyne Radical

We used heats of formation for :CF_2 as adopted by Rodgers (1978) and for :CHF as provided by Pritchard *et al.* (1984). For entropies at standard state and heat capacity data of both species, we used values from the JANAF tables. We note that heats of formation for both species from our BAC-MP4 *ab initio* calculations (Zachariah *et al.*, 1995) are within about 15 kJ/mol of the recommended experimental values.

There are a few sources of thermochemical data for the closed-shell fluoromethylenes (:CHF and :CF_2). Thermochemical data for these species can be found in the JANAF tables (Stull and Prophet, 1971). More recently, Rodgers (1978) has recommended a value for the heat of formation of :CF_2 based largely upon kinetic data. Hsu *et al.* (1978) and Pritchard *et al.* (1984) have independently made a recommendation for the heat of formation of :CHF based upon heat of reaction and kinetic data. Lias *et al.* (1985) have provided values for the heat of formation of both :CHF and :CF_2 based upon appearance and ionization potentials. Unfortunately (since :CHF and :CF_2 are important species), there are significant uncertainties in their heats of formation. The values for :CF_2 are the best (±10 kJ/mol) and are derived from a number of different types of measurements. The uncertainty in the heat of formation for :CHF is even greater (±30 kJ/mol) due to the lack of direct, reliable data.

The experimental data for the heat of formation of :CF_2 comes from a number of different measurements. The heat of formation of :CF_2 has been calculated from heat of reaction or kinetic data from the decomposition of C_2F_4 by Modica and LaGraff (1965, 1966), by Zmbov *et al.* (1968), by Schug and Wagner (1968), and by Carlson (1971). Using equilibrium data in experiments by Farber *et al.* (1969), one can also determine a value. The heat of formation of :CF_2 has also been calculated from the decomposition of various halomethanes: from the decomposition of CHF_3 by Schug and Wagner (1978), from the decomposition of CHF_2Br by Okafo and Whittle (1974), and from the decomposition of CHF_2Cl by Dalby (1964), Gozzo and Patrick (1964), Edwards and Small (1965), and Schug and Wagner (1968). The ionization potential of $:CF_2$ has been used to estimate its heat of formation by Fisher *et al.* (1965), Pottie (1965), and Zmbov *et al.* (1968). Various appearance potential measurements by Walter *et al.* (1969), Berman *et al.* (1981), and Paulino and Squires (1991) have also been used to estimate a value for the heat of formation of $:CF_2$. The ionization and appearance potential measurements have been reviewed in detail by Lias *et al.* (1985) and Paulino and Squires (1991).

Thermochemical data for fluoromethylidyne (•CF) can be found in the JANAF tables (Stull and Prophet, 1971). More recently, Gurvich *et al.* (1991) have also provided thermochemical data for •CF. In the latter review, more recent measurements by Hildenbrand (1975) were also considered, in addition to earlier measurements by Modica (1966) and Farber *et al.* (1969). We used the more recent value from Gurvich *et al.* (1991) for the heat of formation with the entropy and heat capacity data provided in the JANAF tables. The reported uncertainties in the heat of formation are about 10 kJ/mol. We note that our BAC-MP4 *ab initio* heat of formation for •CF is within about 10-20 kJ/mol of the recommended values.

2.3.4. Carbonyl Fluorides and Fluoromethoxy Radicals

Thermochemical data for the carbonyl fluorides ($CHF{=}O$, $CF_2{=}O$, $\bullet CF{=}O$) can be found in the JANAF table. We have employed these data. The uncertainty in the heat of formation of $CF_2{=}O$ is reported to be about 2 kJ/mol. For the other two carbonyl fluorides, where there is little or no experimental data, the estimated uncertainty in their heats of formation are probably at least 15 kJ/mol.

Gurvich *et al.* (1991) have recommended a value for the heat of formation of $\bullet CF{=}O$ that is similar to the JANAF recommendation (about 8 kJ/mol higher). This recommendation is based upon appearance potential measurements of McNeil and Thynee (1969) and heat of reaction measurements by Heras *et al.* (1962).

We note that heats of formation for these species from our BAC-MP4 *ab initio* calculations (Zachariah *et al.*, 1995) are within about 20 kJ/mol of the recommended experimental values, except for $CF_2{=}O$, where the *ab initio* value is about 40 kJ/mol higher. Other *ab initio* calculations (Montgomery *et al.*, 1994; Schnieder and Wallington, 1994) using different approaches also predict a heat of formation for $CF_2{=}O$ that is higher (by about 30 kJ/mol) than the experimental value. Because of this significant difference, both uncertainties in the experimental measurements and *ab initio* calculations warrant further examination.

The biggest uncertainties here are for CHF=O (±20 kJ/mol) and •CF=O (±10 kJ/mol), where there are little or no direct experimental data available and, consequently, their heats of formation were estimated (Stull and Prophet, 1971) using average bond dissociation energies from other related compounds. Given that reliable experimental data exists for the unimolecular decomposition of CHF=O (Saito *et al.*, 1985), uncertainty in its heat of formation may be unimportant. However, under some conditions the bimolecular reaction $\bullet CF=O + H_2O \rightarrow CHF=O + OH$ (roughly 80 kJ/mol endothermic) may contribute. Consequently, uncertainty in the heat of formation of CHF=O may play some role. In contrast, the heat of formation of •CF=O is very important, since there are not experimental data for its unimolecular decomposition, which is a primary decomposition pathway (competing with H atom combination followed by HF elimination).

We used an experimentally derived value for the heat of formation of the perfluoromethoxy radical $CF_3O\bullet$ (Batt and Walsh, 1982) with a reported estimated uncertainty of about 6 kJ/mol. For entropy at standard state and heat capacity data, we used that derived from our BAC-MP4 *ab initio* calculations (Zachariah *et al.*, 1995). The heat of formation of $CF_3O\bullet$ from the *ab initio* calculations is within about 30 kJ/mol of the experimentally derived value.

A number of other species, such as the other fluoromethoxy radicals ($CH_2FO\bullet$, $CHF_2O\bullet$), fluoromethanols (*e.g.*, CF_3OH), or fluoromethylperoxy radicals (*e.g.*, $CF_3OO\bullet$), were initially considered in the mechanism (using *ab initio* thermochemical data). These species were later excluded, because they did not contribute to the overall chemistry. In many cases, these species were present in steady state concentrations and, consequently, the creation and destruction reactions could be combined into a single overall reaction. Although these species may be important in atmospheric chemistry, they are present in extremely low concentrations at high temperatures in hydrocarbon/air flames.

2.4. C_2 Fluorinated Hydrocarbons

2.4.1. Fluoroethanes

We chose to use thermochemical data from a Journal of Physical and Reference Data (JPCRD) review (Chen *et al.*, 1975) for the six simple fluoroethanes (CH_3-CH_2F, CH_3-CHF_2, CH_3-CF_3, CH_2F-CF_3, CHF_2-CF_3, CF_3-CF_3). For CH_2F-CH_2F, we used a heat of formation calculated using the C-C bond dissociation energy as determined by Kerr and Timlin (1971) and the heat of formation for •CH_2F as recommended by McMillen and Golden (1982). We used the heat of formation of CH_2F-CHF_2 as recommended by Lacher and Skinner (1968). For CHF_2-CHF_2, we used a heat of formation calculated using the C-C bond dissociation energy as determined by Millward *et al.* (1971) and the heat of formation for •CHF_2 as recommended by McMillen and Golden (1982). Standard state entropy and heat capacities for these other 3 fluoroethanes were computed based on vibrational frequencies and moments of inertia from our *ab initio* calculations. We note that heats of formation for all of the fluoroethanes from our BAC-MP4 *ab initio* calculations are within about 10-20 kJ/mol of the recommended experimental or empirical values.

We believe some re-examination of all of the heat of formation data is warranted. For example, the heat of formation of CH_3-CF_3 recommended in the JPCRD review is based on old values for •CH_3 and •CF_3. In addition, employing a group additivity scheme with an ionic correction should yield better values for both CH_2F-CH_2F and CHF_2-CHF_2.

There are a number of sources of compiled or evaluated data for the fluoroethanes. Thermochemical data for some of the fluoroethanes can be found in JPCRD (Chen *et al.*, 1975) and the DIPPR compilation (Daubert and Danner, 1985). Recommendations for the heats of formation of some of the fluoroethanes have been made by Kolesov and Papina (1983) and by Pedley *et al.* (1986). There are no experimentally derived heats of formation for two of the fluoroethanes (CH_3-CH_2F, CH_2F-CF_3). These have been estimated using bond additivity, group additivity, or other trends in heats of formation. However, there are significant uncertainties in using these procedures, because of non-covalent or ionic contributions to the stability of these species due to the high electronegativity of fluorine. For example, CH_3-CF_3 is about 33 kJ/mol more stable than predicted using heats of formation of CH_3-CH_3 and CF_3-CF_3. All three of these species have heats of formation that were derived from good quality experimental measurements. The additional stabilization can be rationalized as an ionic contribution to the C-C bond strength because of large differences in net charges on the carbon atoms of the -CH_3 and -CF_3 groups due to the high electronegativity of the F atoms.

There are a number of different sources of experimental data for the heats of formation of the fluoroethanes. These various sources are described in the paragraphs below.

The heat of formation of ethyl fluoride (CH_3-CH_2F) has been estimated (Chen *et al.*, 1975) using group additivity and heat of reaction data for propyl fluoride (Lacher *et al.*, 1956). A recommendation for the heat of formation of ethyl fluoride (CH_3-CH_2F) has recently been given by Luo and Benson (1988) based on electronegativity correlations of heats of formation of substituted alkanes and is significantly lower (15 kJ/mol) than other recommendations. The reasons for this significant difference warrant further examination. CH_3-CH_2F is unlikely to be important as a species in the fluorocarbon-inhibited hydrocarbon flames. However, as a simple, single-substituted fluorinated hydrocarbon (like CH_3F), its heat of formation is important as a reference point for the heats of formation of other species. For example, another -CH_2F substituted fluoroethane, CH_2F-CF_3, has no experimentally derived heats of formation. Any uncertainties in the heats of formation and, consequently, stability of the fluoroethanes will influence product channels for fluoromethyl combinations (*e.g.*, $\bullet CH_3 + \bullet CF_3 \rightarrow CH_3\text{-}CF_3$ versus $\bullet CH_3 + \bullet CF_3 \rightarrow CH_2{=}CF_2 + HF$).

Kolesov *et al.* (1968) have measured the heat of combustion of CH_3-CHF_2, from which one can calculate its heat of formation. The heat of formation of CH_3-CHF_2 could be determined from the enthalpy of hydrogenation of $CF_2{=}CCl_2$ as measured by Lacher *et al.* (1956) given a reliable value for the heat of formation of $CF_2{=}CCl_2$ could be obtained.

We calculated a heat of formation for CH_2F-CH_2F based on the C-C bond dissociation energy (368.6 kJ/mol) as determined by Kerr and Timlin (1971) and the heat of formation for $\bullet CH_2F$ (-32.6 kJ/mol) as recommended by McMillen and Golden (1982). The bond dissociation energy was determined from the critical energy (E_o) calculated using RRKM analysis of experimental kinetic data for thermal (Chang and Setser, 1969) and chemically activated decomposition of CH_2F-CH_2F.

Kolesov *et al.* (1965) have determined a heat of formation for CH_3-CF_3 by measuring its heat of combustion. Kinetic data for the forward and reverse reactions for $\bullet CH_3 + \bullet CF_3 \longleftrightarrow CH_3\text{-}CF_3$ can be used to obtain a heat of formation for 1,1,1-trifluoroethane. Kinetic data for this reaction have been obtained by Giles and Whittle (1965), Pritchard and Perona (1970), and Chang *et al.* (1972). These data have been reviewed by Rodgers and Ford (1973).

The heat of formation of CH_2F-CHF_2 has been determined (Kolesov and Papina, 1983) from the enthalpy of hydrogenation of CF_2=CFCl as measured by Lacher *et al.* (1956).

We have calculated a heat of formation for CHF_2-CHF_2 based on the C-C bond dissociation energy (382.4 kJ/mol) as determined by Millward *et al.* (1971) and the heat of formation for $\bullet CHF_2$ (-247.7 kJ/mol) as recommended by McMillen and Golden (1982). The bond dissociation energy was set equal to the activation energy for thermal decomposition of CHF_2-CHF_2, which was determined from analysis of experimental kinetic data.

The heat of formation of CHF_2-CF_3 can be obtained from equilibrium data with CF_3-CF_2Br (and group additivity) as measured by Whittle and coworkers (Coomber and Whittle, 1967; Ferguson and Whittle, 1972) and from heat of reaction data for the bromination of CF_2=CF_2 (and group additivity) as measured by Lacher *et al.* (1956). In addition, one can calculated a value for the heat of formation for CHF_2-CF_3 from the heat of formation of the perfluoroethyl radical (CF_3-$CF_2\bullet$) and the CF_3CF_2-H bond dissociation energy. Wu and Rodgers (1976) determined the heat of formation of the perfluoroethyl radical by measuring the enthalpy of its reaction with I_2. Values for the bond dissociation energy of CF_3CF_2-H have been determined by Bassett and Whittle (1972) and Martin and Paraskevopoulos (1983).

The heat of formation of CF_3-CF_3 has been determined from equilibrium data with CF_3Br as measured by Coomber and Whittle (1967), with CF_3-CN as measured by Walker *et al.* (1970), and with CF_4 (and NF_3 as the oxidizer) as measured by Sinke (1966).

2.4.2. Fluoroethyl Radicals

In the absence of reliable experimental data, we used the calculated thermochemical data for the fluoroethyl radicals as provided by Tschuikow-Roux and coworkers (Chen *et al.*, 1990a, 1990b; Chen *et al.*, 1991a, 1991b) for consistency. However, we believe some re-examination of all of the heat of formation data (both experimental and *ab initio*) is warranted. For the radical CH_3-CHF•, we used the average of the heats of formation reported by Martin and Paraskevopoulos (1983) and Tschuikow-Roux and Salomon (1987). For the three fluoroethyl radicals, CH_2F-CHF•, CHF_2-CF_2•, and CF_3-CHF•, we calculated heats of formation based on C-H bond dissociation energies determined by Martin and Paraskevopoulos (1983). We note that heats of formations for the fluoroethyl radicals from our BAC-MP4 *ab initio* calculations (Zachariah *et al.*, 1995) are within about 10-20 kJ/mol of the recommended literature values.

There are a number of sources of heats of formation for the fluoroethyl radicals. There are experimentally derived thermochemical data (Rodgers, 1978) for a few of the fluoroethyl radicals (CH_3-CF_2•, CF_3-CH_2•, CF_3-CF_2•). Heats of formation for the others have been estimated using heats of formation for the fluoroethanes and C-H or C-F bond dissociation energies for CH_3-CHF• and CF_3-CHF• by Martin and Paraskevopoulos (1983), for CH_3-CHF• by Tschuikow-Roux and Salomon (1987), and for all of the other fluoroethyl radicals by Burgess and Zachariah (this work). Thermochemistry for all of the fluoroethyl radicals have been calculated using *ab initio* molecular orbital theory by Tschuikow-Roux and coworkers (cited above). They used the experimentally derived heats of formation of the 3 fluoroethyl radicals recommended by Rodgers (1978). For the others, they used their calculated energies in conjunction with isodesmic-homodesmic reactions (with known experimental reaction enthalpies) to provide values that approach the "true" heats of formation.

2.4.3. Fluoroethylenes and Fluorovinyl Radicals

We used the heat of formation of CH_2=CHF as recommended by Gurvich *et al.* (1991). Entropy at standard state and heat capacity data were taken from the DIPPR compilation (Daubert and Danner (1985). These data can also be found in the TRC Thermodynamic Tables (1990). The heat of formation data are based on measurements by Kolesov and Papina (1970) of the heat of combustion of vinyl fluoride. Pedley *et al.* (1986) have also made a recommendation based on this experimental data. A heat of formation was also determined by Williamson *et al.* (1976) based on appearance potential measurements.

We have chosen to use heats of formation for CHF=CHF(*E*) and CHF=CHF(*Z*) based on appearance ionization potential measurements by Stadelman and Vogt (1980) and entropies at standard state and heat capacities based on geometries and vibrational frequencies from our BAC-MP4 *ab initio* calculations (Zachariah *et al.*, 1995). Gurvich *et al.* (1991) have also estimated heats of formation for these species using a bond additivity method. For $CH_2=CF_2$, we used the heat of formation recommended by Gurvich *et al.* (1991) with entropy at standard state and heat capacity data taken from Stull *et al.* (1969). Recommendations for the heat of formation for 1,1-difluoroethylene have also been made by Lacher and Skinner (1968), Stull *et al.* (1969), Cox and Pilcher (1970), and Pedley *et al.* (1970). All of these recommendations are based on heat of combustion measurements by Neugebauer and Margrave (1956) and Kolesov *et al.* (1962).

We used thermochemical data for $CHF=CF_2$ as recommended by Gurvich *et al.* (1991). The heat of formation data is based on an experimental measurement by Kolesov *et al.* (1962) of the heat of combustion of trifluoroethylene. Recommended values (also based on these experiments) can be found in the evaluations of Stull *et al.* (1969), Cox and Pilcher (1970), and Pedley *et al.* (1986).

We used thermochemical data for $CF_2=CF_2$ from the JANAF tables (Stull and Prophet, 1971). The recommended heat of formation is based the heat of reaction data for conversion to amorphous carbon by Neugebauer and Margrave (1956) and Kolesov *et al.* (1962). Lacher and Skinner (1968), Stull *et al.* (1969), Cox and Pilcher (1970), Kolesov and Papina (1983), Pedley *et al.* (1986), and Gurvich *et al.* (1991) have all reviewed the existing experimental data and made recommendations. These evaluations were made based upon a number of different sources of experimental heat of reaction data for perfluoroethylene, including the data of Lacher *et al.* (1949), Lacher *et al.* (1950), Kirkbride and Davidson (1954), von Wartenberg and Schiefer (1955), Duus (1955), Neugebauer and Margrave (1956), Lacher *et al.* (1956), Scott *et al.* (1956), Kolesov *et al.* (1962), and Edwards and Small (1964).

We note that the heats of formation for the fluoroethylenes that we have calculated using the BAC-MP4 *ab initio* method are within about 10 kJ/mol of the recommended experimental values.

There are not any experimentally derived thermochemical data (to our knowledge) for the fluorovinyl radicals, other than the heat of formation for $CF_2=CF\bullet$. The heat of formation of the perfluorovinyl radical has been estimated by Bryant (1962) based on trends in C-F bond dissociation energies for perfluorocarbons. Gurvich *et al.* (1991) recommended a value based on a review of appearance potential measurements by Thynee and MacNeil (1970), Lifshitz and Crajower (1972), and Bibby and Caster (1966). Because of the lack of experimental data for most of the fluorovinyl radicals, we chose to use thermochemical data from our BAC-MP4 *ab initio* calculations (Zachariah *et al.*, 1995) in order to provide a consistent set. We note that our calculated value is within about 10 kJ/mol of the experimentally derived value that was recommended by Gurvich *et al.* (1991).

2.4.4. Fluoroacetylenes, Fluoroketenes, and Fluoroketyl Radical

Data on the thermochemistry of the fluoroacetylenes (C_2HF, C_2F_2) can be found in the JANAF tables (Stull and Prophet, 1971), however, with relatively large uncertainties: ±60 kJ/mol and ±20 kJ/mol in the heats of formation, respectively. Fluoroketenes ($CHF=C=O$ and $CF_2=C=O$) and the fluoroketyl radical ($\bullet CF=C=O$) can be formed through a number of channels. These channels are analogous to those considered in pure hydrocarbon chemistry for ketene ($CH_2=C=O$). To assess the importance of the fluoroketene species and relevant reactions, we included these species in the mechanism. There are not any experimentally derived data for these species. Consequently, we used data from our BAC-MP4 *ab initio* calculations (Zachariah *et al.*, 1995).

A number of other partially oxidized species, such as CH_3-CFO, were excluded from the mechanism based on the assumption that they would be only present in steady state concentrations at flame temperatures. For lower temperatures, these species may become important and, consequently, our assumption should be re-examined. It is possible that perfluoro-oxidized species, such as CF_3-CFO, may be present at flame temperatures. For example, since both $\bullet CF_3$ and $\bullet$CFO are present in significant concentrations, the combination of these species (and stabilization) may be a source of CF_3-CFO. This should be examined in future refinements of this mechanism.

2.5. BAC-MP4 *Ab Initio* Predictions

For a number of species considered in the reaction set, especially the radicals, there are little or no thermochemical data. Consequently, we have estimated that data using BAC-MP4 *ab initio* calculations (see description below). In order to quantify the uncertainties in the calculated data, we have also performed calculations on many related species where there is good quality experimental data.

Structures, energies, and thermochemical data for a large number of C_1 and C_2 hydrocarbons, oxidized hydrocarbons, hydrofluorocarbons, and oxidized hydrofluorocarbons, including radical species, were calculated using the BAC-MP4 procedure as outlined by Melius (1986). This procedure involves *ab initio* molecular orbital calculations using the Gaussian series of programs (Frish *et al.*, 1990), followed by application of a bond additivity correction (BAC) procedure to the *ab initio* calculated energies. The BAC procedure enables energies to be calculated at accuracies that are necessary for chemical applications, without the need to resort to large basis sets or configuration interaction terms. This is a particularly important issue when the goal is the generation of a sufficiently complete data set necessary for development of a detailed chemical mechanism.

Equilibrium geometries, vibrational frequencies, and zero point energies were calculated at the Hartree-Fock level using a 6-31G(d) basis set (HF/6-31G*). Using these geometries, single point energies were calculated with 4th order Moller-Plesset theory using a 6-31G(d,p) basis set (MP4/6-31G**), to which the BAC procedure was applied. In the BAC method, errors in the electronic energy of a molecule are bond-wise additive and depend on bonding partner, distance, and next-nearest neighbors. The energy per bond is corrected by calibration at a given level of theory against molecules of known energy.

Table 4 lists calculated heats of formation for most of the species in the reaction set, as well as literature values (where available). We note that we have calculated thermochemical data for a number of related species that are not included in the reaction set. These data are also included in Table 4 for purposes of comparison. Of the approximately 110 species, where we have calculated heats of formation, about 70 species have literature values. We note that the literature values consist of a number of different types of data, including estimated and calculated values, in addition to those that are derived from experimental measurements.

The average difference between the BAC-MP4 and the literature values is about 9.5 kJ/mol, while the standard deviation is about 7.5 kJ/mol. From these data, we conclude that for the fluorinated hydrocarbon system, that heats of formation calculated using the BAC-MP4 method provide values that are accurate to less than 10 kJ/mol or comparable to the majority of the experimentally derived values. We believe that the precision of the *ab initio* values for any homologous series to be significantly better than that which is typically obtainable from experimental measurements. This becomes evident when calculated bond dissociation energies are compared to those derived from experimental measurements. A more detailed discussion and comparison can be found elsewhere (Zachariah *et al.*, 1995).

Of all the species, $CF_2=O$ has the largest difference between calculated and experimental values. Although the quoted uncertainty for this molecule is small, there is reason to believe that the experimental data may have had side reactions complicating its determination. In addition, other recent calculations (Schnieder and Wallington, 1994; Montgomery *et al.*, 1994) using other *ab initio* methods predict a heat of formation for $CF_2=O$ that is consistent with our BAC-MP4 calculated value. There are a number of other oxyfluoro-species that have significant differences between calculated and literature values. However, the heats of formation of these species were derived based on heats of reactions involving $CF_2=O$. Consequently, if the true value for $CF_2=O$ was closer to the calculated value, then the experimentally derived values for these other species would also be closer to their respective calculated values.

There are a number of other species with significant differences between calculated and literature values. The uncertainties in many of these literature values are high because they are only indirectly tied to experimental measurements. For example, the heat of formation of the HCOO• radical is an estimate based on group additivity. The heats of formation of two fluoroethyl radicals (CF_3-CHF• and CH_2F-CF_2•) were determined from estimated from C-H bond dissociation energies based on correlations between rates of H atom abstractions, C-H bond frequencies, and known C-H bond strengths.

To reiterate, from analysis of the data presented in Table 4, we can conclude that for the fluorinated hydrocarbon system, that heats of formation calculated using the BAC-MP4 method provide values that are accurate to less than 10 kJ/mol or comparable in accuracy to the majority of the experimentally derived values. Furthermore, from trends in bond dissociation energies, we believe that the precision of the *ab initio* values for any homologous series to be significantly better than that which is typically obtainable from experimental measurements.

TABLE 1. Enthalpy of Formation, Entropy, Heat Capacities for H/O, Hydrocarbons

SPECIES	$\Delta H^\circ_f(298)$	$S^\circ(298)$	$C^\circ_p(T)$ J/mol/K								Ref
	kJ/mol	J/mol/K	300	500	800	1000	1200	1500	2000	3000	
N_2	0.0	191.5	29.07	29.63	31.39	32.76	33.70	34.80	35.98	37.02	a
H_2	0.0	130.6	28.87	29.27	29.58	30.16	31.07	32.35	34.23	37.11	a
O_2	0.0	205.0	29.33	31.11	33.75	34.93	35.59	36.49	37.78	39.84	a
H_2O	-241.8	188.7	33.46	35.33	38.58	41.31	43.87	47.10	51.14	55.77	a
H_2O_2	-136.1	232.9	43.57	51.65	59.80	63.64	66.75	70.50	74.80	78.91	a
H	218.0	114.6	20.78	20.78	20.78	20.78	20.78	20.78	20.78	20.78	a
O	249.2	160.9	21.89	21.25	20.98	20.91	20.88	20.84	20.82	20.94	a
OH	39.0	183.6	29.93	29.57	29.84	30.68	31.66	32.94	34.63	36.76	a
HO_2	10.5	229.0	34.87	39.69	45.10	47.64	49.59	52.10	55.33	59.10	a
CH_4	-74.9	186.0	35.26	46.60	62.75	72.15	78.71	86.32	94.49	101.36	a
$\bullet CH_3$	145.7	194.0	38.62	45.33	53.85	59.07	63.19	68.06	73.45	78.30	a
$^1{:}CH_2$	387.0	195.5	34.50	37.15	41.57	44.21	46.36	49.11	52.45	55.33	a
$^3{:}CH_2$	424.7	188.7	33.79	36.00	41.20	44.38	46.63	49.48	52.88	55.58	a
$\bullet CH$	594.1	182.9	29.09	29.49	30.82	32.56	34.38	36.61	39.18	41.44	a
C_2H_6	-83.9	229.0	52.61	77.89	108.05	122.59	132.68	144.83	158.64	171.05	a
$C_2H_5\bullet$	117.2	251.6	47.37	66.73	94.48	106.71	114.07	123.66	135.76	146.83	a
C_2H_4	52.5	219.2	42.82	62.52	83.90	94.17	101.38	109.70	118.54	125.81	a
$C_2H_3\bullet$	294.5	227.9	45.77	57.82	71.91	78.77	83.27	89.21	96.90	104.31	a
C_2H_2	226.7	200.9	44.44	54.73	63.90	68.23	71.97	76.46	81.65	87.09	a
CH_3OH	-201.1	239.6	43.98	59.64	79.80	89.53	96.40	104.66	114.00	121.99	a
$CH_3O\bullet$	16.3	228.5	37.99	52.02	69.58	77.81	83.38	90.00	97.32	103.23	a
$\bullet CH_2OH$	-17.2	246.3	47.38	60.16	73.37	78.62	82.59	87.65	93.73	98.76	a
CH_2O	-115.9	218.6	35.15	43.94	55.90	62.27	66.34	70.99	75.80	79.54	a
$\bullet CHO$	43.5	224.5	34.49	38.81	44.93	48.20	50.22	52.53	54.96	57.04	a
CO	-110.5	197.5	29.08	29.85	31.86	33.25	34.15	35.17	36.27	37.21	a
CO_2	-393.5	213.7	37.28	44.56	51.54	54.36	56.20	58.29	60.43	62.19	a
CH_2CO	-51.9	241.8	52.01	65.54	78.63	84.70	88.88	93.89	99.49	104.15	a
$\bullet CHCO$	177.6	254.1	52.93	59.53	67.25	70.43	72.56	75.24	78.39	80.77	a
$HCCOH$	85.5	245.6	55.30	67.62	80.10	84.94	88.59	93.24	98.81	103.38	a

TABLE 2. Enthalpy of Formation, Entropy, Heat Capacities for H/F/O, C_1 Fluorocarbons

SPECIES	$\Delta H^\circ_f(298)$ kJ/mol	$S^\circ(298)$ J/mol/K	$C^\circ_p(T)$ J/mol/K								Ref
			300	500	800	1000	1200	1500	2000	3000	
F_2	0.0	202.7	31.37	34.34	36.46	37.19	37.66	38.20	38.87	39.87	a
HF	-272.5	173.7	29.12	29.20	29.55	30.14	30.98	32.25	34.01	36.21	a
F	78.9	158.7	22.77	22.10	21.46	21.25	21.14	21.03	20.93	20.84	a
CH_3F	-232.6	222.8	37.50	51.26	68.90	77.30	83.34	90.21	96.81	102.59	b
CH_2F_2	-452.2	246.6	42.96	58.91	76.33	83.55	88.84	94.35	99.47	103.97	b
CHF_3	-697.6	259.6	51.15	69.26	85.10	91.01	94.89	98.83	102.42	105.39	b
CF_4	-933.0	261.3	61.30	80.67	94.49	98.73	101.41	103.67	105.52	106.90	b
$\bullet CH_2F$	-32.6	234.4	38.71	48.67	59.29	64.20	67.92	72.02	76.06	79.71	c,d
$\bullet CHF_2$	-247.7	256.0	42.21	54.10	65.33	69.66	72.60	75.69	78.47	80.92	c,e
$\bullet CF_3$	-467.4	265.0	49.94	63.30	73.24	76.37	78.27	79.92	81.29	82.30	c,e
:CHF	163.2	223.2	34.63	39.25	45.21	47.93	50.05	52.43	55.43	61.04	f,e
$:CF_2$	-186.6	240.7	39.01	46.45	52.35	54.18	55.28	56.31	57.14	58.37	g,e
$\bullet CF$	242.1	212.9	30.05	32.24	34.79	35.77	36.32	36.96	37.53	38.20	p
CHF=O	-376.6	246.7	40.50	51.65	63.12	67.92	71.20	74.70	77.94	80.67	d
$CF_2{=}O$	-638.9	258.8	47.41	60.49	70.82	74.39	76.71	78.78	80.58	81.96	d
$\bullet CF{=}O$	-171.5	248.4	38.99	45.06	50.63	52.76	54.14	55.44	56.57	57.45	d
$CF_3O\bullet$	-655.6	275.2	56.44	73.91	86.83	90.89	93.40	95.56	97.32	98.66	h,e

References for Tables 1-3			
a	Kee et al. (1987)	i	Chen et al. (1975)
b	Kolesov (1978)	j	this work, see text
c	McMillen and Golden (1982)	k	Lacher and Skinner (1968)
d	Stull and Prophet (1971)	l	Chen et al. (1990, 1991)
e	Zachariah et al. (1995)	m	Daubert and Danner (1985)
f	Pritchard et al. (1984)	n	Stadelman and Vogt (1980)
g	Rodgers (1978)	o	Stull et al. (1969)
h	Batt and Walsh (1982)	p	Gurvich et al. (1991)

TABLE 3. Enthalpy of Formation, Entropy, Heat Capacities for C_2 Fluorocarbons

SPECIES	$\Delta H^\circ_f(298)$	$S^\circ(298)$	$C^\circ_p(T)$ J/mol/K								Ref
	kJ/mol	J/mol/K	300	500	800	1000	1200	1500	2000	3000	
CH_3-CH_2F	-263.2	265.0	59.83	87.22	116.47	129.62	139.71	150.28	159.35	164.18	i
CH_2F-CH_2F	-433.9	288.2	67.88	95.13	124.30	136.74	145.96	155.31	162.30	163.96	j,e
CH_3-CHF_2	-500.8	282.5	68.72	97.11	124.65	136.47	145.39	154.49	161.85	165.39	i
CH_2F-CHF_2	-664.8	311.7	75.31	107.53	133.47	143.93	151.98	159.92	169.26	177.71	k,e
CH_3-CF_3	-745.6	287.4	78.81	108.32	133.82	144.08	151.47	158.99	165.10	167.67	i
CHF_2-CHF_2	-877.8	314.8	85.23	115.25	141.25	150.60	156.64	163.29	169.67	173.93	j,e
CH_2F-CF_3	-895.8	316.2	86.58	118.04	143.15	152.09	158.17	164.43	169.66	171.50	i
CHF_2-CF_3	-1104.6	333.8	96.09	127.53	151.13	158.85	164.06	168.60	170.64	169.74	i
CF_3-CF_3	-1342.6	332.1	106.79	139.13	160.34	166.68	169.89	172.97	175.77	177.09	i
CH_2F-CH_2•	-44.6	279.8	58.13	80.27	103.74	114.31	122.42	130.91	138.24	142.37	l
CH_3-CHF•	-76.3	274.0	58.79	79.75	103.33	114.06	122.34	130.91	138.07	141.89	j,l
CH_2F-CHF•	-238.5	293.4	69.59	91.24	111.69	119.75	125.52	131.33	136.07	139.86	j,l
CHF_2-CH_2•	-277.2	297.8	67.06	90.20	111.94	121.10	128.00	135.04	140.63	142.60	l
CH_3-CF_2•	-302.5	290.4	67.34	89.22	111.30	120.80	127.83	135.52	142.85	147.42	g,l
CH_2F-CF_2•	-446.0	311.1	74.07	97.38	118.86	127.24	133.22	139.11	143.42	144.90	l
CHF_2-CHF•	-451.9	310.7	76.14	99.54	119.95	127.91	133.70	139.35	143.30	143.80	l
CF_3-CH_2•	-517.1	302.6	77.37	101.75	121.27	128.88	134.26	139.75	145.42	149.64	g,l
CHF_2-CF_2•	-664.8	328.4	84.32	107.31	127.04	134.10	138.83	143.26	145.92	145.88	j,l
CF_3-CHF•	-680.7	326.3	85.84	109.68	128.34	135.01	139.45	143.76	147.55	149.47	j,l
CF_3-CF_2•	-891.2	340.5	92.84	118.29	136.19	141.80	145.18	148.11	150.50	151.09	g,l
CH_2=CHF	-140.1	262.3	50.61	71.66	91.80	100.57	107.42	114.10	118.92	121.04	p,m
CHF=CHF [*Z*]	-297.1	268.6	58.06	79.62	99.16	107.13	112.47	118.31	124.29	128.86	n,e
CHF=CHF [*E*]	-292.9	267.8	59.82	80.44	99.61	107.53	112.83	118.70	124.91	129.77	n,e
CH_2=CF_2	-336.4	265.2	59.33	81.55	100.20	107.74	113.14	118.70	123.44	125.80	p,o
CHF=CF_2	-491.0	292.7	69.45	90.32	107.48	113.93	118.67	124.16	130.07	134.34	p.o
CF_2=CF_2	-658.5	299.9	80.70	100.40	115.53	120.89	123.89	126.87	129.64	131.27	d
CHF=CH• [*E*]	124.3	258.0	50.61	67.10	81.56	87.66	92.21	97.15	101.75	104.49	e
CHF=CH• [*Z*]	123.0	257.0	50.74	67.33	81.76	87.92	92.44	97.29	101.69	104.19	e
CH_2=CF•	109.2	256.8	50.22	66.10	80.71	86.89	91.30	96.37	101.64	105.58	e
CHF=CF• [*E*]	-41.0	279.3	59.30	74.51	87.79	92.80	96.05	99.66	103.21	105.68	e
CHF=CF• [*Z*]	-42.7	279.3	59.30	74.51	87.79	92.80	96.05	99.66	103.21	105.68	e
CF_2=CH•	-67.8	277.0	59.20	76.36	89.73	94.73	97.78	100.81	103.08	103.88	e
CF_2=CF•	-216.3	300.5	68.26	83.42	95.36	99.41	101.77	104.39	106.90	108.21	e
C_2HF	125.5	231.5	52.48	62.17	69.69	73.22	75.83	78.82	81.96	84.57	d
C_2F_2	20.9	244.0	57.07	67.96	76.67	79.74	81.54	83.46	85.20	86.16	d
CHF=C=O	-147.2	270.5	56.75	71.49	84.93	90.34	94.31	98.24	101.99	102.12	e
CF_2=C=O	-290.4	288.8	68.30	81.79	92.56	96.66	99.61	102.48	104.72	106.77	e
•CF=C=O	69.0	276.2	56.80	65.85	73.77	76.59	94.38	98.22	101.97	103.19	e

Table 4. C_1 and C_2 Fluorinated Hydrocarbon Heats of Formation: Calculated Values (BAC-MP4), Literature Values, and Uncertainties

SPECIES	BAC	Lit	Uncert	Ref	Lit	Ref
CH_4	-74.8	-74.9	0.4	a		
CH_3F	-233.8	-232.6	8.4	b	-247.3	y
CH_2F_2	-451.1	-452.2	1.8	b	-460.7	y
CHF_3	-699.5	-697.6	4.2	b	-697.9	y
CF_4	-934.1	-933.0	0.4	b	-934.3	y
$\bullet CH_3$	146.0	145.7	1.3	a		
$\bullet CH_2F$	-31.4	-32.6	8.4	c	-32.0	aa
$\bullet CHF_2$	-247.3	-247.7	8.4	c	-252.0	aa
$\bullet CF_3$	-471.9	-467.4	8.4	c	-472.0	aa
$:CH_2$	429.8	424.7	4.2	d		
$:CHF$	131.7	163.2	12.6	e	105.0	aa
$:CF_2$	-203.3	-186.6	6.3	f	-180.0	aa
$\bullet CH$	613.7	594.1	0.4	g		
$\bullet CF$	236.3	242.1	10.0	aa	255.2	g
$CH_2{=}O$	-108.5	-108.6	6.3	h		
$CHF{=}O$	-382.3	-376.6	15.0	g		
$CF_2{=}O$	-598.4	-638.9	1.7	g	-640.0	aa
$\bullet CH{=}O$	38.9	37.2	8.4	a		
$\bullet CF{=}O$	-182.9	-175.7	15.0	g	-179.0	aa
CH_3OH	-204.8	-201.2	0.4	a		
CF_3OH	-919.4	-893.3	12.6	i		
CH_3OF	-92.0	-72.4	12.6	i		
CF_3OF	-750.1	-764.8	12.6	a		
$CH_3O\bullet$	27.6	16.7	2.9	j		
$CF_3O\bullet$	-628.3	-655.6	6.3	i		
CH_3OOH	-124.6	-131.0	8.4	h		
CF_3OOH	-807.5	-803.3	15.0	m		
$CH_3OO\bullet$	25.3	28.0	12.6	a		
$CF_3OO\bullet$	-627.5	-602.5	12.6	i		
$HC(O)OH$	-387.3	-378.6	0.4	h		
$FC(O)OH$	-614.9					
$HC(O)O\bullet$	-124.9	-150.6	8.4	k		
$FC(O)O\bullet$	-336.9					
C_2H_6	-86.9	-84.1	0.4	a		
$CH_3\text{-}CH_2F$	-272.4	-263.2	1.6	l		
$CH_2F\text{-}CH_2F$	-446.0	-433.9	11.8	m		
$CH_3\text{-}CHF_2$	-505.3	-500.8	6.3	l	-497.0	q
$CH_2F\text{-}CHF_2$	-671.5	-664.8	4.2	n	-691.0	q
$CH_3\text{-}CF_3$	-755.4	-745.6	1.6	l	-747.3	q
$CHF_2\text{-}CHF_2$	-883.3	-877.8	17.6	m		
$CH_2F\text{-}CF_3$	-913.3	-895.8	4.2	l		
$CHF_2\text{-}CF_3$	-1124.1	-1104.6	4.6	l		
$CF_3\text{-}CF_3$	-1357.0	-1342.7	6.3	l	-1344.0	q

SPECIES	BAC	Lit	Uncert	Ref	Lit	Ref
$C_2H_5\bullet$	120.6	118.5		a		
$CH_2F\text{-}CH_2\bullet$	-56.2	-47.7	1.9	m	-44.6	z
$CH_3\text{-}CHF\bullet$	-75.6	-76.3	5.9	m	-72.4	z
$CH_2F\text{-}CHF\bullet$	-247.3	-238.5	12.5	m	-235.5	z
$CHF_2\text{-}CH_2\bullet$	-280.9	-285.8	15.0	m	-277.2	z
$CH_3\text{-}CF_2\bullet$	-300.2	-302.5	8.4	o		
$CH_2F\text{-}CF_2\bullet$	-460.1	-449.8	15.0	m	-446.0	z
$CHF_2\text{-}CHF\bullet$	-459.8	-456.1	15.0	m	-451.9	z
$CF_3\text{-}CH_2\bullet$	-526.6	-517.1	4.2	o		
$CHF_2\text{-}CF_2\bullet$	-671.1	-660.7	18.7	m	-660.2	z
$CF_3\text{-}CHF\bullet$	-703.0	-680.7	9.6	p	-688.3	z
$CF_3\text{-}CF_2\bullet$	-907.6	-891.2	4.2	o	-896.0	aa
C_2H_4	51.5	52.4	0.8	a		
$CH_2{=}CHF$	-139.2	-140.1	2.5	aa	-138.9	
$CHF{=}CHF$ [*Z*]	-301.3	-297.1	10.0	r	-306.5	aa
$CHF{=}CHF$ [*E*]	-302.2	-292.9	10.0	r	-303.6	aa
$CH_2{=}CF_2$	-340.1	-336.4	4.0	aa	-345.2	s
$CHF{=}CF_2$	-485.6	-491.0	9.0	aa	-495.8	s
$CF_2{=}CF_2$	-653.7	-658.5	2.9	g	-659.5	aa
$C_2H_3\bullet$	297.1	286.2	4.2	a		
$CHF{=}CH\bullet$ [*Z*]	123.1					
$CHF{=}CH\bullet$ [*E*]	124.1					
$CH_2{=}CF\bullet$	109.1					
$CHF{=}CF\bullet$ [*Z*]	-41.1					
$CHF{=}CF\bullet$ [*E*]	-42.5					
$CF_2{=}CH\bullet$	-67.7					
$CF_2{=}CF\bullet$	-216.4	-227.0	20.0	aa	-192.1	t
C_2H_2	226.8	226.7	0.8	a		
C_2HF	117.8	125.5	22.0	g		
C_2F_2	31.8	20.9	21.0	g		
$\bullet C_2H$	550.5	564.8	4.2	c		
$\bullet C_2F$	453.9	460.2	22.0	m		
$CH_2{=}C{=}O$	-40.6	-47.7	2.5	u		
$CHF{=}C{=}O$	-147.2					
$CF_2{=}C{=}O$	-290.4					
$\bullet CH{=}C{=}O$	187.3	177.4	8.4	v		
$\bullet CF{=}C{=}O$	69.0					
$CH_3\text{-}CHO$	-161.1	-166.2	0.4	h		
$CF_3\text{-}CHO$	-774.3					
$CH_3\text{-}CO\bullet$	-7.5	-10.2	1.7	a		
$CF_3\text{-}CO\bullet$	-609.9					

Table 4. C_1 and C_2 Fluorinated Hydrocarbon Heats of Formation: Calculated Values (BAC-MP4), Literature Values, and Uncertainties

a Tsang and Hampson (1986)	q Kolesov and Papina (1970)	
b Kolesov (1978)	r Stadelmann and Vogt (1980)	
c McMillen and Golden (1982)	s Stull et al. (1969)	
d Kee et al (1987)	t Bryant (1962)	
e Pritchard et al (1984)	u Nuttall et al. (1971)	
f Rodgers (1978)	v Lias et al. (1988)	
g Stull and Prophet (1971)	w Kerr and Timlin (1971)	
h Baulch et al (1984)	x Tschuikow-Roux and Salomon (1987)	
i Batt and Walsh (1982)	y Rodgers et al. (1974)	
j Batt et al (1974)	z Chen et al. (1990, 1991)	
k Benson (1976)	aa Gurvich et al (1991)	
l Chen et al. (1975)		
m this work, see text	$H_f(298)$	Calculated Heat of Formation at 298 K
n Lacher and Skinnner (1968)	Lit	Literature Value for $H_f(298)$
o Rodgers (1978)	Uncert	Reported Uncertainty in Literature Value
p Martin and Paraskevopoulos (1983)	Ref	Literature Reference

3. Reaction Kinetics

3.1. Overview

The reaction set or "mechanism" is too large to be described in detail here and, consequently, only an overview of important classes of reactions will be presented. Utilizing the species identified as potentially important, a grid of possible reactions was constructed. Existing chemical rate data involving these fluorinated species was then compiled and evaluated. Where rate data were available, but only over limited temperature ranges or at different pressures (for unimolecular or chemically activated steps), RRKM (Robinson and Holbrook, 1972) and QRRK (Dean and Westmoreland, 1987) methods were used to estimate the temperature dependencies (at 1 atmosphere) of the rates and to predict relative rates where multiple product channels were possible. Where no rate data were available for potential reactions, the rate constants were estimated by analogy to other hydrocarbon or substituted hydrocarbon reactions. The prefactors were adjusted for reaction path degeneracy and the activation energies were adjusted empirically based on relative heats of reaction or relative bond energies (*i.e.*, Evans-Polanyi relationships).

Initially, upper limits were used for estimated rate constants. If as a result of simulations under a variety of conditions (using different agents, flame geometries, etc.), it was observed that a specific reaction with an upper limit rate constant did not significantly contribute to the destruction or creation of any of the species in the "mechanism," then that estimate was continued to be used. However, if a specific reaction contributed to the chemistry and its rate constant was an upper-limit estimate, then its value was re-examined and possibly refined. For important contributing reactions where no good analogy was available, where significant uncertainty existed in the barrier (generally reactions with tight transition states and modest-to-large barriers), or where multiple, energetically similar product channels were possible, we calculated the geometries and energies of the transition states (Zachariah *et al.*, 1995) using the BAC-MP4 *ab initio* method. RRKM methods were then applied to obtain the temperature (and pressure) dependence of the rate constant.

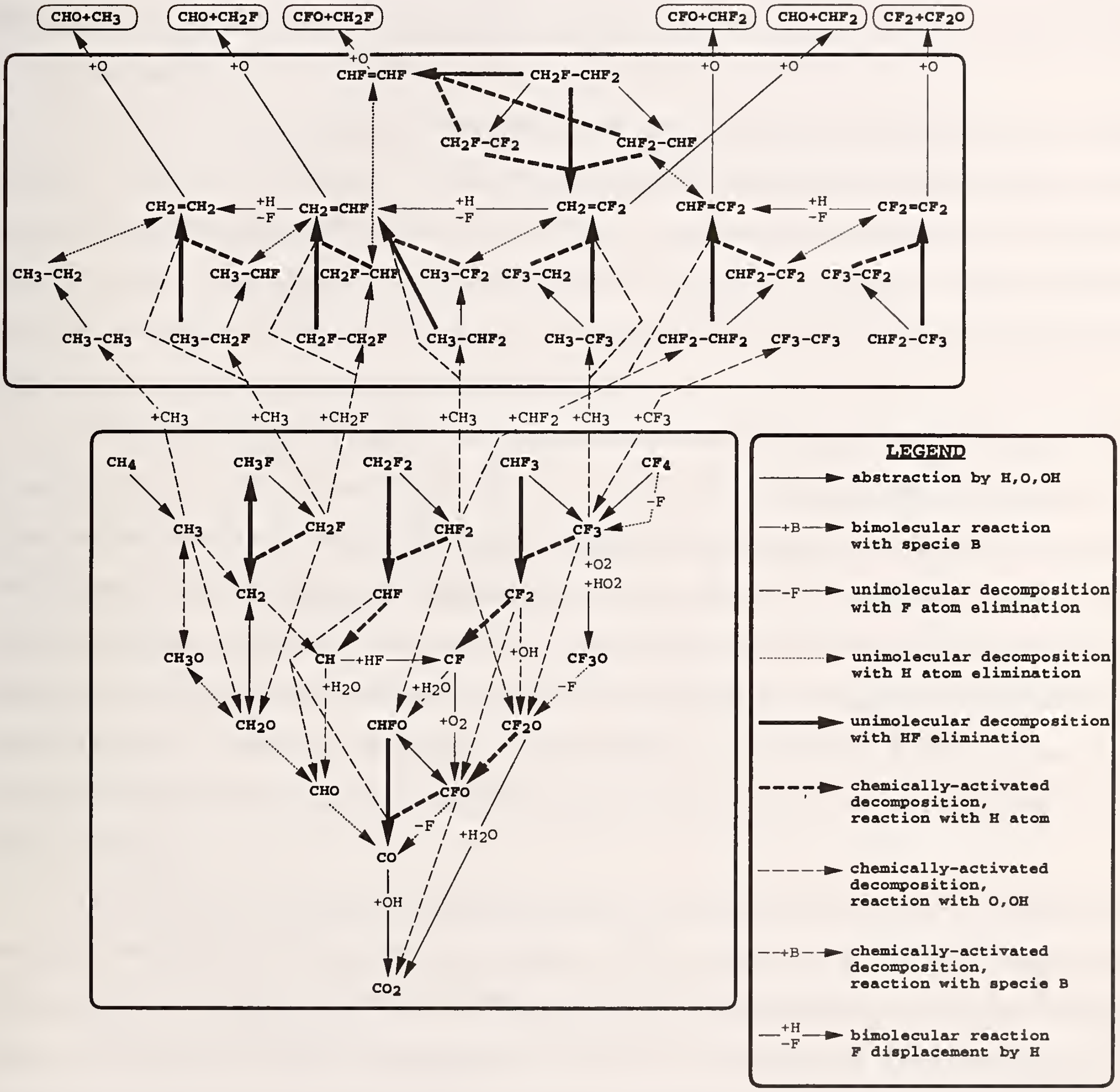
A listing of the rate constants in the reaction set or mechanism used in the simulations is given below in Table 5. In addition, other reactions were also considered but were observed not to contribute under the conditions tested. Many of the relevant rate constants can be found in the "NIST Chemical Kinetics Database" (Mallard *et al.*, 1993).

A qualitative discussion of the uncertainties in the rate expressions is provided with each class of reaction. For rate expressions traceable to experimental measurements, quantitative evaluation of the uncertainties can be found in the original sources.

A schematic of the possible reaction pathways for the fluorinated hydrocarbon mechanism is given in Figure 1. This schematic provides no indication of the relative contributions of each of the possible reaction pathways since this is highly dependent upon conditions. Rather, this schematic gives an indication of the connectivity between all of the species and how the different types of reaction (*e.g.*, thermal decompositions, chemically activated decompositions, abstractions, etc.) provide this connectivity between different types of species. For example, the linkages between each fluoromethane and the corresponding fluoromethylene is due to thermal decomposition and are indicated with bold solid arrows. Other thermal decompositions involving HF elimination (*e.g.*, fluoroethanes → fluoroethylenes, $CHF{=}O \rightarrow CO$) are also represented by bold solid arrows. Thermal decompositions involving H and F atom elimination are represented by plain dotted arrows. H atom addition/elimination reactions are represented by reversible plain dotted arrows (*e.g.*, $CH_3\text{-}CHF\bullet \leftrightarrow CH_2{=}CHF + H$). Similarly, chemically activated decompositions, such as fluoromethyls → ["hot" fluoromethanes] → fluoromethylenes, are represented by bold dashed arrows (for reactions involving H atoms) and plain dashed arrows (for reactions involving O atoms and OH radicals). Abstraction type reactions (*e.g.*, fluoromethanes → fluoromethyls) are represented by plain solid arrows. A few of the potential reaction pathways are not shown in Figure 1 for purposes of maintaing clarity in the schematic representation.

For any given condition (*e.g.*, temperature, concentration) and any given fluorocarbon, only a subset of the reactions pathways will be relevant. For each reaction pathway that is possible, each will have a different relative importance. A discussion of each of the different reaction types for each species type can be found in the following sections.

Figure 1. Fluorinated Hydrocarbon Reaction Pathways



3.2. Hydrocarbon and H/O/F Chemistry

The C/H/O subset is derived from the Miller-Bowman mechanism (Miller and Bowman, 1989) and consists of about 30 species and 140 reactions (see reactions HO-xx, HC-xx in Table 5). Any other hydrocarbon mechanism could be used instead. For example, the GRIMECH set (Bowman *et al.*, 1995) is a new hydrocarbon mechanism that accurately reproduces flame speeds for methane mixtures.

The H/O/F subset consists of 3 species (F, HF) and 8 reactions (reactions HF-xx in Table 5) that are relatively well known. This is the chemistry of fluorine atoms with hydrogen- and oxygen-containing species, such as H_2, OH, and H_2O. There are three reactions of this type that were determined to participate in the chemistry under a variety of conditions. These reactions are the combination of H and F to form HF (and the reverse decomposition) and the hydrogen atom transfer reactions by F atoms from H_2 and H_2O.

The HF decomposition reaction has been measured only at temperatures above about 4000 K (Jacobs *et al.*, 1965; Blauer, 1968, Blauer *et al.*, 1971). Although this reaction in the decomposition direction is unimportant at typical flame temperatures, the reverse $H + F = HF$ combination must be considered. Extrapolating the recommended value (Baulch *et al.*, 1981) for decomposition to 1000 K may result in an uncertainty of as much as a factor of ten, especially when considering non-simple Arrhenius dependence to the rate and different third-body efficiencies. However, since many other reactions ($F + H_2$, H_2O, RH) contribute to F atom destruction, the uncertainty in the absolute rate of the forward or reverse reaction is most likely unimportant.

The hydrogen abstraction reactions of F atoms with H_2 and H_2O have been measured only near room temperature (Wurzberg and Houston, 1980; Stevens *et al.*, 1989; Walther and Wagner, 1983). These values were extended to higher temperatures by fitting the reported values to extended Arrhenius expressions. For the H_2 reaction, an expression with $T^{0.5}$ dependence was chosen consistent with the value recommended by Cohen and Westberg (1983). For the H_2O reaction, an expression with $T^{1.5}$ dependence was chosen by analogy to other reactions.

There are a number of other reactions which were included in the mechanism, but were never observed to contribute significantly to the chemistry. These reactions include the combination of F atoms to form F_2 and the hydrogen abstractions by F atoms from OH, HO_2, and H_2O_2. The oxy-fluoro-species FO•, HOF, FOO•, and F_2O were also initially considered in the mechanism. However, given the very low concentration of F atoms at high temperatures in the hydrocarbon/air flame, these species are present in extremely low concentrations and do not contribute to the overall chemistry. The rate constants used for reactions involving these species will be detailed later in another publication.

3.3. C_1 Fluorinated Hydrocarbon Chemistry

3.3.1. Overview

The C_1 subset of the reaction set (approximately 150 reactions) consists of chemistry of 14 species containing one carbon (and hydrogen/fluorine/oxygen) with H, O, OH, H_2O, and other flame species (see reactions MD-xx, MA-xx, NN-xx, PP-xx, CF-xx in Table 5). The C_1/H/F/O species used in this reaction set are the fluoromethanes (CH_3F, CH_2F_2, CHF_3, CF_4), the fluoromethyl radicals (•CH_2F, •CHF_2, •CF_3), the fluoromethylenes (:CHF, :CF_2), and the fluoromethylidyne radical (•CF). The oxidized C_1 fluorocarbon species contained in this reaction set are the perfluoromethoxy radical (CF_3O•) and the carbonyl fluorides (CHF=O, CF_2=O, •CF=O). Other oxidized C_1 fluorocarbon species were initially considered in the development of the mechanism, but later were excluded, as were the other fluoromethoxy radicals (CH_2FO•, CHF_2O•), the fluorohydroxymethyl radicals (•CHFOH, •CF_2OH), the perfluoromethylperoxy radical (CF_3OO•), and perfluoromethanol (CF_3OH). Although these species (and others) may be important in atmospheric chemistry, our initial simulations suggest that they are present in extremely low concentrations at high temperatures in hydrocarbon/air flames and do not contribute to the overall chemistry.

Both thermally and chemically activated decompositions are considered (*e.g.*, $CH_2F_2 \rightarrow$:CHF + HF and •CHF_2 + H $\rightarrow$:CHF + HF). Fluoromethane decompositions via abstraction of H atoms by H, O, and OH radicals are important pathways. Fluoromethane metathesis reactions with methyl, ethyl, vinyl, and fluoromethyl radicals are also considered. The reaction set also includes reactions of fluoromethyls with O_2, O, and OH to form carbonyl fluorides (*e.g.*, CF_2=O) and other products, and reactions of the fluoromethylenes (*e.g.*, :CF_2) with H to form •CF and O_2, O, or OH to form carbonyl fluorides. The carbonyl fluorides (*i.e.*, CHF=O, CF_2=O, and •CF=O) can be destroyed via unimolecular decomposition, by reactions with H atoms (both abstractions and addition/eliminations), and through reactions with OH radicals (abstractions). Destruction of CF_2=O through complex formation with H_2O and subsequent decompositions are also considered.

3.3.2. Fluoromethanes: Decompositions

The fluoromethanes are primarily destroyed in hydrocarbon flames by H atom abstraction by H and OH and through unimolecular decomposition. Destruction by H atom abstraction by O atoms is a minor channel. The biggest uncertainties for the destruction of the fluoromethanes are the unimolecular decompositions. Although there are good quality experimental data for these reactions, their strong temperature and pressure dependence results in a level of uncertainty to these reactions at flame temperatures. Further mechanism refinements should provide better rate expressions for these reactions.

Both thermally and chemically activated decompositions of the fluoromethanes were considered (*e.g.*, $CHF_3 \rightarrow :CF_2 + HF$ and $\bullet CHF_2 + H \rightarrow :CF_2 + HF$). There have been a number of measurements of the unimolecular decomposition of fluoromethanes (with HF elimination). We employed rate expressions for HF elimination from CH_3F and CHF_3 that are fits using an extended Arrhenius form to the experimental data of Schug and Wagner (1973) and Hidaka *et al.* (1991), respectively. These experimental data were obtained at different temperatures and pressures than are relevant to atmospheric flames. The experimental data were interpolated or extrapolated and fit using temperature dependencies (T^b) that were consistent with the experimental data and our RRKM calculations. For HF elimination from CH_2F_2, we employed a rate expression from our BAC-MP4/RRKM calculations, although there is reasonable experimental data by Politanskii and Shevchuk (1968). For H_2 elimination (minor channel) from CH_3F and CH_2F_2, we used rate expressions from our RRKM calculations using our BAC-MP4 *ab initio* barriers (Zachariah *et al.*, 1995). F atom eliminations from the fluoromethanes are negligible decomposition channels, except for CF_4, where it is the only possible pathway. For this reaction, we used a rate expression from our RRKM calculations that is based on the room-temperature measurement of the reverse reaction ($\bullet CF_3 + F$) by Plumb and Ryan (1986).

There have been no measurements (to our knowledge) for reactions involving chemically activated or "hot" fluoromethanes other than room temperature measurements of the rate constant for $CF_3 + H \rightarrow$ Products (*e.g.*, Ryan and Plumb, 1984; Tsai and McFadden, 1989). In order to estimate values for these various reactions, as well as for the stabilized fluoromethane channels, we used RRKM methods with experimental (where they existed) or our BAC-MP4 *ab initio* barriers (Zachariah *et al.*, 1995) for insertion of :CHF and :CF_2 into HF and H_2 and the energetics of the reaction pathways. Although there are no experimental rate measurements at flame temperatures for chemically activated fluoromethane decompositions and these are primary pathways for destruction of fluoromethyl radicals, the corresponding uncertainties in the rates are small, since these are barrierless combinations.

There have been a number of measurements of the unimolecular decomposition of fluoromethanes (with HF elimination): at least two for CH_3F (Politanskii and Shevchuk, 1967; Schug and Wagner, 1973), at least one for CH_2F_2 (Politanskii and Shevchuk, 1968), and several for CHF_3 (Tschuikow-Roux, 1965; Tschuikow-Roux and Marte, 1965; Modica and LaGraff, 1966; Politanskii and Shevchuk, 1968; Biordi *et al.*, 1978; Schug *et al.*, 1979; Hidaka *et al.*, 1991). In addition, there have been quite a few measurements of the unimolecular decomposition of other halomethanes (eliminating HF, HCl, or HBr) such as CHF_2Cl (Norton, 1957; Edwards and Small, 1964; Gozzo and Patrick, 1964; Edwards and Small, 1965; Gozzo and Patrick, 1966; Barnes *et al.*, 1971; Kushina *et al.*, 1972; Schug *et al.*, 1979; Zhitnev *et al.*, 1990; Zhitnev *et al.*, 1991), CHF_2Br (Cox and Simmons, 1971) , $CHFCl_2$ (Kushina *et al.*, 1972), and $CHCl_3$ (Shilov and Sabirova, 1960; Schug *et al.*, 1979). All of these halomethane decomposition reactions have a small-to-moderate barrier in the reverse direction (*i.e.*, carbene insertion into HF, HCl, or HBr) of 10-40 kJ/mol. Consequently, all of the halomethane measurements are important from the point of evaluating the fluoromethane values (both experimental and calculated) for consistency. Furthermore, the barriers-to-insertion for :CHF and :CF_2 in these reactions can be used as reference reactions for reactions of :CHF and :CF_2 with many other important molecules where there is no or little information available (*i.e.*, the reactions of :CHF and :CF_2 with H_2, H_2O, CH_4, C_2H_6, fluoromethanes, fluoromethyls, etc.).

3.3.3. Fluoromethanes: H Abstractions by H Atoms

In this work, we have used our fits to extended Arrhenius form to the experimental data of Westenberg and deHaas (1975), Ridley *et al.* (1972), and Arthur and Bell (1978) for H atom abstraction from CH_3F, CH_2F_2, and CHF_3, respectively. A temperature dependence of $T^{3.0}$ was used in analogy to the recommended value (Tsang and Hampson, 1986) for H atom abstraction from methane (CH_4). The experimental data were all obtained at modest temperatures (600 K-900 K) and, consequently, the uncertainties in extrapolation of these data to flame decomposition temperatures are most likely acceptable. We note that based on our limited evaluation (Burgess *et al.*, 1994), the trends in the rate expressions for this homologous series appear to be consistent with the number of H atoms in the molecules and the C-H bond strengths (or heats of reaction).

There have been a quite a number of measurements for H atom abstractions from fluoromethanes by H radicals, but only a few for H atom abstraction by O or OH radicals. For H atom abstraction by H radicals, there have been at least four measurements for CH_3F (Parsamyan *et al.*, 1967; Hart *et al.*, 1974; Westenberg and deHaas, 1975; Aders *et al.*, 1975), at least two measurements for CH_2F_2 (Parsamyan and Nalbanddyan, 1968; Ridley *et al.*, 1972), and quite a few for CHF_3 (Ayscough and Polanyi, 1956; Pritchard *et al.*, 1956; Skinner and Ringrose, 1965; Amphlett and Whittle, 1967; Arthur and Bell, 1968; Fagarash and Moin, 1968, Kibby and Weston, 1968; Berces *et al.*, 1972; Kondratiev, 1972; Arthur *et al.*, 1975; Arthur and Bell, 1978; Richter *et al.*, 1994). We should note that many of the measurements for the CHF_3 reactions are actually measurements of the reverse rate or $\bullet CF_3 + H_2 \rightarrow CHF_3 + H$. Two of the citations (Kondratiev, 1972; Arthur and Bell, 1978) are evaluations of the experimental data. We have also calculated (Zachariah *et al.*, 1995) the structure and energy of each transition state for these H atom abstraction reactions from the fluoromethanes using the BAC-MP4 *ab initio* method. The calculated energy barriers compare well with the experimental values.

For the CH_3F + H reaction, all of the workers cited above incorrectly identified the reaction as abstraction of F atoms rather than H atoms. These workers only measured the disappearance of the reactants and simply assigned the product channel by analogy to the CH_3Br

+ H reaction, where it is known that the halogen atom (Br) is abstracted. However, the C-F bond is much stronger than the C-Br bond or even the C-H bond. Consequently, in CH_3F, the H atom, rather than the F atom, is abstracted. Our *ab initio* calculations (Zachariah *et al.*, 1995) also support this argument, where H atom abstractions from the fluoromethanes by H atoms were calculated to have energy barriers of 49.4, 40.6, 53.6 kJ/mol for the CH_3F, CH_2F_2, CHF_3 series, respectively. These same calculations yield barriers-to-abstraction of F atoms of 131.4, 142.7, 168.6, 171.1 kJ/mol for the CH_3F, CH_2F_2, CHF_3, CF_4 series, respectively. This is a significant difference and clearly supports assignment of H atom abstraction as the dominant channel.

Richter *et al.* (1994) have recently measured the rate of H atom abstraction from CHF_3 by H in H_2/O_2 premixed flames and report an activation energy of about 73 kJ/mol. This barrier would appear to be inconsistent with and significantly higher than typical values of 40-50 kJ/mol for H atom abstraction by H from hydrocarbons (*e.g.*, CH_4, C_2H_6) and other fluoromethanes (see references above).

3.3.4. Fluoromethanes: H Abstractions by O Atoms and OH Radicals

In this work, for H atom abstraction by O atoms, we fit experimental data for CH_3F (Parsamyan *et al.*, 1967), CH_2F_2 (Parsamyan and Nalbandyan, 1968), and CHF_3 (Jourdain *et al.*, 1978) using an extended Arrhenius expression with a temperature dependence ($T^{1.5}$) by analogy to methane (Tsang and Hampson, 1986). For H atom abstraction by OH radicals, we used rate expressions recommended by Cohen and Benson (1987a, 1987b) that have temperature dependencies based on transition state theory. These recommendations are based on experimental measurements at relatively low temperatures (about 300 K-500 K). Since these reactions are primary decomposition pathways for the fluoromethanes, it would be valuable to have experimental measurements of these rates at higher temperatures (closer to flame conditions). We note that based on our limited evaluation, the trends in the rate expressions for these homologous series (both O and OH) appear to be consistent with changes in the number of H atoms and the C-H bond strengths or heats of reaction.

There have been a quite a number of measurements for H atom abstractions from fluoromethanes by H radicals, but only a few for H atom abstraction by O or OH radicals. Parsamyan and coworkers have measured the rate of reaction for $CH_3F + O$ (Parsamyan *et al.*, 1967) and for $CH_2F_2 + O$ (Parsamyan and Nalbandyan, 1968). Jourdain *et al.* (1978) and Miyoshi *et al.* (1993) have measured the rate of reaction for $CHF_3 + O$. We have not used the more recent value by Miyoshi *et al.* (1993), because it appears that these data may be complicated by the $CHF_3 \rightarrow :CF_2 + HF$ decomposition reaction at the highest temperatures. This should be examined in more detail, since our conclusion was based on a limited evaluation of the data. Richter *et al.* (1994) have recently measured the rate of H atom abstraction from CHF_3 by O in H_2/O_2 premixed flames and report an activation energy of about 13 kJ/mol. This barrier would appear to be inconsistent with and significantly lower than typical values of 35-40 kJ/mol for H atom abstraction by O from hydrocarbons (*e.g.*, CH_4, C_2H_6) and other fluoromethanes (see references above).

As indicated above, Cohen and Benson (1987a, 1987b) used transition-state theory calculations to analyze and predict rate coefficients for reaction of OH radicals in a series of halogen-substituted methanes and ethanes. Much of their analysis is based on the experimental data of Jeong and Kaufman (1982), but it is also consistent with other measurements for fluoromethanes (Howard and Evenson, 1976; Clyne and Holt, 1979; Nip *et al.*, 1979; Talukdar *et al.*, 1991).

3.3.5. Fluoromethanes: H Abstractions by F and F Abstractions by H

There have been a number of measurements of H atom abstraction from methane (CH_4) by F atoms near room temperature (Wagner *et al.*, 1971; Pollock and Jones, 1973; Williams and Rowland, 1973; Manning *et al.*, 1975; Smith *et al.*, 1977; Clyne and Hodgson, 1983; Pagsberg *et al.*, 1988). In our work, we used a fit to extended Arrhenius form to the rate constant of recommended by Atkinson *et al.* (1992) using a reasonable temperature dependence ($T^{0.5}$) in order to extend the rate expression to flame temperatures. Although there is some uncertainty here in extrapolating the rate constant to flame temperatures, it is most likely unimportant. This is because this reaction occurs on almost every collision (that is, the rate cannot change by much). Furthermore, there are many other reactions (*e.g.*, F + H_2, F + H_2O, and F + other hydrocarbons) that contribute to F atom destruction.

For completeness in the reaction set (although it is unlikely that they will contribute), we have also included H atom abstractions from the fluoromethanes by F atoms. There have been a number of measurements for these reactions near room temperature for CH_3F (Pollock and Jones, 1973; Smith *et al.*, 1977; Manocha *et al.*, 1983), for CH_2F_2 (Pollock and Jones, 1973; Smith *et al.*, 1977; Manocha *et al.*, 1983, Clyne and Hodgson, 1985; Nielsen *et al.*, 1992), and for CHF_3 (Pollock and Jones, 1973; Goldberg and Schneider, 1976; Smith *et al.*, 1977; Clyne and Hodgson, 1983; Maricq and Szente, 1992). For these reactions, rate expressions were used where the rate constant prefactor relative to that recommended by Atkinson *et al.*, 1992) for CH_4 + F was adjusted to account for reaction path degeneracy (*i.e.*, fewer number of H atoms) and the activation energy was adjusted such that the rate was consistent with the measurements at room temperature. Use of extended Arrhenius form in these cases is not justified, because of the lack of temperature-dependent experimental measurements.

For F atom abstractions from CH_3F, CH_2F_2, and CHF_3 by H radicals, we employed rate expressions derived from our BAC-MP4 *ab initio* calculations (Zachariah *et al.*, 1995). The F atom abstraction pathways are negligible channels and these reactions were included simply for completeness in development of this reaction set. However, for reaction of H atoms with CF_4, the only possible pathway is F atom abstraction. For this reaction, we have used the experimentally derived rate expression of Kochubei and Moin (1969, 1971). This reaction is very important pathway for CF_4 destruction, competing with the only other possible channel - unimolecular decomposition of CF_4 to $\bullet CF_3$ and F.

3.3.6. Fluoromethanes: Metathetical Reactions

There have been quite a few measurements of metathetical reactions of methyl/fluoromethyl radicals with methane/fluoromethanes. These will not be reviewed here. In our work, we used the recommendations of Kerr and Parsonage (1976), which are consistent with the majority of the experimental data and empirical relationships for the barriers-to-reactions (activation energies). The values recommended by Kerr and Parsonage are largely based on the pioneering work in this area by Pritchard and coworkers (*e.g.*, Pritchard *et al.*, 1965), Whittle and coworkers (*e.g.*, Chamberlain and Whittle, 1972), and Arthur and coworkers (*e.g.*, Arthur and Bell, 1978). We note that based on our limited evaluation, the trends in the preexponentials and activation energies in the rate expressions for this homologous series appear to be consistent with changes in the number of H atoms and the C-H bond strengths or heats of reaction, respectively.

Although there have been no experimental measurements of metathetical reactions of vinyl radicals (C_2H_3) with the fluoromethanes, one can estimate their rates by analogy to the methyl radical (CH_3) reactions. We used rate expressions for these reactions, where the activation energy was reduced by 10%. This amount determined using the roughly 6 kJ/mol decrease in the heat of reaction and an empirical relationship we determined for a series of abstraction reactions (Burgess *et al.*, 1994).

Given the abundance of H and OH radicals in hydrocarbon flames and the somewhat higher barrier for H atom abstraction by methyl/fluoromethyl and vinyl radicals, these are secondary reaction pathways. However, under pyrolytic conditions they may contribute (especially the C_2H_3 reactions which have the lowest barriers) and, consequently, for completeness should be retained in the reaction set. The experimental measurements for H atom abstractions by the methyl/fluoromethyl radicals were all made at relatively low temperatures (about 300 K-600 K). Extrapolation of these measurements to flame decomposition temperatures may introduce significant uncertainty in the rates, especially since these reactions should have considerable non-simple Arrhenius temperature dependencies. In further refinement of this mechanism, these data should be critically evaluated. Experimental measurements at significantly higher temperatures would also be extremely valuable.

3.3.7. Fluoromethyl Radical Destruction

Fluoromethyl radicals are destroyed by three general pathways whose relative importances are sensitive to conditions. 1) They can combine with H atoms forming chemically activated fluoromethanes that eliminate HF (creating methylene/fluoromethylenes). 2) They can react with oxygen-containing species (*i.e.*, O_2, O, OH), resulting in the formation of fluoromethoxy radicals and carbonyl fluoride species. 3) They can combine with methyl or fluoromethyl radicals, forming chemically activated fluoroethanes that may be either stabilized or eliminate HF (creating ethylene/fluoroethylenes). This latter class of reactions is included with the fluoroethane (C_2) chemistry.

The fluoromethyl radicals are primarily formed by H atom abstractions from the fluoromethanes. However, there are several other channels that can contribute to their formation and are classified as C_2 chemistry. For example, the reactions $CH_2{=}CHF + O \rightarrow \bullet CH_2F + HCO$ and $CHF_2\text{-}CF_2\bullet + H \rightarrow \bullet CHF_2 + \bullet CHF_2$ contribute to the formation of fluoromethyl radicals. Similarly, there are a number of other decomposition channels that can be classified as C_2 or C_3 chemistry, such as $\bullet CH_2F + C_2H_4 \rightarrow \bullet CH_2\text{-}CH_2\text{-}CH_2F$.

There are four potential reaction product channels following association of fluoromethyl radicals (*e.g.*, $\bullet CHF_2$) with O_2 (by analogy to hydrocarbon and chlorinated hydrocarbon chemistry). 1) Stabilization of the fluoromethylperoxy radicals (*e.g.*, $CHF_2OO\bullet$ product). 2) Internal abstraction of a hydrogen atom followed by O-O bond breakage (*e.g.*, $CF_2{=}O + OH$ products). 3) Internal abstraction of a fluorine atom followed by O-O bond breakage (*e.g.*, $CHF{=}O + OF$ products). 4) Direct dissociation of the O-O bond (*e.g.*, $CHF_2O\bullet + O$ products). The first channel (stabilization) should be negligible at flame temperatures, but may need to be considered at lower temperatures and for ignition delays. The second channel (H abstraction) should be a secondary pathway at flame temperatures, but clearly should be re-examined at lower temperatures. The third channel (F abstraction) can clearly be disregarded, because of the strong C-F bond. This contrasts to the analogous reactions that are assumed to occur in chlorinated hydrocarbon chemistry (*e.g.*, Ho *et al.*, 1992). Consequently, eliminating the first three potential pathways, we must only explicitly consider the fourth channel (direct O-

O bond dissociation) to form fluoromethoxy radicals and oxygen atoms (*e.g.*, $CHF_2O\bullet$ + O products).

There have been a number of rate measurements for the reaction of $\bullet CF_3$ with O_2 near room temperature (Vedeneev *et al.*, 1978; Ryan and Plumb, 1982; Caralp *et al.*, 1986; Cooper *et al.*, 1988; Orlando and Smith, 1988), but none (to our knowledge) for reaction of the other fluoromethyl radicals with O_2. At low temperatures the only possible product pathway is formation of the fluoromethylperoxy radical. These types of radical species are known to play a role in atmospheric chemistry. At high temperatures in a flame, these species will be present in significantly smaller concentrations and there are other possible product pathways for the fluoromethyl + O_2 reactions. For $\bullet CF_3 + O_2 \rightarrow CF_3O\bullet + O$, we estimated a rate expression from our RRKM calculations using the reasonable assumption that there is no barrier in the reverse direction. For the other two fluoromethyl reactions, we assumed the fluoromethoxy radical would be present in steady state concentrations and that they would rapidly eliminating HF after being formed. Based on these assumptions then, we simply used the $\bullet CF_3$ rate expression after adjusting for reaction enthalpies. For lower temperature conditions (than flames), these assumptions and the relevant reaction pathways and rate expressions should be re-examined.

For reaction of the perfluoromethyl radical ($\bullet CF_3$) with O atoms (eliminating F), we used a rate constant corresponding to the room temperature value measured by McFadden and coworkers (Tsai *et al.*, 1989). For reaction of the other fluoromethyl radicals with O atoms (eliminating H), we used rate constants scaled between that for $\bullet CH_3$ and $\bullet CF_3$. For reaction of the fluoromethyl radicals with OH radicals, we used rate constants identical to that for $\bullet CH_3$.

Fluoromethyl radicals are primarily destroyed in hydrocarbon flames through reactions with H, OH, and $\bullet CH_3$ radicals. Reactions with O atoms are minor channels. The biggest uncertainty here is likely the reactions with $\bullet CH_3$ radicals (HF elimination versus stabilization), which are very temperature and pressure dependent. Further refinements of this mechanism should provide better rate expressions for these reactions, benchmarking them to experimental data that exists (see brief discussion in Fluoroethane Chemistry section).

Reaction of fluoromethyl radicals with HO_2 may be important for correctly describing ignition delays. There are two possible product channels: $\bullet CHF_2 + HO_2 \rightarrow CH_2F_2 + O_2$

(disproportionation and chain termination) versus $\bullet CHF_2 + HO_2 \rightarrow CHF_2O\bullet + OH$ (combination/elimination and chain propagation). We estimated rate expression by analogy to the corresponding reaction. We assumed the fluoromethoxy radicals immediately eliminate an H atom, since the C-H bond strengths are only 25-30 kJ/mol. This eliminates the need for explicitly including these species in the mechanism. For the $CF_3O\bullet$ product, a fast subsequent F atom elimination step (which is explicitly included in the reaction mechanism) does not happen immediately, since the C-F bond dissociation energy is about 110 kJ/mol. If these reactions (for $CH_2FO\bullet$ and $CHF_2O\bullet$) are shown to be important for ignition delays, then the rates and branching ratios should be re-examined.

3.3.8. Fluoromethylene Destruction

Estimates for the rates of reactions of the fluoromethylenes (:CHF and :CF_2) with many species are somewhat uncertain, because reactions involving these species are significantly slower than the analogous reactions for singlet methylene (^{1}:CH_2). There also appear to be conflicting experimental data on their reactivities. This will not be discussed here. The fluoromethylenes can be destroyed in a number of different ways.

1) They can be destroyed by reaction with H atoms, where we used rate expressions consistent with the room temperature values measured by McFadden and coworkers (Tsai and McFadden, 1989; Tsai and McFadden, 1990). For :CF_2 + H (which was slightly slower), this necessitates a small barrier (5 kJ/mol) to be used.

2) They can be destroyed by reaction with O atoms, where we used rate expressions consistent with the room temperature values measured by McFadden and coworkers (Tsai and McFadden, 1990). A small barrier (4 kJ/mol) for the :CF_2 reaction was used.

3) They can be destroyed by reaction with OH radicals, where we used rate expressions consistent with the value for CF_2: determined by Biordi *et al.* (1978) in their flame measurements. Again a small barrier (14 kJ/mol) was used for :CF_2 and no barrier for :CHF.

4) They can be destroyed by reaction with O_2, where we used the rate expression for :CF_2 measured by Keating and Matula (1977). For :CHF, we used an equivalent rate expression (after adjusting for reaction enthalpy) with a significantly reduced, but still modest (24 kJ/mol) barrier. Since the :CHF reaction barrier has no experimental basis, if it is identified as a reaction that significantly contributes to the destruction of :CHF, then this reaction should be re-examined. An *ab initio* transition state calculation would be extremely useful in resolving this uncertainty.

5) They can be destroyed via insertion into H_2O (a major flame species). We estimated barriers to reaction of 25 and 100 kJ/mol for :CHF and :CF_2, respectively, from our BAC-MP4 *ab initio* calculations.

6) The fluoromethylenes can also be destroyed via reaction with hydrocarbons (see brief discussion in Fluoroethane Chemistry section).

The fluoromethylenes (:CHF and :CF_2) are largely destroyed in hydrocarbon flames via reaction with H atoms. Reactions with O and OH radicals are minor channels. There are good quality experimental data for all of the reactions, which proceed with small barriers. An open question here is the probable addition of the fluoromethylenes to ethylene. This class of reactions has been ignored in this mechanism in order to minimize the number of species in the reaction set, because these reactions would lead to the formation of C_3 fluorinated hydrocarbons.

3.3.9. Fluoromethylidyne Destruction

The rates of reactions of fluoromethylidyne (•CF) with many species are somewhat uncertain given they are significantly slower than the analogous reactions for methylidyne (•CH). There also appear to be conflicting experimental data on its reactivity. This will not be discussed here. For the reactions of •CF with O_2, H, and O, we used rate expressions with reasonable prefactors and barriers that are consistent with the room temperature rate measurements of McFadden and coworkers (Tsai *et al.*, 1989; Tsai and McFadden, 1990) and Peeters *et al.* (1992). We note that to date we have (mis)assigned the products of the reaction •CF + H → C + HF (about 25 kJ/mol exothermic) as CH + F (about 20 kJ/mol endothermic). This was done to eliminate C, C_2H, C_4H_2, and other fuel rich species in order to minimize the number of species in the reaction set. If a hydrocarbon sub-mechanism is used that includes these species, the correct product channel should be used. For •CF + OH → CO + HF, we assumed that there was no barrier to reaction. For •CF + H_2O → Products, we estimated an activation energy of 70 kJ/mol by analogy to other Radical + H_2O reactions. •CF can also be formed via CH + HF → •CF + H_2 (roughly 70 kJ/mol exothermic). For reaction of •CF with other molecules, we assumed upper limits that should be re-examined if those reactions are observed to contribute to •CF destruction.

In the reaction set, fluoromethylidyne (•CF) is largely destroyed via reaction with O_2 and OH. Reaction with H atoms and H_2O are minor channels. Given that there is no experimental measurements for reaction of •CF with H_2O, limited (and inconsistent) data for reaction with O_2, and both of these reactions are likely to have modest barriers, these reactions provide a significant uncertainty to this reaction set. Further refinements of this mechanism should address these issues for :CHF, :CF_2, and •CF.

3.3.10. Carbonyl Fluoride Chemistry

An important set of species to fluorocarbon species are the carbonyl fluorides (CHF=O, CF_2O, •CF=O). CHF=O can be destroyed via unimolecular decomposition and H atom abstraction by H, O, and OH radicals. For the unimolecular decomposition (eliminating HF), we have fit the experimental data of Saito *et al.* (1985) using an extended Arrhenius expression (using the value for E_0 (threshold energy) that they recommend based on their analysis). For the abstractions, we have substituted accepted rate expressions for the analogous $CH_2=O$ reactions. However, there is some significant uncertainty for abstraction by H atoms. The C-H bond dissociation energy in CHF=O is about 45-50 kJ/mol stronger than in $CH_2=O$. Consequently, as an abstraction the barrier should be somewhat higher. On the other hand, H atom addition followed by H_2 elimination could be more facile than the pure abstraction.

$CF_2=O$ can be destroyed via unimolecular decomposition (F atom elimination), by reactions with H atoms, through reactions with OH radicals, and through reactions, potentially, with H_2O. The unimolecular decomposition is likely a minor channel due to the strong C-F bond. There are a number of possible reactions with H atoms: 1) direct abstraction of a F atom abstraction; 2) addition to the oxygen followed by 1,2 elimination of HF; and 3) addition to the carbon followed by 1,1 elimination of HF. Biordi *et al.* (1974) have estimated a rate constant for the net reaction of H with $CF_2=O$ at 1800 K based on their molecular beam sampling measurements in low pressure flames. More recently, Richter *et al.* (1994) have estimated a rate expression based upon measurements at several different temperatures. We have also BAC-MP4 *ab initio* transition state calculations (Zachariah *et al.*, 1995) followed by RRKM analysis to provide rate expressions for each of the possible channels. Our calculations are in excellent agreement with the experimental values and indicate that the addition/1,2 elimination channel dominates (92 kJ/mol barrier), the addition/1,1 elimination channel is about a factor of ten slower (101 kJ/mol barrier), and the direct abstraction channel is negligible (188 kJ/mol barrier). $CF_2=O$ may also be destroyed via addition of OH to the carbon atom followed by 1,2-elimination of HF. However, this is likely a minor channel for destruction, since from our BAC-MP4 *ab initio* transition state calculations (Zachariah *et al.*, 1995), we estimate a barrier of about 105 kJ/mol. Because of the low reactivity of $CF_2=O$ and the large amounts of H_2O

in hydrocarbon flames, CF_2O + H_2O reactions must be considered. We have calculated (Zachariah *et al.*, 1995) rate expressions for $CF_2{=}O$ + H_2O complex formation followed by HF elimination. Modeling results suggest that it is a secondary destruction pathway to the H atom addition/1,2 elimination pathway, but, nevertheless, still needs to be considered.

•CF=O can be destroyed via unimolecular decomposition and reactions with H, O, OH, and $\bullet CH_3$ radicals. Modeling results suggest that the unimolecular decomposition and the reaction with H atoms are the primary decomposition pathways. For reaction with H atoms, we used a rate constant identical to that for the analogous HCO reaction. For the unimolecular decomposition, we determined a rate expression based on the reasonable assumption that combination reaction (reverse direction) is barrierless. There is significant uncertainty in the heat of formation of •CF=O and, consequently, there is significant uncertainty in this rate. Future refinements of this mechanism should address this issue.

3.4. C_2 Fluorinated Hydrocarbon Chemistry

3.4.1. Overview

The C_2 subset of the reaction set (approximately 370 reactions) consists of chemistry of 34 species containing two carbons (and hydrogen/fluorine/oxygen) with H, O, OH, H_2O, and other flame species (see reactions ED-xx, EC-xx, EA-xx, ER-xx, GG-xx, JD-xx, JA-xx, JO-xx, KK-xx, CF-xx in Table 5). The $C_2/H/F/O$ species used in this reaction set are the 9 fluoroethanes (*e.g.*, $CH_2F\text{-}CF_3$), the 11 fluoroethyl radicals (*e.g.*, $CH_2F\text{-}CF_2\bullet$), the 6 fluoroethylenes (*e.g.*, $CHF{=}CF_2$), the 7 fluorovinyl radicals (*e.g.*, $CF_2{=}CH\bullet$), the fluoroacetylenes (C_2HF, C_2F_2), and the fluoroketenes and fluoroketyl radical ($CHF{=}CO$, $CF_2{=}CO$, $\bullet CF{=}CO$). This reaction set will not be described here in detail. Briefly, the fluoroethane destruction pathways (like fluoromethanes) consist of thermally and chemically activated decompositions and H atom abstraction reactions. Fluoroethyl radicals can react with H atoms creating fluoroethylenes via chemically activated fluoroethanes and HF elimination. Fluoroethyl radicals can also react with oxygen-containing species (O_2, O, OH), resulting in the formation of oxidized fragments (*e.g.*, $CF_3\text{-}CF_2\bullet + O \rightarrow \bullet CF_3 + CF_2{=}O$). Fluoroethylenes (produced from thermally and chemically activated fluoroethane decompositions) are predominantly destroyed via reaction with O radicals, resulting in the formation of oxidized fragments (*e.g.*, $CH_2{=}CF_2 + O \rightarrow \bullet CH{=}O + \bullet CHF_2$). Fluoroethylenes are also destroyed to a lesser degree through H atom abstraction by radicals such as OH, resulting in formation of fluorovinyl radicals (*e.g.*, $CH_2{=}CF_2 + OH \rightarrow CF_2{=}CH\bullet + H_2O$). Fluorovinyl radicals (like fluoromethyl and fluoroethyl radicals) are destroyed via reactions with H radicals, as well as with oxygen-containing species.

3.4.2. Fluoroethanes: Thermally and Chemically Activated Decompositions

Both thermally and chemically activated decompositions of the fluoroethanes were considered, as well as stabilization of hot fluoroethanes (*e.g.*, $CH_3\text{-}CF_3 \rightarrow CH_2{=}CF_2 + HF$, $\bullet CH_3 + \bullet CF_3 \rightarrow CH_2{=}CF_2 + HF$, and $\bullet CH_3 + \bullet CF_3 \rightarrow CH_3\text{-}CF_3$). There have been quite a few measurements (mainly in shock tubes) of the unimolecular decomposition of the fluoroethanes. The kinetics of decomposition of most of the fluoroethanes (HF elimination) has been measured in a comprehensive series of work by Tschuikow-Roux and coworkers (Tschuikow-Roux *et al.*, 1970; Tschuikow-Roux and Quiring, 1971; Tschuikow-Roux *et al.*, 1971; Millward *et al.*, 1971; Millward and Tschuikow-Roux, 1972; Sekhar and Tschuikow-Roux, 1974). Data for HF elimination from the other fluoroethanes have been obtained by Kerr and Timlin (1971) and Trotman-Dickenson and coworkers (Day and Trotman-Dickenson, 1969; Cadman *et al.*. 1970). Fluoroethane decomposition kinetics have also been measured by a few other workers (Kochubei *et al.*, 1980; Mitin *et al.*, 1988). We selected experimental values from these and other sources and used them without modification. The validity of employing these high pressure limit values should be re-examined for those fluoroethanes which have only a few fluorine substitutions, especially when using the reaction set at low pressures (and high temperatures).

There have been a number of measurements for reactions of a few of the chemically activated or "hot" fluoroethanes produced by combination of fluoromethyl radicals by Kim *et al.* (1973), by Trotman-Dickenson and coworkers (Kirk *et al.*, 1968; Phillips and Trotman-Dickenson, 1968; Cadman *et al.*, 1976), and by Pritchard and coworkers (Pritchard *et al.*, 1964; Bryant and Pritchard, 1967; Bryant *et al.*, 1967; Pritchard and Thommarson, 1967; Perona *et al.*, 1968; Pritchard and Bryant, 1968; Pritchard and Perona, 1970; Follmer and Pritchard, 1974). Some of this work includes measurements of branching ratios between product channels (*i.e.*, HF elimination versus stabilization). There are no measurements (to our knowledge) for decomposition of hot fluoroethanes following combination of fluoroethyl radicals and H atoms. We used rate expressions for all of the hot fluoroethanes for the various product channels based on our RRKM calculations in order to provide a consistent set. Further refinements of this mechanism should include using the existing experimental data as reference values for the RRKM calculations.

3.4.3. Fluoroethanes: Fluoromethyl Disproportionations, Fluoromethylene Insertions

There has been a number of measurements of disproportionations between methyl and fluoromethyl radicals (Pritchard and Follmer, 1973; Nilsson and Pritchard, 1982; Pritchard *et al.*, 1984, 1985, 1987, 1990, 1991, 1992). These studies suggest a branching ratio for disproportionation versus combination (HF elimination or stabilization) of about 10-20% at 350-500 K. We employed these data in combination with estimated barriers from our BAC-MP4 *ab initio* calculations and determined rate expressions consistent with the available experimental data. The activation energies or barriers-to-disproportionation are about 3-9 kJ/mol for reactions involving $\bullet CHF_2$ (*i.e.*,$:CF_2$ product) and 14-19 kJ/mol for reactions involving $\bullet CH_2F$ (*i.e.*, $:CHF$ product). $:CHF$ and $:CF_2$ may also insert into C-H bonds in methane and fluoromethanes. We used rate expressions based on estimated barriers from our BAC-MP4 *ab initio* calculations of 63 and 130 kJ/mol for insertions of $:CHF$ and $:CF_2$, respectively. These are rather significant when compared to $:CH_2$, which inserts into C-H bonds with little barrier. Our BAC-MP4 *ab initio* calculations suggest these barriers result from ionic repulsion between the electropositive H atom on the (fluoro)methane and the highly electropositive carbon atom on the fluoromethylene. For example, the H atom on CH_4 has a Mulliken charge of $+0.17$ and the C atom on $:CF_2$ has a Mulliken charge of $+0.54$. However, there is some experimental evidence to suggest that the barriers are significantly smaller (DiFelice and Ritter, 1994). This apparent conflict for these important species should be addressed in future mechanism refinements.

3.4.4. Fluoroethanes: Abstractions

There have been quite a few measurements of H atom abstractions from fluoroethanes by OH radicals. Cohen and coworkers (Cohen and Benson, 1980; Cohen and Westberg, 1987) have used transition-state theory calculations to analyze and predict rate coefficients for a series of halogen-substituted methanes and ethanes. Much of their analysis is based on the experimental data of Clyne and Holt (1979) and Jeong *et al.* (1984). Other experimental data included in their analysis was from the measurements by Howard and Evenson (1976), Handwerk and Zellner (1978), Nip *et al.* (1979), and Martin and Paraskevopoulos (1983). In our work to date, we have used values recommended by Cohen and Benson (1987). For the three asymmetric fluoroethanes (CH_3-CH_2F, CH_3-CHF_2, CH_2F-CHF_2), where there are different functional H substitutions, we have estimated the branching ratios (based on relative bond strengths). Recently, there have been a number of precise measurements for these abstraction reactions for a number of the fluoroethanes by Huie and coworkers (Liu *et al.*, 1990; Zhang *et al.*, 1992), by Ravishankara and coworkers (Talukdar *et al.*, 1991; Gierczak *et al.*, 1991), and by Nielsen (1991). Based on some of the more recent measurements there are newer recommendations by Cohen and Westberg (1991) for some of these reactions. The biggest changes are for reactions involving CH_3-CHF_2 and CHF_2-CF_3. However, the changes in the rate expressions are only significant at temperatures well below flame temperatures (because of T^b dependence). These recommendations are based on experimental measurements at relatively low temperatures (about 300 K-500 K) and these reactions are primary decomposition pathways for the fluoroethanes at significantly higher temperatures. Consequently, it would be valuable to have experimental measurements of these rates at near flame temperatures. We note that based on our limited evaluation, the trends in the rate expressions for this homologous series appear to be consistent with changes in the number of H atoms and the C-H bond strengths or heats of reaction.

Although there have been a number of measurements of H atom abstractions by OH radicals from many of the fluoroethanes, there have been no measurements (to our knowledge) for H atom abstractions by H and O atoms from any of the fluoroethanes. Consequently, we utilized an empirical correlation that we determined for other H abstraction reactions (Burgess *et al.*, 1994). For abstraction by H atoms, we used activation energies that were a factor of 2.5 times that for the analogous abstraction by OH radicals. For abstraction by O atoms, a factor of 2.7 was employed.

The fluoroethanes are largely destroyed via unimolecular decomposition and abstraction by OH radicals. Good quality experimental data are available. Future refinements of this mechanism need only to re-evaluate this work.

3.4.5. Fluoroethyl Radical Destruction

Fluoroethyl radicals can be destroyed via reaction with the flame species O_2, H, O, OH, and $\bullet CH_3$. For reaction with O_2, O, and OH, we used the accepted rate expressions for the analogous ethyl radical reactions. Reactions of fluoroethyl radicals with H atoms form hot fluoroethanes and we used rate expressions from our RRKM calculations as mentioned previously. Fluoroethyl radicals may combine with $\bullet CH_3$ to form hot fluoropropanes (which most likely will be stabilized except at the highest temperature). Fluoroethyl radicals may also disproportionate with $\bullet CH_3$ to form CH_4 and fluoroethylenes. The first channel (combination) was simply ignored in order to exclude C_3 fluorinated species from the reaction set. The rate constants for the second channel (disproportionation) were set identical to that accepted for the reaction $\bullet C_2H_5 + \bullet CH_3 \rightarrow C_2H_4 + CH_4$.

3.4.6. Fluoroethylene Chemistry

There are experimental measurements (Simmie and Tschuikow-Roux, 1970; Simmie *et al.*, 1970) for the rate of pyrolysis of at least two of the fluoroethylenes (eliminating HF). For the other fluoroethylenes, we used these rate expressions as reference points and adjusted the activation energy based on the reaction enthalpy. For thermal decomposition or pyrolysis of perfluoroethylene ($CF_2{=}CF_2 \rightarrow :CF_2 + :CF_2$), we used rate expressions from our RRKM fits to the experimental data of Schug and Wagner (1978). These data are also consistent with experimental rate expression of Modica and LaGraff (1966). For the other thermally and chemically activated fluoroethylene decompositions (*e.g.*, $:CHF + :CHF \rightarrow CHF{=}CHF$ or $C_2HF + HF$), we used rate expressions from our RRKM calculations (based on the reverse reaction or combination). Fluoroethylenes are primarily destroyed via reaction with O atoms (*e.g.*, $CH_2{=}CF_2 + O \rightarrow \bullet CHF_2 + HCO$). For these reactions, we used the recommendations of Cvetanovic (1987). There is some evidence (Gilbert *et al.*, 1976) to suggest that the assumed methyl+formyl products (*e.g.*, $\bullet CHF_2 + HCO$) may not be the only product channel (*e.g.*, $CHF{=}CHF + O \rightarrow CHF{=}C{=}O + HF$ or $CHF{=}CHF + O \rightarrow CHF{=}O + :CHF$). Future refinements of this mechanism should resolve this issue.

Fluoroethylenes can also be destroyed via reaction with H atoms. This includes H atom addition followed by stabilization of the fluoroethyl radical produced (*e.g.*, $CH_2{=}CF_2 + H \rightarrow CH_3\text{-}CF_2\bullet$ or $CHF_2\text{-}CH_2\bullet$), as well as H atom addition followed by F atom elimination (*e.g.*, $CH_2{=}CF_2 + H \rightarrow CH_2{=}CHF + F$). There are some experimental data for these reactions, however, there appears to be some conflict between them. Consequently, in this mechanism, we simply employed an accepted rate expression for the H atom addition/stabilization for the analogous ethylene reaction. That is, we used rate expressions for the reactions of fluoroethylenes with H atoms by analogy to the recommendations of Tsang and Hampson (1986) for the two pathways $C_2H_4 + H \rightarrow C_2H_5$ and $C_2H_4 + H \rightarrow C_2H_3 + H_2$.

For the F atom eliminations, we assumed barrierless addition in the reverse direction. However, there are some significant uncertainties here. First, it is likely the barrier to addition will be influenced by the degree of fluorine substitution on the alpha carbon. Secondly, the efficiency of stabilization of the chemically activated or "hot" fluoroethyl radical will be strongly influenced by the degree of fluorine substitution. Fluoroethylenes may also be destroyed by OH addition/elimination reactions. This would result in the formation of (fluoro)vinoxy radicals (*e.g.*, CHO-CHF•). However, in order to minimize the number of species in the reaction set, we have not considered these reactions. Future refinements of this mechanism should investigate whether or not these types of reactions significantly contribute to the chemistry.

Fluoroethylenes may also be destroyed via reaction with OH radicals. We have only considered H atom abstraction (and not addition/elimination). For abstraction of H atoms from the fluoroethylenes by OH radicals, we have used our fit (with an estimated $T^{2.0}$ dependence) to the values recommended by Baulch *et al.* (1992) for $C_2H_4 + OH \rightarrow C_2H_3 + H_2O$, which is based on a measurement by Tully (1988). Clearly the C-H bond strength will be significantly influenced by fluorine substitution. This issue should be addressed in future refinements of this mechanisms.

We have not considered another possible reaction pathway with OH; that is, OH addition followed by HF elimination (*e.g.*, $CF_2{=}CF_2 + OH \rightarrow [\bullet CF_2\text{-}CF_2\text{-}OH] \rightarrow \bullet CF_2\text{-}CF{=}O$). There are a number of uncertainties here and, consequently, this reaction pathway was simply not pursued (because of potential complexities). First, this pathway results in the production of a number of new species in the reaction set (fluorovinoxy radicals, *e.g.*, $\bullet CF_2\text{-}CF{=}O$), whose thermochemistry is unknown. Second, the effect of fluorine substitution on the barrier to OH addition is not known (but probably could be estimated reasonably well). Third, the relative rates for three competing reactions must be known; that is, 1) stabilization of the fluorohydroxyethyl radicals (*e.g.*, $\bullet CF_2\text{-}CF_2\text{-}OH$), 2) reversion to reactants, and 3) HF elimination. Furthermore, if the fluorohydroxyethyl radicals are sufficiently stabilized, then they are a new set of species that must be considered. Fourth, there are a number of reactions which must be considered for the fluorovinoxy radicals. Future refinements of this mechanism should investigate the potential importance of the OH addition/HF elimination reactions for the fluoroethylenes. Most likely, only the perfluorocompounds may need to be considered (by analogy to the sole importance of the perfluoromethoxy radical).

There have been quite a few measurements of the reactions of O atoms with fluoroethylenes. These will not be reviewed here. In our work, we have used our fits to extended Arrhenius form to the recommendations of Cvetanovic (1987) in order to extrapolate the low temperature values (300-500 K) to flame temperatures. A temperature dependence of $T^{1.0}$ was used in analogy to other reactions. The recommended values by Cvetanovic are largely based on work in this area by Herron and Huie (1973), Jones and Moss (1974), Atkinson and Pitts (1977), and Gutman and coworkers (Park *et al.*, 1984).

For this class of reactions, it is generally understood that the dominant pathway is where the products are the fluoromethyl and (fluoro)formyl radical (*e.g.* $CH_2=CHF + O \rightarrow HCO + \bullet CH_2F$) following dissociation of the chemically activated fluoroethylene oxide formed by O atom attack on the double bond. That is, the O atom first "adds" to the carbon with the least number of electronegative substituents (in this case F). An H atom on this carbon, then "migrates" to the other carbon. The numerous other possible channels are generally considered to be minor pathways: fluorine-substitute analogs of 1) stabilized ethylene oxide, 2) stabilized acetaldehyde, 3) formaldehyde + methylene, 4) acetyl radical + H, 5) ketene + H_2, and 6) vinyl radical + OH. The latter, abstraction of H atom, is a separate reaction from the first four (addition/elimination). For completeness in the reaction set, we have included the latter abstraction reaction and used rate expressions based on analogy to the value estimated by Fontijn and coworkers (Mahmud *et al.*, 1987) for the unsubstituted ethylene reaction. It should be noted that for perfluoroethylene, the only possible channel is $CF_2=CF_2 + O \rightarrow CF_2=O + :CF_2$ (*i.e.*, no H migration possible). It should also be noted that for $CH_2=CHF$ there are two possible channels ("addition" of the O atom to one side or the other). We have used an estimated additional 4 kJ/mol for "addition" of the O atom to the fluorinated carbon. This is consistent with an upper limit measurement at room temperature for this reaction by Gutman and coworkers (Slagle *et al.*, 1974). Given that this is a primary decomposition pathway for the fluoroethylenes and that the rate expression that we have chosen to use is based on experimental measurements at low temperatures (300 K-500 K), it would be very valuable to have measurements of these reactions and product channels at near flame temperatures.

3.4.7. Fluorovinyl Radical Destruction

Westmoreland (1992) has calculated the temperature (and pressure) dependencies of the rate for the chemically activated reaction $C_2H_3 + O_2 \rightarrow CH_2O + HCO$. We have used these values for the analogous fluorovinyl radical reactions. In our work, we have used the values recommended by Warnatz (1984) and Tsang and Hampson (1986) for the $C_2H_3 + O \rightarrow$ Products and $C_2H_3 + OH \rightarrow$ Products reactions, respectively, for the analogous fluorovinyl radical reactions. The values recommended by Warnatz for the first reaction is based on measurements by Heinemann *et al.* (1988).

3.4.8. Fluoroethyne, Fluoroketene, and Fluoroketyl Radical Chemistry

For reactions involving the fluoroethynes (C_2HF, C_2F_2), the fluoroketenes ($CHF=C=O$, $CF_2=C=O$), and the fluoroketyl radical ($\bullet CF=C=O$), we have used rate expressions by analogy to the corresponding hydrocarbons (C_2H_2, CH_2CO, $\bullet HCCO$). For reaction of H atoms with the two fluoroacetylenes (C_2HF, C_2F_2), we have used rate expressions derived from the recommendation of Warnatz (1984) for $C_2H_2 + H \rightarrow C_2H_3$, which is based on measurements by Payne and Stief (1976). For these H atom addition reactions, we employed third-body stabilization efficiencies and low pressure limits identical to that for acetylene. Future refinements of this mechanism should provide better estimates for these reactions.

3.5. BAC-MP4 *Ab Initio* Predictions

For a number of reactions considered in the mechanism, there are no or little experimental rate data. Consequently, we have estimated that data using BAC-MP4 *ab initio* calculations of the transition state geometries and energies and RRKM/master equation analysis. A short description of the BAC-MP4 *ab initio* calculations is given in the section titled Thermochemistry: BAC-MP4 *Ab Initio* Predictions. The transition state for a reaction was obtained by searching for a geometry with one negative eigenvalue. This corresponds to a saddle point on the potential energy surface. This is then followed by a steepest-descent reaction path analysis to ensure that the calculated transition state corresponds to the appropriate reactants and products. BAC corrections are then assigned in the same manner as with the equilibrium structures. In order to quantify the uncertainties in the calculated data, we have also performed calculations on a number of related reactions where there is good quality experimental data.

We have calculated transition states for a number of sets of reactions, including the following:

1. HF elimination from the fluoromethanes (*e.g.*, $CH_3F \rightarrow :CH_2 + HF$);
2. H_2 elimination from the fluoromethanes (*e.g.*, $CH_3F \rightarrow :CHF + H_2$);
3. H atom abstraction by H from the fluoromethanes (*e.g.*, $CH_3F + H \rightarrow \bullet CH_2F + H_2$);
4. F atom abstraction by H from the fluoromethanes (*e.g.*, $CH_3F + H \rightarrow \bullet CH_3 + HF$);
5. reactions of H_2O with the fluoromethylenes (*e.g.*, $:CHF + H_2O \rightarrow CH_2FOH \rightarrow CH_2O + HF$);
6. reactions of H_2O with carbonyl difluoride (*e.g.*, $CF_2{=}O + H_2O \rightarrow FCO_2H + HF$);
7. F atom abstraction by H from carbonyl difluoride (*i.e.*, $CF_2{=}O + H \rightarrow \bullet CF{=}O + HF$);
8. H atom addition to carbonyl difluoride (*e.g.*, $CF_2{=}O + H \rightarrow \bullet CF_2OH \rightarrow \bullet CF{=}O + HF$);
9. OH addition to carbonyl difluoride (*i.e.*, $CF_2{=}O + OH \rightarrow \bullet OCF_2(OH) \rightarrow FC(O)O\bullet + HF$).

The *ab initio* geometries and energies of the transition states were then used as inputs to RRKM/master equation analysis in order to calculate rate expressions. The calculated rate expressions agree well with those derived from experimental measurements (where they exist). Further discussion of the *ab initio* transition state calculations can be found elsewhere (Zachariah *et al.*, 1995).

There is one reaction that is very important to the chemistry of fluorinated hydrocarbon destruction and where the calculated rate expression can be compared with good quality experimental measurements. The rate of reaction of H atoms with $CF_2{=}O$ has been estimated based on measurements in flames of the rate of disappearance of carbonyl difluoride. Biordi *et al.* (1974) estimated a rate constant at 1800 K for this reaction in CF_3Br inhibited methane/oxygen/argon premixed flames. More recently, Richter *et al.* (1994) have determined rate coefficients at 1175-1490 K for this reaction in CF_3H inhibited hydrogen/oxygen/argon premixed flames.

The reaction of H atoms with $CF_2{=}O$ has three distinct pathways, one is a direct abstraction and the other two are addition/elimination reactions.

First, H atoms can abstract fluorine (*i.e.*, $CF_2{=}O + H \rightarrow {\bullet}CF{=}O + HF$). Our BAC-MP4 transition state calculations suggest a barrier of about 150 kJ/mol for this reaction and barriers of about 130-170 kJ/mol for F atom abstraction from the fluoromethanes. These barriers are consistent with that measured by Kochubei and Moin (1971) for F atom abstraction by H from CF_4. They reported an activation energy of about 190 kJ/mol at 1200 K-1600 K. This would suggest a barrier of about 160 kJ/mol assuming a T^2 dependence to the rate.

The second pathway consists of H atom addition to the carbon atom on the carbonyl difluoride followed by 1,1 elimination of HF from the chemically activated fluoromethoxy intermediate (*i.e.*, $CF_2{=}O + H \rightarrow [CHF_2O{\bullet}]^* \rightarrow {\bullet}CF{=}O + HF$). The third pathway is also an addition/elimination reaction, but consists of H atom addition in this case to the oxygen atom on the carbonyl difluoride followed by 1,2 elimination of HF from the "hot" hydroxyfluoromethyl intermediate ($CF_2{=}O + H \rightarrow [{\bullet}CF_2OH]^* \rightarrow {\bullet}CF{=}O + HF$).

Our *ab initio* transition state calculations suggest barriers of about 50 kJ/mol and 65 kJ/mol for addition to the carbon and oxygen sides of the carbonyl difluoride, respectively. It is slightly more energetically favorable for the H atom to add to the carbon side. However, the subsequent 1,1 HF elimination step in this case in order to form the ${\bullet}CF{=}O$ product involves a transition state that is an additional 80 kJ/mol higher (a total of 130 kJ/mol). The overall energetics of this pathway is significantly less favorable than the 1,2 HF elimination step that follows H atom addition to the oxygen side. This involves a transition state that is only additional 15 kJ/mol higher (a total of 80 kJ/mol). We have derived rate expressions based on RRKM/master equation calculations using the geometries and energies of the *ab initio* transition states. These calculated rate expressions (Zachariah *et al.*, 1995) agree extremely well with the experimental rate constants reported by Biordi *et al.* (1974) and Richter *et al.* (1994).

Further discussion of the *ab initio* transition state calculations can be found elsewhere (Zachariah *et al.*, 1995).

4. Future Mechanism Refinement

4.1. Overview

The purpose of this section is to highlight uncertainties in the reaction set that may impact its ability to predict adequately the chemistry of fluorinated hydrocarbon destruction and the behavior of fluorinated hydrocarbon-inhibited hydrocarbon flames. We will mention known significant uncertainties, both those that may influence and those that are unlikely to influence the overall chemistry. For example, the heats of formation of many of the species must be estimated using empirical methods, such as group additivity. However, much of the chemistry of the destruction of fluorinated hydrocarbon species in hydrocarbon flames is irreversible. That is, it is the rates of mainly highly exothermic steps that are important and not thermodynamic considerations (free energies) or endothermic steps. For example, although there is significant uncertainty in the heat of formation of :CHF, this should have little impact on the chemistry in hydrocarbon flames, since :CHF is overwhelmingly destroyed through reactions with radicals such as H and OH, and not through unimolecular decompositions. In general, the uncertainties in the reaction set will only be highlighted here.

The reaction set presented here should be considered a framework for development of a model that accurately describes the decomposition of fluorinated hydrocarbons and their impact on hydrocarbon flame inhibition chemistry. It should not be considered a finished product, since to date there has been very little comparison of its predictions with experimental measurements. Future refinement and validation of the mechanism will require input from measurements of flame speed, flame temperature, concentration profiles, and temperature profiles in fluorinated hydrocarbon-inhibited flames.

In the reaction set or mechanism presented here, there are a number of species with uncertain thermochemistry and a number of reactions with uncertain rate expressions. These can be divided (arbitrarily) into several classes. 1) In most cases, the uncertainties are derived from the lack of direct or even indirect experimental data for these species and reactions. 2) In some cases, certain classes of species and reactions were not included in the reaction set, because of lack of experimental data and uncertainty in the chemistry. 3) In the other cases, experimental data exist, but because of the magnitude of the reaction set, we have not yet verified that the rate expressions employed in the reaction set are fully consistent with the available experimental data.

For example, the JANAF recommended heat of formation for $CHF{=}O$ is simply the average of the heats of formation of the analogous $CH_2{=}O$ and $CF_2{=}O$. Consequently, there is significant uncertainty introduced from this procedure (bond dissociation energies are strongly dependent upon alpha-substitution), irrespective of the uncertainties in the heats of formation of the reference compounds. For example, using the heats of formation of CH_4 (-75 kJ/mol) and CH_2F_2 (-453 kJ/mol), one would estimate using this procedure a heat of formation for CH_3F of -264 kJ/mol that is 26 kJ/mol lower than the accepted value (-238 kJ/mol).

An analogous example for estimated rate constants is for the hydrogen abstraction $CHF{=}O + H \rightarrow \bullet CF{=}O + H_2$. In this case, we have simply used an accepted rate expression for the analogous reaction $CH_2{=}O + H \rightarrow HCO + H_2$. Given that the C-H bond dissociation energy in $CHF{=}O$ is about 45-55 kJ/mol stronger than in $CH_2{=}O$, it is likely that the barrier to abstraction for the $CHF{=}O$ reaction is somewhat higher than the barrier for the $CH_2{=}O$ reaction. Although we have estimated that the barrier is about 10 kJ/mol higher (based upon trends in other halogen-substituted hydrocarbons), we have not (to date) employed this estimate because of some uncertainties. For example, it is likely that this reaction is not an abstraction, but rather an addition to the oxygen (*e.g.*, $CH_2{=}O + H \rightarrow \bullet CH_2OH$) followed by a 1,2-elimination of H_2, because H atom abstractions by H should have a barrier closer to 40 kJ/mol (like $CH_4 + H \rightarrow \bullet CH_3 + H_2$). Consequently, the effective "barrier" may not be significantly influenced by the C-H bond strength.

Another important example of uncertainties in rate constants can found for H atom addition/stabilization to the fluoroethylenes (*e.g.*, $CH_2{=}CF_2 + H \rightarrow CH_3\text{-}CF_2\bullet$ and $CHF_2\text{-}CH_2\bullet$). We have simply employed an accepted rate expression for the H atom addition/stabilization for the analogous $C_2H_4 + H \rightarrow \bullet C_2H_5$ reaction. However, there are some significant uncertainties here. First, it is likely the barrier to addition will be influenced by the degree of fluorine substitution on the alpha carbon. For example, the barrier to addition for the above reaction involving $CH_2{=}CF_2$ may be on the order of 8 kJ/mol versus 30 kJ/mol for addition to the unsubstituted versus substituted carbon, respectively. Secondly, the efficiency with which the "hot" fluoroethyl radical is stabilized will be strongly influenced by the degree of fluorine substitution (*e.g.*, CHF_2-CF_2• versus CH_3-CHF•). The relative barriers to addition and relative stabilization efficiencies could be calculated satisfactorily using *ab initio* and RRKM methods, respectively. However, to date we have not done these calculations.

4.2. Thermochemistry

There are a number of other species in this reaction set that have significant uncertainties in their heats of formation, because of lack of direct experimental data.

The heat of formation of CH_3F has been estimated based on trends in the heats of formation of the other fluoromethanes. Although CH_3F is unlikely to be a key species in fluorinated hydrocarbon-inhibited hydrocarbon flames, as the simplest fluorinated hydrocarbon, its heat of formation is significant as a reference point for heats of formation of other fluorinated hydrocarbons. An experimentally derived heat of formation for CH_3F would be very valuable.

The value recommended in the JANAF tables for the heat of formation of :CHF is based on the average of the heats of formation of $:CH_2$ and $:CF_2$. Other values are based on estimates of bond dissociation energies or the absence of :CHF as a product in certain reactions (Staemmler, 1974; Hsu *et al.*, 1978; Pritchard *et al.*, 1984). Consequently, there are significant uncertainties introduced from these procedures (*i.e.*, bond dissociation energies are strongly dependent upon alpha-substitution). Most reactions that create or destroy :CHF are highly irreversible reactions (*e.g.*, $:CHF + H \rightarrow CH + HF$) and, consequently, are unaffected by the energetics of the reactions. However, disproportionation reactions involving :CHF may proceed with small barriers and have modest heats of reaction (*e.g.*, $\bullet CH_3 + \bullet CH_2F \rightarrow CH_4 + :CHF$). For these reactions, the uncertainty in the heat of formation of :CHF may be important.

The literature value for the heat of formation of $CF_2=O$ is reported with a relatively low uncertainty. However, our BAC-MP4 *ab initio* calculations predict a value that is about 40 kJ/mol higher than the experimental number. Other *ab initio* calculations (Montgomery *et al.*, 1994; Schnieder and Wallington, 1994) using different approaches also predict a heat of formation for $CF_2=O$ that is higher (by about 30 kJ/mol) than the experimental value. There is reason to believe that there may have been side or wall reactions that complicated the measurement. Furthermore, the heats of formation of all the other oxygenated C_1 fluorocarbons (*e.g.*, $CF_3O\bullet$, $\bullet CF=O$, etc.) are referenced to $CF_2=O$. Because of these issues, both uncertainties in the experimental measurements and *ab initio* calculations warrant further examination. A new, reliable experimental measurement would be ideal.

The JANAF recommended heat of formation for $CHF{=}O$ is based on the average of the heats of formation of the analogous $CH_2{=}O$ and $CF_2{=}O$. Although this procedure introduces significant uncertainty, it may not be important, since there are relatively good experimentally derived rate expressions for thermal decomposition of formyl fluoride ($CHF{=}O \rightarrow CO + HF$).

The literature value for the heat of formation of $CF_2{=}O$ is reported with a relatively low uncertainty. However, our BAC-MP4 *ab initio* calculations predict a value that is about 40 kJ/mol higher than the experimental number. Other *ab initio* calculations (Montgomery *et al.*, 1994; Schnieder and Wallington, 1994) using different approaches also predict a heat of formation for $CF_2{=}O$ that is higher (by about 30 kJ/mol) than the experimental value. There is reason to believe that there may have been side or wall reactions that complicated the measurement. Furthermore, the heats of formation of all the other oxygenated C_1 fluorocarbons (*e.g.*, $CF_3O\bullet$, $\bullet CF{=}O$, etc.) are referenced to $CF_2{=}O$. Because of these issues, both uncertainties in the experimental measurements and *ab initio* calculations warrant further examination. A new, reliable experimental measurement would be ideal.

The value recommended in the JANAF tables for the heat of formation of $\bullet CF{=}O$ is based on estimates of the C-F bond dissociation energy in $CF_2{=}O$. In contrast to that for $CHF{=}O$, the heat of formation of $\bullet CF{=}O$ is important, since there are no experimental data for the unimolecular decomposition $\bullet CF{=}O \rightarrow CO + F$, which is a primary destruction pathway for $\bullet CF{=}O$ (competing with H atom combination followed by HF elimination). Therefore, it would be very useful to obtain a better value (smaller uncertainty) for the heat of formation of $\bullet CF{=}O$ that is based on some type of experimental measurement.

There are no experimentally derived heats of formation for many of the fluoroethanes (CH_3-CH_2F, CHF_2-CHF_2, CH_2F-CF_3). These have been estimated using bond additivity, group additivity, or other empirical trends in heats of formation. However, there are significant uncertainties in using these procedures, because of non-covalent or ionic contributions to the stability of these species due the high electronegativity of fluorine. Furthermore, the stability of the fluoroethanes will influence product channels for fluoromethyl combination reactions (e.g., $\bullet CH_3 + \bullet CF_3 \rightarrow CH_3\text{-}CF_3$ versus $\bullet CH_3 + \bullet CF_3 \rightarrow CH_2{=}CF_2 + HF$).

There are experimentally derived heats of formation (*i.e.*, heat of reaction data) for only three of the fluoroethyl radicals (CH_3-CF_2•, CF_3-CH_2•, CF_3-CF_2•). Values for the eight other fluoroethyl radicals have been estimated using heats of formation of the parent fluoroethanes (which is some cases are also estimates) and C-H and C-F bond dissociation energies (largely estimates). The stability of the fluoroethyl radicals can be of importance for destruction of fluoroethylenes (*e.g.*, $CH_2=CF_2 + H \longleftrightarrow CH_3\text{-}CF_2\bullet$ and $CH_3\text{-}CF_2\bullet + H \rightarrow CH_2=CHF + HF$).

There are no experimentally derived heats of formation for the fluorovinyl radicals and these values cannot be estimated empirically. Consequently, in this reaction set we have employed values that we have calculated using *ab initio* methods. However, the uncertainties in these values may not be significant, since these species are largely formed via H atom abstraction (by OH) and consumed via combination with flame radicals such as H atoms. One possible uncertainty here is the effect of reaction energy on product channels for combination of H atoms (e.g. $CF_2=CH\bullet + H \rightarrow CH_2=CF_2$ [stabilized] versus $C_2HF + HF$ [elimination]).

There are no experimentally derived heats of formation for the fluoroketenes ($CHF=C=O$, $CF_2=C=O$) and the fluoroketyl radical ($\bullet CF=C=O$). In order to include these potential important species in the mechanism, it was necessary to use thermochemical data from our *ab initio* calculations. There are a number of reversible reactions involving these species that are important under stoichiometric to fuel rich conditions. Consequently, the uncertainties in the heats of formation of these species may contribute to uncertainties in flame speeds, flame temperatures, and flame products. These uncertainties should be better quantified in future mechanism refinements.

4.3. Kinetics

A brief discussion of the major uncertainties in the rate expressions used in this mechanism can be found in each individual section.

5. Reaction Set

5.1. Description of Listing

The reaction set listing (Table 5) is divided into sets of similar reaction types (e.g., Fluoromethanes: thermally and chemically activated decompositions, Fluoromethanes: atom abstraction and metathesis, Fluoromethyls: oxidation, etc.). For each reaction, the reaction number and reaction are given and followed by the Arrhenius parameters. The listing is essentially a CHEMKIN II reaction input file (Kee *et al.*, 1989).

The reactions are numbered according to the following scheme.

HO-xx	Hydrogen/Oxygen Chemistry
HC-xx	Hydrocarbon Chemistry
HF-xx	Hydrogen/Oxygen/Fluorine Chemistry
MD-xx	Fluoromethanes: Thermal and Activated Decompositions
MA-xx	Fluoromethanes: Abstractions
NN-xx	Fluoromethyl, Fluoromethylene, Fluoromethylidne Chemistry
PP-xx	Carbonyl Fluorides and Fluoromethoxy Chemistry
ED-xx	Fluoroethanes: Thermal and Activated Decompositions
EC-xx	Hot Fluoroethanes & Fluoroethyls: Fluoromethylene Reactions
EA-xx	Fluoroethanes: Abstractions by X (H, O, OH)
ER-xx	Fluoroethanes: Abstractions by R (CxHy)
GG-xx	Fluoroethyl Chemistry
JD-xx	Fluoroethylenes: Thermal and Activated Decompositions
JA-xx	Fluoroethylenes: Additions and Abstractions
JO-xx	Fluoroethylenes & Fluorovinyls: Oxidations
KK-xx	Fluoroethynes & Fluoroketenes Chemistry
CF-xx	H Atom Abstractions by F

The symbol "=" in the reaction indicates a reversible reaction and the symbol "=>" indicates an irreversible reaction. For reference purposes, the heat of reaction is also given for a number of the reactions (but not all). In addition, a notation and references are given to provide traceability on each rate expression. A detailed legend for the notation given for each reaction is at the end of Table 5. For example in the listing, $CH_3F + H = CH_2F + H_2$ (reaction MA-13) has Arrhenius parameters A=2.70E03, b=3.00, E/R=2667., where the rate expression is $k = A*T^b*\exp(-E/RT)$. The units are A_1=mol/s, A_2=mol/cm^3/s, A_3=mol/cm^6/s (for first, second, and third order reactions, respectively), T=K, E=kJ/mol, and R=8.314 J/mol/K or 1.987 cal/mol/K). Please note 1 cal = 4.184 J (for conversion from SI units). For this reaction example, the notation and references "xf", "75WES/DEH", and "nist" indicate that the rate expression is our fit to the experimental data of Westenberg and deHaas (1975).

A number of the unimolecular reactions have rate expressions with third-body efficiencies and/or low pressure fall-off parameters. For example, $H + O_2 \rightarrow HO_2 + M$ (reaction HO-13) has explicit third-body efficiencies for $M = H_2O$, CO_2, H_2, CO, and N_2. An example, of a rate expression with low pressure fall-off parameters is the reaction $CH_3 + CH_3 \rightarrow C_2H_6 + M$ (reaction HC-16), where "LOW" and "TROE" are low pressure and Troe fall-off parameters. The reader is referred to Kee *et al.* (1989) for more details on third-body efficiencies and fall-off parameters.

For reference purposes at the end of Table 5, the experimental rate expression (A=1.80E13, b=0.00, E/R=4803.) and the temperature range (T=600-900K) from this work (75WES/DEH) are also given. In some cases, where rate expressions were estimated relative to a reference reaction, the A-factor or activation energy were adjusted. For example in the listing, the reaction $CH_3F + C_2H_3 = CH_2F + C_2H_4$ (reaction MA-20) has the notations "r CH3" and "E*0.9". These indicate that an activation energy was used that was 90% of the activation energy for the analogous abstraction by CH_3, a reaction that is slightly more exothermic.

In order to reduce (slightly) the number of species in the reaction set, the isomers CHF=CHF(*E*), CHF=CH(*E*), and CHF=CF(*E*) were excluded (retaining the *Z* isomers). The differences in energies and chemistries are sufficiently small that this is justified. We note that a number of the fluoroethanes and fluoroethyl radicals have both *trans* and *gauche* forms. In this work, we used thermochemistry for the most stable or *trans* isomers.

The hydrogen/oxygen and hydrocarbon reaction subsets of the mechanism are derived from the Miller-Bowman mechanism (Miller and Bowman, 1989) and consists of about 30 species and 140 reactions. Any other hydrocarbon mechanism could be used instead. For example, the GRIMECH set (Bowman *et al.*, 1995) is a recent hydrocarbon mechanism that accurately reproduces flame speeds for methane mixtures.

In this work, some modifications to the Miller-Bowman mechanism were made. All nitrogen-containing species and reactions were removed. A number of the rich species (*e.g.*, C_2H, C_4H_2) were eliminated from the mechanism in order to keep the number of species in the mechanism to a manageable level. A number of species (*e.g.*, CH_3OH) were also added to the mechanism. In addition to these addition and deletions, a number of rate constants for a number of reactions (*e.g.*, CH_3+OH) were adjusted to provide correct falloff and product-channel ratios. In this section of the reaction set, the notation for the reference is slightly different. For example, for $CH_4 + H = CH_3 + H_2$ (reaction HC-1), the notation "73CLA/DOV MBA004" means that this rate expression was determined by Clark and Dove (1973) and was reaction #4 in table A of the Miller-Bowman mechanism (Miller and Bowman, 1989). Where only the Miller-Bowman reference is given, either the expression is directly attributable to that work or the origins/traceability of the expression is not clear.

HO	H2/O2 System: Combination, Decomposition	A	b	E/R	note	ref1	ref2	Hr
1	H + H + M = H2 + M	1.00E+18	-1.00	0.			MBA139	
	H2/0/ H2O/0/ CO2/0/							
2	H + H + H2 = H2 + H2	9.20E+16	-0.60	0.			MBA140	
3	H + H + H2O = H2 + H2O	6.00E+19	-1.25	0.			MBA141	
4	H + H + CO2 = H2 + CO2	5.49E+20	-2.00	0.			MBA142	
5	O + O + M = O2 + M	1.89E+13	0.00	-900.		86TSA/HAM	MBA145	
6	H + OH + M = H2O + M	1.60E+22	-2.00	0.			MBA143	
	H2O/5/							
7	H + O + M = OH + M	6.20E+16	-0.60	0.			MBA144	
	H2O/5/							
	H2/O2 System: Atom Transfers							
8	O + OH = O2 + H	4.00E+14	-0.50	0.		81HOW/SMI	MBA132	
9	O + H2 = OH + H	5.06E+04	2.67	3166.		88SUT/MIC	MBA133	
10	OH + OH = O + H2O	6.00E+08	1.30	0.			MBA138	
11	H2 + O2 = OH + OH	1.70E+13	0.00	24046.		71JAC/HOU	MBA130	
12	OH + H2 = H2O + H	1.17E+09	1.30	1825.		79COH/WES	MBA131	
	H2/O2 System: Peroxyl and Peroxide							
13	H + O2 + M = HO2 + M	3.61E+17	-0.72	0.			MBA134	
	H2O/18.6/ CO2/4.2/ H2/2.9/ CO/2.1/ N2/1.3/							
14	H + HO2 = H2 + O2	1.25E+13	0.00	0.			MBA146	
15	O + HO2 = O2 + OH	1.40E+13	0.00	540.			MBA137	
16	OH + HO2 = H2O + O2	7.50E+12	0.00	0.			MBA135	
17	H2O2 + M = OH + OH + M	1.30E+17	0.00	22899.			MBA148	
18	H + HO2 = OH + OH	1.40E+14	0.00	540.			MBA136	
19	HO2 + HO2 = H2O2 + O2	2.00E+12	0.00	0.		84WAR	MBA147	
20	H2O2 + H = HO2 + H2	1.60E+12	0.00	1912.			MBA149	
21	H2O2 + OH = H2O + HO2	1.00E+13	0.00	906.			MBA150	

Table 5. NIST HFC Mechanism

HC	C1 Hydrocarbons: Methane	A	b	E/R	note	ref1	ref2	Hr
1	CH4 + H = CH3 + H2	2.20E+04	3.00	4404.		73CLA/DOV	MBA004	
2	CH4 + O = CH3 + OH	1.02E+09	1.50	4330.		86SUT/MIC	MBA005	
3	CH4 + OH = CH3 + H2O	1.60E+06	2.10	1238.		83BAU/CRA	MBA005	
4	CH4 + O2 = CH3 + HO2	7.90E+13	0.00	28183.		72SKI/LIF	MBA003	
5	CH4 + HO2 = CH3 + H2O2	1.80E+11	0.00	9411.		72SKI/LIF	MBA006	
	C1 Hydrocarbons: Methyl							
6	CH3 + H (+M) = CH4 (+M)	6.00E+16	-1.00	0.		84WAR	MBA002	
	LOW/8.00E26 -3.0 0./					89STE/SMI		
	SRI/0.45 797. 979./							
	H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/							
7	CH3 + H = CH2 + H2	9.00E+13	0.00	7599.			MBA013	
8	CH3 + O = CH2O + H	8.00E+13	0.00	0.			MBA009	
9	CH3 + OH = CH2 + H2O	7.50E+06	2.00	2516.			MBA012	
10	CH3 + OH = CH3OH	2.24E+40	-8.20	5875.		87DEA/WES		
11	CH3 + OH = CH2OH + H	2.64E+19	-1.80	4060.		87DEA/WES		
12	CH3 + OH = CH3O + H	5.74E+12	-0.23	7011.		87DEA/WES		
13	CH3 + OH = CH2SING + H2O	8.90E+19	-1.80	4060.		87DEA/WES		
14	CH3 + O2 = CH3O + O	2.05E+18	-1.57	14710.		86TSA/HAM	MBA008	
15	CH3 + HO2 = CH3O + OH	2.00E+13	0.00	0.		86TSA/HAM	MBA007	
16	CH3 + CH3 (+M) = C2H6 (+M)	9.03E+16	-1.20	329.		88WAG/WAR	MBA001	
	LOW/3.18E41 -7.0 2762./					88WAG/WAR		
	TROE/0.6401 6927. 132./							
	H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/							

HC	C1 Hydrocarbons: Methylene (triplet)					A	b	E/R	note	ref1	ref2	Hr
17	CH2	+ OH	=	CH2O	+ H	2.50E+13	0.00	0.			MBA026	
18	CH2	+ O	=	CO	+ H +H	5.00E+13	0.00	0.			MBA043	
19	CH2	+ CO2	=	CH2O	+ CO	1.10E+11	0.00	503.			MBA042	
20	CH2	+ O	=	CO	+ H2	3.00E+13	0.00	0.			MBA044	
21	CH2	+ O2	=	CO2	+ H +H	1.60E+12	0.00	503.			MBA045	
22	CH2	+ O2	=	CH2O	+ O	5.00E+13	0.00	4529.			MBA046	
23	CH2	+ O2	=	CO2	+ H2	6.90E+11	0.00	252.			MBA047	
24	CH2	+ O2	=	CO	+ H2O	1.90E+10	0.00	-503.			MBA048	
25	CH2	+ O2	=	CO	+ OH+H	8.60E+10	0.00	-252.			MBA049	
26	CH2	+ O2	=	HCO	+ OH	4.30E+10	0.00	-252.			MBA050	
27	CH2	+ CH3	=	C2H4	+ H	3.00E+13	0.00	0.			MBA072	
28	CH2	+ CH2	=	C2H2	+ H2	4.00E+13	0.00	0.			MBA114	
	C1 Hydrocarbons: Methylene (singlet)											
29	CH2SING	+ M	=	CH2	+ M	1.00E+13	0.00	0.			MBA106	
	H/0.0/											
30	CH2SING	+ H	=	CH2	+ H	2.00E+14	0.00	0.			MBA111	
31	CH2SING	+ O2	=	CO	+ OH+H	3.00E+13	0.00	0.			MBA109	
32	CH2SING	+ H2	=	CH3	+ H	7.00E+13	0.00	0.			MBA110	
33	CH2SING	+ CH4	=	CH3	+ CH3	4.00E+13	0.00	0.			MBA107	
34	CH2SING	+ C2H6	=	CH3	+ C2H5	1.20E+14	0.00	0.			MBA108	
	C1 Hydrocarbons: Methylidyne											
35	CH2	+ H	=	CH	+ H2	1.00E+18	-1.56	0.			MBA024	
36	CH2	+ OH	=	CH	+ H2O	1.13E+07	2.00	1510.			MBA025	
37	CH	+ O2	=	HCO	+ O	3.30E+13	0.00	0.		82BER/FLE	MBA027	
38	CH	+ O	=	CO	+ H	5.70E+13	0.00	0.		81MES/FIL	MBA028	
39	CH	+ OH	=	HCO	+ H	3.00E+13	0.00	0.			MBA029	
40	CH	+ CO2	=	HCO	+ CO	3.40E+12	0.00	347.		82BER/FLE	MBA030	
41	CH	+ H2O	=	CH2O	+ H	1.17E+15	-0.75	0.			MBA032	
42	CH	+ CH2O	=	CH2CO	+ H	9.46E+13	0.00	-259.		88ZAB/FLE	MBA033	
43	CH	+ CH2	=	C2H2	+ H	4.00E+13	0.00	0.			MBA035	
44	CH	+ CH3	=	C2H3	+ H	3.00E+13	0.00	0.			MBA036	
45	CH	+ CH4	=	C2H4	+ H	6.00E+13	0.00	0.		80BUT/FLE	MBA037	
46	C2H3	+ CH	=	CH2	+ C2H2	5.00E+13	0.00	0.			MBA086	
47	HCCO	+ CH	=	C2H2	+ CO	5.00E+13	0.00	0.			MBA104	

Table 5. NIST HFC Mechanism

HC	Oxidized C1 Hydrocarbons: Methanol	A	b	E/R	note	ref1	ref2	Hr
48	CH3OH + H = CH3O + H2	8.00E+12	0.00	3067.		90NOR		
49	CH3OH + OH = CH3O + H2O	1.50E+13	0.00	2999.		75BOW		
50	CH3OH + CH3 = CH3O + CH4	1.45E+01	3.10	3490.		90NOR		
51	CH3OH + O2 = CH2OH + HO2	2.05E+13	0.00	22505.		90NOR		
52	CH3OH + H = CH2OH + H2	3.20E+13	0.00	3067.		90NOR		
53	CH3OH + O = CH2OH + OH	3.88E+05	2.50	1550.		90NOR		
54	CH3OH + OH = CH2OH + H2O	1.50E+13	0.00	2999.		75BOW		
55	CH3OH + HO2 = CH2OH + H2O2	3.98E+13	0.00	9763.		90NOR		
56	CH3OH + CH3 = CH2OH + CH4	3.19E+01	3.17	3609.		90NOR		
	Oxidized C1 Hydrocarbons: Methoxy, Hydroxymethyl							
57	CH3O + M = CH2O + H + M	1.00E+14	0.00	12582.			MBA014	
58	CH3O + O2 = CH2O + HO2	6.30E+10	0.00	1309.			MBA022	
59	CH3O + H = CH2O + H2	2.00E+13	0.00	0.			MBA016	
60	CH3O + O = CH2O + OH	1.00E+13	0.00	0.			MBA020	
61	CH3O + OH = CH2O + H2O	1.00E+13	0.00	0.			MBA018	
62	CH2OH + M = CH2O + H+M	1.00E+14	0.00	12582.			MBA015	
63	CH2OH + O2 = CH2O + HO2	1.48E+13	0.00	755.			MBA023	
64	CH2OH + H = CH2O + H2	2.00E+13	0.00	0.			MBA017	
65	CH2OH + O = CH2O + OH	1.00E+13	0.00	0.			MBA021	
66	CH2OH + OH = CH2O + H2O	1.00E+13	0.00	0.			MBA019	
	Oxidized C1 Hydrocarbons: Formaldehyde and Formyl							
67	CH2O + M = HCO + H + M	3.31E+16	0.00	40765.		80DEA/JOH	MBA053	
68	CH2O + H = HCO + H2	2.19E+08	1.77	1510.		86TSA/HAM	MBA052	
69	CH2O + O = HCO + OH	1.80E+13	0.00	1550.		80KLE/SKO	MBA054	
70	CH2O + OH = HCO + H2O	3.43E+09	1.18	-225.		86TSA/HAM	MBA051	
71	HCO + M = CO + H+M	2.50E+14	0.00	8456.		84WAR	MBA056	
	CO/1.9/ H2/1.9/ CH4/2.8/ CO2/3.0/ H2O/5.0/							
72	HCO + H = CO + H2	1.19E+13	0.25	0.			MBA057	
73	HCO + O = CO + OH	3.00E+13	0.00	0.		84WAR	MBA058	
74	HCO + O = CO2 + H	3.00E+13	0.00	0.		84WAR	MBA059	
75	HCO + OH = CO + H2O	1.00E+14	0.00	0.		84TEM/WAG	MBA055	
76	HCO + O2 = CO + HO2	3.30E+13	-0.40	0.		81VEY/LES	MBA060	
	Oxidized C1 Hydrocarbons: Carbon Monoxide							
77	CO + O + M = CO2 + M	6.17E+14	0.00	1510.		86TSA/HAM	MBA061	
78	CO + OH = CO2 + H	1.51E+07	1.30	-381.			MBA062	
79	CO + O2 = CO2 + O	1.60E+13	0.00	20634.		71BRA/BEL	MBA063	
80	CO + HO2 = CO2 + OH	5.80E+13	0.00	11542.		77ATR/BAL	MBA064	

Table 5. NIST HFC Mechanism

HC	**C2 Hydrocarbons: Ethane**	A	b	E/R	note	ref1	ref2	Hr
81	C2H6 + H = C2H5 + H2	5.40E+02	3.50	2622.		73CAL/DOV	MBA066	
82	C2H6 + O = C2H5 + OH	3.00E+07	2.00	2574.		84WAR	MBA067	
83	C2H6 + OH = C2H5 + H2O	8.70E+09	1.05	911.		83TUL/RAV	MBA068	
84	C2H6 + CH3 = C2H5 + CH4	5.50E-01	4.00	4177.		73CLA/DOV	MBA065	
	C2 Hydrocarbons: Ethyl							
85	C2H5 + H = CH3 + CH3	1.00E+14	0.00	0.			MBA074	
86	C2H5 + O = CH2O + CH3	1.60E+13	0.00	0.		86TSA/HAM		
87	C2H5 + O2 = C2H4+HO2	2.56E+19	-2.77	995.		90BOZ/DEA		
	C2 Hydrocarbons: Ethylene							
88	C2H4 + M = C2H2 + H2 + M	1.50E+15	0.00	28083.		83KIE/KAP	MBA128	
89	C2H4 + M = C2H3 + H + M	1.40E+16	0.00	41449.			MBA129	
90	C2H4 + H (+M) = C2H5 (+M)	8.40E+08	1.50	498.		86TSA/HAM		
	LOW/6.37E27 -2.8 -54./						MBA073	
	H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/						MBA073	
91	C2H4 + H = C2H3 + H2	1.10E+14	0.00	4278.		73PEE/MAH	MBA069	
92	C2H4 + O = CH3 + HCO	1.60E+09	1.20	375.		84WAR	MBA070	
93	C2H4 + OH = C2H3 + H2O	4.50E+06	2.00	1434.	rf			
	C2 Hydrocarbons: Vinyl							
94	C2H3 + H = C2H2 + H2	1.20E+13	0.00	0.		92BAU/COB		
95	C2H3 + OH = C2H2 + H2O	5.00E+12	0.00	0.			MBA083	
96	C2H3 + CH2 = C2H2 + CH3	3.00E+13	0.00	0.			MBA084	
97	C2H3 + O2 = CH2O + HCO	1.05E+38	-8.22	3538.	a/s	92WES		
98	C2H3 + O2 = CH2O + HCO	4.48E+26	-4.55	2758.	direct	92WES		
99	C2H3 + O = CH2CO + H	3.00E+13	0.00	0.		84WAR	MBA081	
	C2 Hydrocarbons: Acetylene							
100	C2H2 + H (+M) = C2H3 (+M)	5.54E+12	0.00	1213.		76PAY/STI	MBA079	
	LOW/2.67E27 -3.5 2410./							
	H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/							
101	C2H2 + OH = HCCOH + H	5.04E+05	2.30	6794.			MBA088	
102	C2H2 + OH = CH2CO + H	2.18E-04	4.50	-503.			MBA089	
103	C2H2 + OH = CH3 + CO	4.83E-04	4.00	-1007.			MBA090	
104	C2H2 + O = CH2 + CO	1.02E+07	2.00	956.			MBA076	
105	C2H2 + O = HCCO + H	1.02E+07		956.			MBA077	
106	C2H2 + O2 = HCCO + OH	2.00E+08	1.50	15148.			MBA126	

Table 5. NIST HFC Mechanism

HC	Oxidized C2 Hydrocarbons: Ketene, HCCOH	A	b	E/R	note	ref1	ref2	Hr
107	HCCOH + H = CH2CO + H	1.00E+13	0.00	0.			MBA091	
108	CH2CO + H = CH3 + CO	1.13E+13	0.00	1725.		79MIC/NAV	MBA094	
109	CH2CO + H = HCCO + H2	5.00E+13	0.00	4026.			MBA095	
110	CH2CO + O = CO2 + CH2	1.75E+12	0.00	679.		83WAS/HAT	MBA093	
111	CH2CO + O = HCCO + OH	1.00E+13	0.00	4026.			MBA096	
112	CH2CO + OH = HCCO + H2O	7.50E+12	0.00	1007.			MBA097	
113	CH2CO (+M) = CH2 + CO (+M)	3.00E+14	0.00	35722.			MBA098	
	LOW/3.60E15 0.0 59270./							
114	**Oxidized C2 Hydrocarbons: Ketyl**							
115	HCCO + H = CH2SING + CO	1.00E+14	0.00	0.			MBA101	
116	HCCO + O = H + 2CO	1.00E+14	0.00	0.			MBA102	
117	HCCO + O2 = 2CO + OH	1.60E+12	0.00	430.		92BAU/COB	MBA103	
118	HCCO + HCCO = C2H2 + 2CO	1.00E+13	0.00	0.			MBA105	
119	HCCO + CH2 = C2H3 + CO	3.00E+13	0.00	0.			MBA115	

Table 5. NIST HFC Mechanism

HF	H/F/O Chemistry				A	b	E/R	note	ref1	ref2	Hr
1	HF	+ M	= H	+ F	3.12E+13	0.00	49985.	xh	81BAU/DUX		135
2	H2	+ F	= H	+ HF	2.56E+12	0.50	327.	xf	89STE/BRU	nist	-32
3	OH	+ F	= O	+ HF	2.00E+13	0.00	0.	r	H+HNO3	nist	-34
4	HO2	+ F	= O2	+ HF	2.89E+12	0.50	0.	xf	83WAL/WAG	nist	-86
5	H2O	+ F	= OH	+ HF	1.30E+09	1.50	0.	xf	83WAL/WAG	nist	-17
6	H2O2	+ F	= HO2	+ HF	1.73E+12	0.50	0.	xf	83WAL/WAG	nist	-49

Table 5. NIST HFC Mechanism

MD	Fluoromethanes: Thermal Decomposition				A	b	E/R	note	ref1	ref2	Hr
7	CH2SING	+ HF	= CH3F		1.91E+23	-3.62	896.	xg	73SCH/WAG	nist	-89
8	CHF	+ H2	= CH3F		2.25E+17	-2.85	6543.	ak		nist	-83
9	CH2F	+ H	= CH3F		3.03E+21	-3.38	1741.	ak		nist	-97
10	CHF	+ HF	= CH2F2		3.64E+24	-4.26	2043.	ak		nist	-72
11	CF2	+ H2	= CH2F2		1.70E+06	-0.71	20584.	ak		nist	-62
12	CHF2	+ H	= CH2F2		2.75E+06	-0.32	3870.	ak		nist	-99
13	CHF3	+ M	= CF2	+ HF	2.39E+30	-4.00	34751.	xg	91HID/NAK	nist	61
14	CF3	+ F	= CF4		1.60E+39	-7.90	4504.	xk	86PLU/RYA	nist	-130
	Fluoromethanes: Activated Decomposition										
15	CH2F	+ H	= CH2SING	+ HF	8.19E+15	-0.63	254.	ak		nist	-9
16	CH2F	+ H	= CHF	+ H2	5.21E+08	1.16	503.	ak		nist	-15
17	CH2SING	+ HF	= CHF	+ H2	2.08E+07	1.27	4192.	ak		nist	-6
18	CH3	+ F	= CH2SING	+ HF	1.62E+16	-0.88	-494.	k		nist	-18
19	CH3	+ F	= CH2F	+ H	1.36E+12	-0.39	-133.	k		nist	-9
20	CHF2	+ H	= CHF	+ HF	1.49E+14	-0.11	51.	ak		nist	-27
21	CHF2	+ H	= CF2	+ H2	5.50E+03	2.42	-211.	ak		nist	-37
22	CHF	+ HF	= CF2	+ H2	5.77E+06	1.35	9009.	ak		nist	-10
23	CH2F	+ F	= CHF	+ HF	5.00E+13	0.00	0.	k		nist	-46
24	CF3	+ H	= CF2	+ HF	5.50E+13	0.00	0.	xk	89TSA/MCF	nist	-46
25	CHF2	+ F	= CF2	+ HF	3.00E+13	0.00	0.	k		nist	-69
MA	Fluoromethanes: H Atom Abstraction by H, O, OH, HO2										
1	CH3F	+ H	= CH2F	+ H2	2.70E+03	3.00	2667.	xf	75WES/DEH	nist	-6
2	CH2F2	+ H	= CHF2	+ H2	1.65E+03	3.00	2818.	xf	72RID/DAV	nist	-4
3	CHF3	+ H	= CF3	+ H2	9.00E+03	3.00	4680.	xf	78ART/BEL	nist	5
4	CH3F	+ O	= CH2F	+ OH	6.50E+07	1.50	3523.	xf	67PAR/AZA	nist	-4
5	CH2F2	+ O	= CHF2	+ OH	2.25E+07	1.50	3070.	xf	68PAR/NAL	nist	-2
6	CHF3	+ O	= CF3	+ OH	1.00E+08	1.50	4655.	xf	78JOU/LEB	nist	7
7	CH3F	+ OH	= CH2F	+ H2O	2.60E+08	1.50	1480.	xt	82JEO/KAU	91COH/WES	-20
8	CH2F2	+ OH	= CHF2	+ H2O	2.80E+07	1.70	1278.	xt	82JEO/KAU	91COH/WES	-19
9	CHF3	+ OH	= CF3	+ H2O	5.77E+06	1.80	2160.	xt	82JEO/KAU	87COH/BEN	-10
10	CH2F	+ H2O2	= CH3F	+ HO2	1.20E+10	0.00	-302.	r CH3	E*1.0	nist	-11
11	CHF2	+ H2O2	= CH2F2	+ HO2	1.20E+10	0.00	-302.	r CH3	E*1.0	nist	-13
12	CF3	+ H2O2	= CHF3	+ HO2	1.20E+10	0.00	-302.	r CH3	E*1.0	nist	-21

Table 5. NIST HFC Mechanism

MA	Fluoromethanes: F Atom Abstraction by H					A	b	E/R	note	ref1	ref2	Hr
13	CH3F	+ H	=	CH3	+ HF	2.75E+14	0.00	15803.	a		nist	-28
14	CH2F2	+ H	=	CH2F	+ HF	5.50E+13	0.00	17162.	a		nist	-17
15	CHF3	+ H	=	CHF2	+ HF	8.00E+13	0.00	20282.	a		nist	-5
16	CF4	+ H	=	CF3	+ HF	1.10E+15	0.00	22446.	x	71KOC/MOI		-5
	Fluoromethanes: H Atom Abstraction by CH3, C2H3											
17	CH3F	+ CH3	=	CH2F	+ CH4	1.50E+11	0.00	5737.	x	65PRI/BRY		-6
18	CH2F2	+ CH3	=	CHF2	+ CH4	8.70E+10	0.00	5133.	x	65PRI/BRY		-5
19	CF3	+ CH4	=	CHF3	+ CH3	8.34E+11	0.00	5496.	x	78ART/BEL		-4
20	CH3F	+ C2H3	=	CH2F	+ C2H4	1.50E+11	0.00	5184.	r CH3	E*0.9	nist	-10
21	CH2F2	+ C2H3	=	CHF2	+ C2H4	9.00E+10	0.00	4630.	r CH3	E*0.9	nist	-9
22	CF3	+ C2H4	=	CHF3	+ C2H3	8.00E+11	0.00	6039.	r CH3	E*1.1	nist	0
	Fluoromethanes: H Atom Abstraction by Fluoromethyls											
23	CH3F	+ CF3	=	CH2F	+ CHF3	1.35E+12	0.00	5637.	x	67GIL/QUI		-10
24	CH2F2	+ CH2F	=	CHF2	+ CH3F	9.00E+10	0.00	7046.	r CH3	E*1.4	nist	1
25	CH2F2	+ CF3	=	CHF2	+ CHF3	7.20E+11	0.00	5637.	x	67GIL/QUI		-8
	Fluoromethanes: H Atom Abstraction from CH2O, CH3OH, HCO by Fluoromethyls											
26	CH2O	+ CH2F	=	HCO	+ CH3F	5.54E+03	2.81	4177.	r CH3	E*1.4	nist	-9
27	CH2O	+ CHF2	=	HCO	+ CH2F2	5.54E+03	2.81	3926.	r CH3	E*1.3	nist	-10
28	CH2O	+ CF3	=	HCO	+ CHF3	5.54E+03	2.81	2315.	r CH3	E*.79	nist	-19
29	HCO	+ CH2F	=	CO	+ CH3F	9.00E+13	0.00	0.	r CH3		nist	-83
30	HCO	+ CHF2	=	CO	+ CH2F2	9.00E+13	0.00	0.	r CH3		nist	-84
31	HCO	+ CF3	=	CO	+ CHF3	9.00E+13	0.00	0.	r CH3		nist	-93
32	HCO	+ CH2F	=	CH2CO	+ HF	2.70E+13	0.00	0.	rul		nist	-82
33	HCO	+ CHF2	=	CHFCO	+ HF	2.70E+13	0.00	0.	rul		nist	-51
34	HCO	+ CF3	=	CF2CO	+ HF	2.70E+13	0.00	0.	rul		nist	-31

Table 5. NIST HFC Mechanism

NN	Fluoromethyls: Oxidation	A	b	E/R	note	ref1	ref2	Hr
1	CH2F + O2 = CHF:O + O +H	2.26E+09	1.14	14343.	r CF3	dH	nist	28
2	CHF2 + O2 = CF2:O + O +H	2.26E+09	1.14	8304.	r CF3	dH	nist	
3	CF3 + O2 = CF3O + O	2.26E+09	1.14	10820.	k		nist	21
4	CH2F + O = CHF:O + H	5.70E+13	0.00	0.	r CH3	CF3	nist	-91
5	CHF2 + O = CF2:O + H	3.70E+13	0.00	0.	r CH3	CF3	nist	-103
6	CF3 + O = CF2:O + F	1.87E+13	0.00	0.	x	89TSA/BEL	nist	-81
7	CH2F + OH = CH2O + HF	2.50E+13	0.00	0.	r CH3		nist	-95
8	CHF2 + OH = CHF:O + HF	2.50E+13	0.00	0.	r CH3		nist	-105
9	CF3 + OH = CF2:O + HF	2.00E+13	0.00	0.	r CH3		nist	-115
10	CH2F + HO2 = CH3F + O2	3.00E+12	0.00	0.	r CH3		nist	-49
11	CHF2 + HO2 = CH2F2 + O2	3.00E+12	0.00	0.	r CH3		nist	-50
12	CF3 + HO2 = CHF3 + O2	2.00E+12	0.00	0.	r CH3		nist	-59
13	CH2F + HO2 = CHF:O + OH + H	1.50E+13	0.00	0.	r CH3		nist	-24
14	CHF2 + HO2 = CF2:O + OH + H	1.50E+13	0.00	0.	r CH3		nist	-37
15	CF3 + HO2 = CF3O + OH	1.00E+13	0.00	0.	r CH3		nist	-32

Table 5. NIST HFC Mechanism

NN	Fluoromethylenes: Oxidation	A	b	E/R	note	ref1	ref2	Hr
16	CHF + H2O = CH2O + HF	5.00E+12	0.00	3271.	a		nist	29
17	CF2 + H2O = CHF:O + HF	5.00E+12	0.00	12582.	a		nist	52
18	CHF + O2 = CHF:O + O	2.00E+13	0.00	8304.	r CF2	E-10	nist	-60
19	CF2 + O2 = CF2:O + O	2.01E+13	0.00	13337.	x	77KEA/MAT		-51
20	CHF + O = CO + HF	8.43E+13	0.00	0.	x	90TSA/MCF		-181
21	CF2 + O = CF:O + F	7.00E+13	0.00	503.	xf	90TSA/MCF	nist	-38
22	CHF + OH = HCO + HF	2.00E+13	0.00	0.	r CF2		nist	-95
23	CF2 + OH = CF:O + HF	2.00E+13	0.00	1761.	r CF2		nist	
24	CHF + OH = CHF:O + H	2.00E+13	0.00	0.	r CF2		nist	-78
25	CF2 + OH = CF2:O + H	2.00E+13	0.00	1761.	xf	78BIO/LAZ	nist	-68
26	CHF + HO2 = CHF:O + OH	2.00E+13	0.00	0.	ul		nist	
27	CF2 + HO2 = CF2:O + OH	2.00E+13	0.00	0.	ul		nist	
28	CHF + HO2 = CH2F + O2	5.00E+12	0.00	0.	ul		nist	
29	CF2 + HO2 = CHF2 + O2	5.00E+12	0.00	0.	ul		nist	
	Fluoromethylenes: Destruction							
30	CHF + H = CH + HF	2.95E+14	0.00	0.	x	90TSA/MCF		-5
31	CF2 + H = CF + HF	2.00E+14	0.00	629.	xf	89TSA/MCF	nist	-12
32	CH2O + CHF = HCO + CH2F	1.00E+13	0.00	7549.	r CH4		nist	1
33	CH2O + CHF = CH2CO + HF	1.00E+13	0.00	7549.	r CH4		nist	-81
34	CH2O + CF2 = HCO + CHF2	1.00E+13	0.00	20634.	r CH4		nist	23
35	CH2O + CF2 = CHFCO + HF	1.00E+13	0.00	20634.	r CH4		nist	-28
36	HCO + CHF = CO + CH2F	2.00E+13	0.00	7549.	r CH4		nist	-74
37	HCO + CF2 = CO + CHF2	2.00E+13	0.00	20634.	r CH4		nist	-52

Table 5. NIST HFC Mechanism

NN	Fluoromethylidyne: Oxidation				A	b	E/R	note	ref1	ref2	Hr
38	CF	+ O2	= CF:O	+ O	2.00E+13	0.00	906.	xf	92PEE/VAN	nist	-43
39	CF	+ H2O	= CHF:O	+ H	2.00E+13	0.00	8556.	r Cl		nist	-42
40	CF	+ O	= CO	+ F	4.00E+13	0.00	503.	xf	90TSA/MCF	nist	-128
41	CF	+ OH	= CO	+ HF	3.00E+13	0.00	503.	r O		nist	-162
42	CF	+ HO2	= CF:O	+ OH	1.00E+13	0.00	0.	ul		nist	-95
	Fluoromethylidyne: Destruction										
43	CH	+ HF	= CF	+ H2	3.00E+13	0.00	0.	r CH		nist	-17
44	CF	+ H	= CH	+ F	4.00E+13	0.00	377.	xf	89TSA/MCF	nist	
			= C	+ HF	use these products (correct) if C is in mechanism						
45	CF	+ CH3	= CH2:CF	+ H	3.00E+13	0.00	0.	ul		nist	-20
46	CF	+ C2H3	= C2HF	+ CH2	3.00E+13	0.00	0.	ul		nist	-9
47	CF	+ CH2	= C2HF	+ H	3.00E+13	0.00	0.	ul		nist	-73
48	CF	+ CH2SING	= C2HF	+ H	3.00E+13	0.00	0.	ul		nist	-82
49	CF	+ CH4	= CH2:CHF	+ H	5.00E+12	0.00	5033.	ul		nist	-24
50	CF	+ C2H4	= C2H2	+ CH2F	1.00E+13	0.00	0.	ul		nist	-27
51	CF	+ F	= CF2		6.00E+13	0.00	0.	ul		nist	-123
PP	**Fluoromethoxys: Destruction**										
1	CF3O	+ M	= CF2:O	+ F	9.03E+26	-3.42	10921.	k		nist	17
2	CF3O	+ H	= CF2:O	+ HF	1.00E+14	0.00	0.	ul		nist	-118
3	CF3O	+ H2	= CF2:O	+ HF + H	1.00E+13	0.00	2516.	ul		nist	
4	CF3O	+ H2O	= CF2:O	+ HF + OH	1.00E+13	0.00	2516.	ul		nist	
5	CF3O	+ CH4	= CF2:O	+ HF + CH3	8.00E+12	0.00	1158.	r C2H6		nist	
6	CF3O	+ C2H6	= CF2:O	+ HF + C2H5	1.20E+13	0.00	1158.	xf	92CHE/ZHU	nist	
7	CF3O	+ C2H4	= CF2:O	+ HF + C2H3	1.00E+13	0.00	2516.	ul		nist	
8	CF3O	+ C2H2	= CF2:O	+ CH2:CF	1.00E+13	0.00	2516.	ul		nist	
9	CF3O	+ CH2O	= CF2:O	+ HF + HCO	5.00E+12	0.00	2516.	ul		nist	
10	CF3O	+ HCO	= CF2:O	+ HF + CO	5.00E+12	0.00	2516.	ul		nist	

Table 5. NIST HFC Mechanism

PP	Carbonyl Fluorides: CHF=O, CF2=O					A	b	E/R	note	ref1	ref2	Hr
11	CF:O	+ F	=	CF2:O		1.00E+12	0.00	0.	ul		nist	-131
12	CHF:O	+ M	=	CO	+ HF	2.48E+25	-3.00	21641.	xg	85SAI/KUR	nist	-2
13	CF2:O	+ H2O	=	CO2	+ 2HF	7.40E-03	3.84	12632.	ak	th/ FC(O)OH	nist	-13
14	CF2:O	+ H	=	CF:O	+ HF	5.50E+08	1.42	9512.	ak	Oadd	nist	-3
15	CF2:O	+ H	=	CF:O	+ HF	1.20E+10	0.83	11223.	ak	Cadd	nist	-3
16	CF2:O	+ H	=	CF:O	+ HF	2.40E+07	1.88	18067.	ak	abstract	nist	-3
17	CF2:O	+ OH	=	CO2	+ HF + F	2.70E+03	2.38	10569.	ak	Oadd th/FCO2	nist	-3
18	CHF:O	+ H	=	CF:O	+ H2	1.10E+08	1.77	1510.	r CH2O	A/2	nist	-4
19	CHF:O	+ O	=	CF:O	+ OH	9.00E+12	0.00	1550.	r CH2O		nist	-2
20	CHF:O	+ OH	=	CF:O	+ H2O	1.72E+09	1.18	-225.	r CH2O		nist	-18
21	CF:O	+ H2O2	=	CHF:O	+ HO2	1.00E+11	0.00	1963.	r	E*0.56	nist	-13
22	CHF:O	+ CH3	=	CF:O	+ CH4	2.00E+12	0.00	4529.	rul		nist	-4
23	CHF:O	+ CH2F	=	CF:O	+ CH3F	2.00E+12	0.00	4529.	rul		nist	2
24	CHF:O	+ CHF2	=	CF:O	+ CH2F2	2.00E+12	0.00	4529.	r		nist	1
25	CHF:O	+ CF3	=	CF:O	+ CHF3	2.00E+12	0.00	4529.	r		nist	-8
26	CHF:O	+ C2H3	=	CF:O	+ C2H4	2.00E+12	0.00	2516.	r	E*0.9	nist	-8
	Carbonyl Fluorides: CF=O											
27	CO	+ F + M	=	CF:O		1.03E+19	-1.40	-245.	k		nist	33
28	CF:O	+ O2	=	CO2	+ F + O	2.00E+13	0.00	12079.	ul		nist	25
29	CF:O	+ H	=	CO	+ HF	1.20E+14	0.00	0.	r HCO		nist	-102
30	CF:O	+ O	=	CO2	+ F	3.00E+13	0.00	0.	r HCO		nist	-94
31	CF:O	+ OH	=	CO2	+ HF	3.00E+13	0.00	0.	r HCO		nist	-128
32	CF:O	+ HO2	=	CO2	+ F + OH	3.00E+13	0.00	0.	r HCO		nist	-28
33	CF:O	+ CH3	=	CH2CO	+ HF	2.70E+13	0.00	0.	ul		nist	-85
34	CF:O	+ CH2F	=	CHFCO	+ HF	2.70E+13	0.00	0.	ul		nist	-52
35	CF:O	+ CHF2	=	CF2CO	+ HF	2.70E+13	0.00	0.	ul		nist	-35

Table 5. NIST HFC Mechanism

ED	Fluoroethanes: Thermal Decomposition	A	b	E/R	note	ref1	ref2	Hr
1	CH3-CH2F = C2H4 + HF	2.63E+13	0.00	30146.	x	70CAD/DAY		11
2	CH3-CHF2 = CH2:CHF + HF	7.94E+13	0.00	31152.	x	70TSC/QUI		22
3	CH3-CF3 = CH2:CF2 + HF	1.00E+14	0.00	34575.	x	71TSC/QUI		
4	CH2F-CH2F = CH2:CHF + HF	2.50E+13	0.00	31656.	x	71KER/TIM		5
5	CH2F-CHF2 = CHF:CHF-Z + HF	1.26E+14	0.00	34776.	x	74SEK/TSC		
6	CH2F-CHF2 = CH2:CF2 + HF	1.00E+13	0.00	32914.	x	74SEK/TSC		8
7	CH2F-CF3 = CHF:CF2 + HF	2.63E+13	0.00	35581.	x	72MIL/TSC		37
8	CHF2-CHF2 = CHF:CF2 + HF	2.00E+13	0.00	34927.	x	71MIL/HAR		32
9	CHF2-CF3 = CF2:CF2 + HF	4.00E+13	0.00	36034.	x	71TSC/MIL		41
	Fluoroethanes: Activated Decomposition, Ethyl + H (HF elimination)							
10	CH2F-CH2 + H = C2H4 + HF	1.44E+20	-2.12	871.	k		nist	
11	CH3-CHF + H = C2H4 + HF	2.27E+20	-2.21	981.	k		nist	
12	CH2F-CHF + H = CH2:CHF + HF	2.06E+23	-3.23	1147.	k		nist	
13	CHF2-CH2 + H = CH2:CHF + HF	5.24E+16	-0.93	443.	k		nist	
14	CH3-CF2 + H = CH2:CHF + HF	2.09E+16	-0.85	427.	k		nist	
15	CHF2-CHF + H = CHF:CHF-Z + HF	1.86E+20	-2.29	881.	k		nist	
16	CHF2-CHF + H = CH2:CF2 + HF	9.95E+19	-2.34	896.	k		nist	
17	CH2F-CF2 + H = CHF:CHF-Z + HF	6.32E+19	-2.21	820.	k		nist	
18	CH2F-CF2 + H = CH2:CF2 + HF	3.36E+19	-2.26	835.	k		nist	
19	CF3-CH2 + H = CH2:CF2 + HF	1.12E+21	-2.27	1127.	k		nist	
20	CHF2-CF2 + H = CHF:CF2 + HF	1.81E+22	-2.92	1545.	k		nist	
21	CF3-CF2 + H = CF2:CF2 + HF	1.41E+21	-2.40	1827.	k		nist	
	Fluoroethanes: Activated Decomposition, Ethyl + H (methyl formation)							
22	CH2F-CH2 + H = CH3 + CH2F	3.80E+11	0.64	319.	k		nist	
23	CH3-CHF + H = CH3 + CH2F	3.47E+10	0.90	689.	k		nist	
24	CH2F-CHF + H = CH2F + CH2F	1.79E+14	-0.11	664.	k		nist	
25	CHF2-CH2 + H = CH3 + CHF2	2.02E+06	2.16	227.	k		nist	
26	CH3-CF2 + H = CH3 + CHF2	1.62E+05	2.50	689.	k		nist	
27	CHF2-CHF + H = CH2F + CHF2	6.36E+12	0.32	735.	k		nist	
28	CH2F-CF2 + H = CH2F + CHF2	3.64E+12	0.33	594.	k		nist	
29	CF3-CH2 + H = CH3 + CF3	2.48E+11	0.82	1444.	k		nist	
30	CHF2-CF2 + H = CHF2 + CHF2	3.25E+15	-0.52	1510.	k		nist	
31	CF3-CF2 + H = CHF2 + CF3	4.37E+16	-0.75	2194.	k		nist	

Table 5. NIST HFC Mechanism

ED	Fluoroethanes: Activated Decomposition, Ethyl + H (stabilization)		b	E/R	note	ref1	ref2	Hr
32	CH2F-CH2 + H = CH3-CH2F	1.19E+35	-8.51	4097.	k		nist	
33	CH3-CHF + H = CH3-CH2F	9.57E+38	-9.24	3704.	k		nist	
34	CH2F-CHF + H = CH2F-CH2F	1.56E+45	10.80	4061.	k		nist	
35	CHF2-CH2 + H = CH3-CHF2	2.96E+37	-9.05	3603.	k		nist	
36	CH3-CF2 + H = CH3-CHF2	3.11E+40	-9.59	3619.	k		nist	
37	CHF2-CHF + H = CH2F-CHF2	1.20E+45	-10.60	3785.	k		nist	
38	CH2F-CF2 + H = CH2F-CHF2	2.74E+43	-10.50	3860.	k		nist	
39	CF3-CH2 + H = CH3-CF3	7.27E+42	-9.86	3704.	k		nist	
40	CHF2-CF2 + H = CHF2-CHF2	3.77E+46	-10.80	4519.	k		nist	
41	CF3-CF2 + H = CHF2-CF3	1.12E+47	-10.80	2063.	k		nist	
	Fluoroethanes: Activated Decomposition, Ethyl + H (H atom elimination)							
42	CH2F-CH2 + H = CH3-CHF + H	1.87E+01	3.10	69.	k		nist	
43	CHF2-CH2 + H = CHF2-CH2 + H	1.59E-03	4.35	79.	k		nist	
44	CH2F-CF2 + H = CHF2-CHF + H	6.40E-01	3.53	921.	k		nist	
	Fluoroethanes: Activated Decomposition, Methyl + Methyl (HF elimination)							
45	CH3 + CH2F = C2H4 + HF	2.35E+19	-1.86	941.	k		nist	
46	CH2F + CH2F = CH2:CHF + HF	7.56E+21	-2.79	1303.	k		nist	
47	CH3 + CHF2 = CH2:CHF + HF	1.90E+15	-0.59	319.	k		nist	
48	CH2F + CHF2 = CHF:CHF-Z + HF	3.88E+20	-2.35	1453.	k		nist	
49	CH2F + CHF2 = CH2:CF2 + HF	2.23E+20	-2.41	1465.	k		nist	
50	CH3 + CF3 = CH2:CF2 + HF	5.53E+19	-1.94	1228.	k		nist	
51	CHF2 + CHF2 = CHF:CF2 + HF	2.20E+19	-1.95	2063.	k		nist	
52	CHF2 + CF3 = CF2:CF2 + HF	7.00E+16	-1.17	2179.	k		nist	
	Fluoroethanes: Activated Decomposition, Methyl + Methyl (stabilization)							
53	CH3 + CH2F = CH3-CH2F	1.57E+31	-6.27	2235.	k		nist	
54	CH2F + CH2F = CH2F-CH2F	2.37E+24	-3.79	1152.	k		nist	
55	CH3 + CHF2 = CH3-CHF2	1.93E+35	-7.69	2899.	k		nist	
56	CH2F + CHF2 = CH2F-CHF2	9.61E+38	-8.36	3493.	k		nist	
57	CH3 + CF3 = CH3-CF3	1.78E+33	-6.64	2526.	k		nist	
58	CHF2 + CHF2 = CHF2-CHF2	2.26E+24	-3.50	1691.	k		nist	
59	CHF2 + CF3 = CHF2-CF3	2.61E+26	-4.16	2063.	k		nist	
60	CF3 + CF3 = CF3-CF3	1.63E+36	-7.26	3548.	xvk		nist	

Table 5. NIST HFC Mechanism

EC	Fluoroethanes: Methyl + Methyl Disproportionation (carbene formation)						E/R	note	ref1	ref2	Hr
1	CH3	+ CH2F	= CH4	+ CHF	3.00E+13	0.00	1711.	ra CF2		nist	
2	CH2F	+ CH2F	= CH3F	+ CHF	3.00E+13	0.00	2416.	r CF2		nist	
3	CHF2	+ CH2F	= CH2F2	+ CHF	3.00E+13	0.00	2214.	r CF2		nist	
4	CF3	+ CH2F	= CHF3	+ CHF	3.00E+13	0.00	2315.	r CF2		nist	
5	CH3	+ CHF2	= CH4	+ CF2	3.00E+13	0.00	403.	xfa	67BRY/PRI	nist	
6	CH2F	+ CHF2	= CH3F	+ CF2	3.00E+13	0.00	1107.	xf	74FOL/PRI	nist	
7	CHF2	+ CHF2	= CH2F2	+ CF2	3.00E+13	0.00	805.	xf	84PRI/NIL	nist	
8	CF3	+ CHF2	= CHF3	+ CF2	3.00E+13	0.00	1007.	xf	69PRI/FOL	nist	
	Fluoroethanes: Carbene Insertion into Fluoromethanes										
9	CH3F	+ CH2SING	= C2H4	+ HF	3.00E+13	0.00	0.	r		nist	-101
10	CH2F2	+ CH2SING	= CH2:CHF	+ HF	2.00E+13	0.00	0.	r		nist	-91
11	CHF3	+ CH2SING	= CH2:CF2	+ HF	1.00E+13	0.00	0.	r		nist	-77
12	CF4	+ CH2SING	= CHF:CF2	+ HF	4.00E+13	0.00	15601.	a		nist	-62
13	CH4	+ CHF	= C2H4	+ HF	4.00E+13	0.00	7549.	a		nist	-66
14	CH3F	+ CHF	= CH2:CHF	+ HF	3.00E+13	0.00	7549.	r CH4		nist	-74
15	CH2F2	+ CHF	= CH2:CF2	+ HF	1.00E+13	0.00	7549.	r CH4		nist	-70
16	CH2F2	+ CHF	= CHF:CHF-Z	+ HF	1.00E+13	0.00	7549.	r CH4		nist	-63
17	CHF3	+ CHF	= CHF:CF2	+ HF	1.00E+13	0.00	7549.	r CH4		nist	-47
18	CF4	+ CHF	= CF2:CF2	+ HF	4.00E+13	0.00	15601.	a		nist	-30
19	CH4	+ CF2	= CH2:CHF	+ HF	4.00E+13	0.00	20634.	a		nist	-36
20	CH3F	+ CF2	= CH2:CF2	+ HF	1.50E+13	0.00	20634.	r CH4		nist	-49
21	CH3F	+ CF2	= CHF:CHF-Z	+ HF	1.50E+13	0.00	20634.	r CH4		nist	-42
22	CH2F2	+ CF2	= CHF:CF2	+ HF	2.00E+13	0.00	20634.	r CH4		nist	-37
23	CHF3	+ CF2	= CF2:CF2	+ HF	1.00E+13	0.00	20634.	r CH4		nist	-11
24	CF4	+ CF2	= CF3-CF3		4.00E+13	0.00	25667.	r CH4+10		nist	-56

Table 5. NIST HFC Mechanism

EC	**Fluoroethyls: Carbene Insertion into Fluoromethyls**	**A**	**b**	**E/R**	**note**	**ref1**	**ref2**	**Hr**
25	CH2F + CH2 = CH2:CHF + H	4.00E+13	0.00	0.	r CH3		nist	-66
26	CH2F + CH2 = C2H4 + F	4.00E+13	0.00	0.	r CH3		nist	-54
27	CHF2 + CH2 = CH2:CF2 + H	4.00E+13	0.00	0.	r CH3		nist	-63
28	CHF2 + CH2 = CH2:CHF + F	4.00E+13	0.00	0.	r CH3		nist	-47
29	CF3 + CH2 = CH2:CF2 + F	4.00E+13	0.00	0.	r CH3		nist	-41
30	CH2F + CH2SING = CH2:CHF + H	4.00E+12	0.00	0.	r CH3		nist	-75
31	CH2F + CH2SING = C2H4 + F	2.00E+12	0.00	0.	r CH3		nist	-63
32	CHF2 + CH2SING = CH2:CF2 + H	2.00E+12	0.00	0.	r CH3		nist	-72
33	CHF2 + CH2SING = CH2:CHF + F	4.00E+12	0.00	0.	r CH3		nist	-55
34	CF3 + CH2SING = CH2:CF2 + F	6.00E+12	0.00	0.	r CH3		nist	-50
35	CH3 + CHF = CH2:CHF + H	1.00E+12	0.00	1007.	ul		nist	-46
36	CH2F + CHF = CHF:CHF-Z + H	1.00E+12	0.00	1007.	ul		nist	-46
37	CH2F + CHF = CH2:CHF + F	1.00E+12	0.00	1007.	ul		nist	-37
38	CHF2 + CHF = CHF:CF2 + H	1.00E+12	0.00	1007.	ul		nist	-42
39	CHF2 + CHF = CHF:CHF-Z + F	1.00E+12	0.00	1007.	ul		nist	-27
40	CF3 + CHF = CHF:CF2 + F	1.00E+12	0.00	2516.	ul		nist	-20
41	CH3 + CF2 = CH2:CF2 + H	1.10E+11	0.00	2617.	r		nist	-21
42	CH2F + CF2 = CHF:CF2 + H	1.10E+11	0.00	2617.	r		nist	-20
43	CH2F + CF2 = CH2:CF2 + F	1.10E+11	0.00	2617.	r		nist	-12
44	CHF2 + CF2 = CF2:CF2 + H	1.10E+11	0.00	2617.	r		nist	-6
45	CHF2 + CF2 = CHF:CF2 + F	1.10E+11	0.00	2617.	r		nist	-1

Table 5. NIST HFC Mechanism

EA	Fluoroethanes: H Atom Abstraction by H, O, OH					A	b	E/R	note	ref1	ref2	Hr
1	CH3-CH2F	+ H	=	CH2F-CH2	+ H2	5.50E+08	1.60	4580.	r OH	10AE+8	nist	2
2	CH3-CH2F	+ O	=	CH2F-CH2	+ OH	2.90E+08	1.60	3070.	r OH	5AE+5	nist	3
3	CH3-CH2F	+ OH	=	CH2F-CH2	+ H2O	5.50E+07	1.60	550.	rxt	91COH/WES	nist	-13
4	CH3-CH2F	+ H	=	CH3-CHF	+ H2	3.30E+08	1.60	4580.	r OH	10AE+8	nist	
5	CH3-CH2F	+ O	=	CH3-CHF	+ OH	1.60E+08	1.60	3070.	r OH	5AE+5	nist	
6	CH3-CH2F	+ OH	=	CH3-CHF	+ H2O	3.30E+07	1.60	550.	rxt	91COH/WES	nist	
7	CH3-CHF2	+ H	=	CHF2-CH2	+ H2	1.50E+08	1.60	4831.	r OH	10A E+8	nist	
8	CH3-CHF2	+ O	=	CHF2-CH2	+ OH	7.50E+08	1.60	3322.	r OH	A*5 E+5	nist	
9	CH3-CHF2	+ OH	=	CHF2-CH2	+ H2O	1.54E+07	1.60	570.	rxt	91COH/WES	nist	
10	CH3-CHF2	+ H	=	CH3-CF2	+ H2	4.40E+07	1.60	4680.	r OH	A*10 E+8	nist	
11	CH3-CHF2	+ O	=	CH3-CF2	+ OH	2.20E+07	1.60	3171.	r OH	A*5 E+5	nist	
12	CH3-CHF2	+ OH	=	CH3-CF2	+ H2O	4.40E+06	1.60	670.	rxt	91COH/WES	nist	
13	CH3-CF3	+ H	=	CF3-CH2	+ H2	4.00E+10	1.10	6392.	r OH	A*10E+8	nist	3
14	CH3-CF3	+ O	=	CF3-CH2	+ OH	2.00E+10	1.10	4882.	r OH	A*5E+5	nist	4
15	CH3-CF3	+ OH	=	CF3-CH2	+ H2O	4.08E+09	1.10	2350.	xt	79CLY/HOL	87COH/BEN	-12
16	CH2F-CH2F	+ H	=	CH2F-CHF	+ H2	6.00E+08	1.70	4831.	r OH	A*10 E+8	nist	-11
17	CH2F-CH2F	+ O	=	CH2F-CHF	+ OH	3.00E+08	1.70	3322.	r OH	A*5 E+5	nist	-10
18	CH2F-CH2F	+ OH	=	CH2F-CHF	+ H2O	6.16E+07	1.70	810.	xt	83MAR/PAR	91COH/WES	-26
19	CH2F-CHF2	+ H	=	CHF2-CHF	+ H2	2.00E+08	1.70	4932.	r OH	A*10 E+8	nist	
20	CH2F-CHF2	+ O	=	CHF2-CHF	+ OH	1.00E+08	1.70	3422.	r OH	A*5 E+5	nist	
21	CH2F-CHF2	+ OH	=	CHF2-CHF	+ H2O	2.05E+07	1.70	906.	rxt	87COH/BEN	nist	
22	CH2F-CHF2	+ H	=	CH2F-CF2	+ H2	1.00E+08	1.70	5536.	r OH	A*10 E+8	nist	
23	CH2F-CHF2	+ O	=	CH2F-CF2	+ OH	5.00E+07	1.70	4026.	r OH	A*5 E+5	nist	
24	CH2F-CHF2	+ OH	=	CH2F-CF2	+ H2O	1.06E+07	1.70	1510.	rxt	87COH/BEN	nist	
25	CH2F-CF3	+ H	=	CF3-CHF	+ H2	2.00E+08	1.70	5284.	r OH	A*10 E+8	nist	-2
26	CH2F-CF3	+ O	=	CF3-CHF	+ OH	1.00E+08	1.70	3775.	r OH	A*5 E+5	nist	-1
27	CH2F-CF3	+ OH	=	CF3-CHF	+ H2O	2.10E+07	1.70	1270.	xt	79CLY/HOL	87COH/BEN	-17
28	CHF2-CHF2	+ H	=	CHF2-CF2	+ H2	1.60E+07	1.70	5335.	r OH	A*10 E+8	nist	
29	CHF2-CHF2	+ O	=	CHF2-CF2	+ OH	8.00E+07	1.70	3825.	r OH	A*5 E+5	nist	
30	CHF2-CHF2	+ OH	=	CHF2-CF2	+ H2O	1.60E+07	1.70	1330.	xt	79CLY/HOL	87COH/BEN	
31	CHF2-CF3	+ H	=	CF3-CF2	+ H2	1.40E+07	1.60	5133.	r OH	A*10 E+8	nist	0
32	CHF2-CF3	+ O	=	CF3-CF2	+ OH	7.00E+07	1.60	3624.	r OH	A*5 E+5	nist	1
33	CHF2-CF3	+ OH	=	CF3-CF2	+ H2O	1.40E+07	1.60	1130.	xt	79CLY/HOL	87COH/BEN	-15
	Fluoroethanes: F Atom Abstraction by H											
34	CF3-CF3	+ H	=	CF3-CF2	+ HF	1.00E+15	0.00	15098.	r CF4		nist	

Table 5. NIST HFC Mechanism

EA	**Fluoroethanes: Association with HO2**	**A**	**b**	**E/R**	**note**	**ref1**	**ref2**	**Hr**
35	CH3-CHF + H2O2 = CH3-CH2F + HO2	9.00E+09	0.00	503.	r C2H5		nist	
36	CH3-CF2 + H2O2 = CH3-CHF2 + HO2	9.00E+09	0.00	503.	r C2H5		nist	
37	CH2F-CH2 + H2O2 = CH3-CH2F + HO2	9.00E+09	0.00	503.	r C2H5		nist	
38	CH2F-CHF + H2O2 = CH2F-CH2F + HO2	9.00E+09	0.00	503.	r C2H5		nist	
39	CH2F-CF2 + H2O2 = CH2F-CHF2 + HO2	9.00E+09	0.00	503.	r C2H5		nist	
40	CHF2-CH2 + H2O2 = CH3-CHF2 + HO2	9.00E+09	0.00	503.	r C2H5		nist	
41	CHF2-CHF + H2O2 = CH2F-CHF2 + HO2	9.00E+09	0.00	503.	r C2H5		nist	
42	CHF2-CF2 + H2O2 = CHF2-CHF2 + HO2	9.00E+09	0.00	503.	r C2H5		nist	
43	CF3-CH2 + H2O2 = CH3-CF3 + HO2	9.00E+09	0.00	503.	r C2H5		nist	
44	CF3-CHF + H2O2 = CH2F-CF3 + HO2	9.00E+09	0.00	503.	r C2H5		nist	
45	CF3-CF2 + H2O2 = CHF2-CF3 + HO2	9.00E+09	0.00	503.	r C2H5		nist	

Table 5. NIST HFC Mechanism

ER	**Fluoroethanes: H Atom Abstraction by CH3, C2H3**	**A**	**b**	**E/R**	**note**	**ref1**	**ref2**	**Hr**
1	CH3-CH2F + CH3 = CH2F-CH2 + CH4	2.00E+11	0.00	6744.	r		nist	1
2	CH3-CH2F + C2H3 = CH2F-CH2 + C2H4	2.00E+11	0.00	5033.	r CH3	E-3	nist	4
3	CH3-CH2F + CH3 = CH3-CHF + CH4	1.50E+11	0.00	5033.	r		nist	
4	CH3-CH2F + C2H3 = CH3-CHF + C2H4	1.50E+11	0.00	3523.	r CH3	E-3	nist	
5	CH3-CHF2 + CH3 = CHF2-CH2 + CH4	2.00E+11	0.00	6039.	r		nist	
6	CH3-CHF2 + C2H3 = CHF2-CH2 + C2H4	2.00E+11	0.00	4529.	r CH3	E-3	nist	
7	CH3-CHF2 + CH3 = CH3-CF2 + CH4	8.00E+10	0.00	5033.	r		nist	
8	CH3-CHF2 + C2H3 = CH3-CF2 + C2H4	8.00E+10	0.00	3523.	r CH3	E-3	nist	
9	CH3-CF3 + CH3 = CF3-CH2 + CH4	2.00E+11	0.00	6039.	r		nist	2
10	CH3-CF3 + C2H3 = CF3-CH2 + C2H4	2.00E+11	0.00	4529.	r CH3	E-3	nist	5
11	CH2F-CH2F + CH3 = CH2F-CHF + CH4	3.00E+11	0.00	5234.	r		nist	-12
12	CH2F-CH2F + C2H3 = CH2F-CHF + C2H4	3.00E+11	0.00	3523.	r CH3	E-3	nist	-9
13	CH2F-CHF2 + CH3 = CHF2-CHF + CH4	2.00E+11	0.00	5033.	r		nist	
14	CH2F-CHF2 + C2H3 = CHF2-CHF + C2H4	2.00E+11	0.00	3523.	r CH3	E-3	nist	
15	CH2F-CHF2 + CH3 = CH2F-CF2 + CH4	1.00E+11	0.00	4831.	r		nist	
16	CH2F-CHF2 + C2H3 = CH2F-CF2 + C2H4	1.00E+11	0.00	3523.	r CH3	E-3	nist	
17	CH2F-CF3 + CH3 = CF3-CHF + CH4	2.00E+11	0.00	5033.	r		nist	-3
18	CH2F-CF3 + C2H3 = CF3-CHF + C2H4	2.00E+11	0.00	3523.	r CH3	E-3	nist	0
19	CHF2-CHF2 + CH3 = CHF2-CF2 + CH4	3.00E+11	0.00	5033.	r		nist	
20	CHF2-CHF2 + C2H3 = CHF2-CF2 + C2H4	3.00E+11	0.00	3523.	r CH3	E-3	nist	
21	CHF2-CF3 + CH3 = CF3-CF2 + CH4	5.70E+10	0.00	4781.	x	64PRI/THO		-1
22	CHF2-CF3 + C2H3 = CF3-CF2 + C2H4	6.00E+10	0.00	3523.	r CH3	E-3	nist	2

Table 5. NIST HFC Mechanism

ER	Fluoroethanes: H Atom Abstraction by Fluoromethyls	A	b	E/R	note	ref1	ref2	Hr
23	CH3-CH2F + CH2F = CH2F-CH2 + CH3F	2.00E+11	0.00	6543.	r CH3		nist	6
24	CH3-CH2F + CH2F = CH3-CHF + CH3F	1.50E+11	0.00	5033.	r CH3		nist	
25	CH3-CHF2 + CH2F = CHF2-CH2 + CH3F	2.00E+11	0.00	6039.	r CH3		nist	
26	CH3-CHF2 + CH2F = CH3-CF2 + CH3F	8.00E+10	0.00	5033.	r CH3		nist	
27	CH3-CF3 + CH2F = CF3-CH2 + CH3F	2.00E+11	0.00	6039.	r CH3		nist	7
28	CH2F-CH2F + CH2F = CH2F-CHF + CH3F	3.00E+11	0.00	5033.	r CH3		nist	-7
29	CH2F-CHF2 + CH2F = CHF2-CHF + CH3F	2.00E+11	0.00	5033.	r CH3		nist	
30	CH2F-CHF2 + CH2F = CH2F-CF2 + CH3F	1.00E+11	0.00	5033.	r CH3		nist	
31	CH2F-CF3 + CH2F = CF3-CHF + CH3F	2.00E+11	0.00	5033.	r CH3		nist	2
32	CHF2-CHF2 + CH2F = CHF2-CF2 + CH3F	3.00E+11	0.00	5536.	r CH3		nist	10
33	CHF2-CF3 + CH2F = CF3-CF2 + CH3F	2.00E+11	0.00	5033.	r CH3		nist	4
34	CH3-CH2F + CHF2 = CH2F-CH2 + CH2F2	2.00E+11	0.00	6543.	r CH3		nist	
35	CH3-CH2F + CHF2 = CH3-CHF + CH2F2	1.50E+11	0.00	5033.	r CH3		nist	
36	CH3-CHF2 + CHF2 = CHF2-CH2 + CH2F2	2.00E+11	0.00	6039.	r CH3		nist	
37	CH3-CHF2 + CHF2 = CH3-CF2 + CH2F2	8.00E+10	0.00	5033.	r CH3		nist	
38	CH3-CF3 + CHF2 = CF3-CH2 + CH2F2	2.00E+11	0.00	6039.	r CH3		nist	
39	CH2F-CH2F + CHF2 = CH2F-CHF + CH2F2	3.00E+11	0.00	5033.	r CH3		nist	
40	CH2F-CHF2 + CHF2 = CHF2-CHF + CH2F2	2.00E+11	0.00	5033.	r CH3		nist	
41	CH2F-CHF2 + CHF2 = CH2F-CF2 + CH2F2	1.00E+11	0.00	5033.	r CH3		nist	
42	CH2F-CF3 + CHF2 = CF3-CHF + CH2F2	2.00E+11	0.00	5033.	r CH3		nist	
43	CHF2-CHF2 + CHF2 = CHF2-CF2 + CH2F2	3.00E+11	0.00	5033.	r CH3		nist	
44	CHF2-CF3 + CHF2 = CF3-CF2 + CH2F2	2.00E+11	0.00	5033.	r CH3		nist	
45	CH3-CH2F + CF3 = CH2F-CH2 + CHF3	9.50E+11	0.00	4127.	x	71QUI/WHI		
46	CH3-CH2F + CF3 = CH3-CHF + CHF3	9.50E+11	0.00	4127.	x	71QUI/WHI		
47	CH3-CHF2 + CF3 = CHF2-CH2 + CHF3	3.10E+10	0.00	3573.	x	66OKS/PRA		
48	CH3-CHF2 + CF3 = CH3-CF2 + CHF3	3.10E+10	0.00	3573.	x	66OKS/PRA		
49	CH3-CF3 + CF3 = CF3-CH2 + CHF3	1.45E+12	0.00	6794.	x	67GIL/QUI		
50	CH2F-CH2F + CF3 = CH2F-CHF + CHF3	5.00E+11	0.00	3825.	r		nist	
51	CH2F-CHF2 + CF3 = CHF2-CHF + CHF3	3.00E+11	0.00	3624.	r		nist	
52	CH2F-CHF2 + CF3 = CH2F-CF2 + CHF3	2.00E+11	0.00	4026.	r		nist	
53	CH2F-CF3 + CF3 = CF3-CHF + CHF3	3.00E+11	0.00	3221.	r		nist	
54	CHF2-CHF2 + CF3 = CHF2-CF2 + CHF3	5.70E+11	0.00	5989.	x	67GIL/QUI		
55	CHF2-CF3 + CF3 = CF3-CF2 + CHF3	1.40E+11	0.00	5083.	x	67GIL/QUI		

Table 5. NIST HFC Mechanism

GG	Fluoroethyls: Association with O2	A	b	E/R	note	ref1	ref2	Hr
1	CH3-CHF + O2 = CH2:CHF + HO2	2.56E+19	-2.77	995.	r C2H5		nist	
2	CH3-CF2 + O2 = CH2:CF2 + HO2	2.56E+19	-2.77	995.	r C2H5		nist	
3	CH2F-CH2 + O2 = CH2:CHF + HO2	2.56E+19	-2.77	995.	r C2H5		nist	
4	CH2F-CHF + O2 = CHF:CHF-Z + HO2	2.56E+19	-2.77	995.	r C2H5		nist	
5	CH2F-CF2 + O2 = CHF:CF2 + HO2	2.56E+19	-2.77	995.	r C2H5		nist	
6	CHF2-CH2 + O2 = CH2:CF2 + HO2	2.56E+19	-2.77	995.	r C2H5		nist	
7	CHF2-CHF + O2 = CHF:CF2 + HO2	2.56E+19	-2.77	995.	r C2H5		nist	
8	CHF2-CF2 + O2 = CF2:CF2 + HO2	2.56E+19	-2.77	995.	r C2H5		nist	
9	CF3-CH2 + O2 = CF3 + CH2O + O	1.30E+13	0.00	22144.	r CF3		nist	
10	CF3-CHF + O2 = CF3 + CHF:O+ O	1.30E+13	0.00	11575.	r CF3		nist	
11	CF3-CF2 + O2 = CF3 + CF2:O+ O	1.30E+13	0.00	11575.	r CF3		nist	
	Fluoroethyls: Association with O							
12	CH2F-CH2 + O = CH2O + CH2F	6.60E+13	0.00	0.	r C2H5	3A/3	nist	
13	CHF2-CH2 + O = CH2O + CHF2	6.60E+13	0.00	0.	r C2H5	3A/3	nist	
14	CF3-CH2 + O = CH2O + CF3	6.60E+13	0.00	0.	r C2H5	3A/3	nist	
15	CH3-CHF + O = CHF:O + CH3	4.40E+13	0.00	0.	r C2H5	2A/3	nist	
16	CH2F-CHF + O = CHF:O + CH2F	4.40E+13	0.00	0.	r C2H5	2A/3	nist	
17	CHF2-CHF + O = CHF:O + CHF2	4.40E+13	0.00	0.	r C2H5	2A/3	nist	
18	CF3-CHF + O = CHF:O + CF3	4.40E+13	0.00	0.	r C2H5	2A/3	nist	
19	CH3-CF2 + O = CF2:O + CH3	2.20E+13	0.00	0.	r C2H5	1A/3	nist	
20	CH2F-CF2 + O = CF2:O + CH2F	2.20E+13	0.00	0.	r C2H5	1A/3	nist	
21	CHF2-CF2 + O = CF2:O + CHF2	2.20E+13	0.00	0.	r C2H5	1A/3	nist	
22	CF3-CF2 + O = CF2:O + CF3	2.20E+13	0.00	0.	r C2H5	1A/3	nist	

Table 5. NIST HFC Mechanism

GG	Fluoroethyls: Assocation with HO2	A	b	E/R	note	ref1	ref2	Hr
23	CH3-CHF + HO2 = CH3 + CHF:O+OH	3.00E+13	0.00	0.	r C2H5		nist	
24	CH3-CF2 + HO2 = CH3 + CF2:O+OH	3.00E+13	0.00	0.	r C2H5		nist	
25	CH2F-CH2 + HO2 = CH2F + CH2O+ OH	3.00E+13	0.00	0.	r C2H5		nist	
26	CH2F-CHF + HO2 = CH2F + CHF:O+OH	3.00E+13	0.00	0.	r C2H5		nist	
27	CH2F-CF2 + HO2 = CH2F + CF2:O+OH	3.00E+13	0.00	0.	r C2H5		nist	
28	CHF2-CH2 + HO2 = CHF2 + CH2O+ OH	3.00E+13	0.00	0.	r C2H5		nist	
29	CHF2-CHF + HO2 = CHF2 + CHF:O+OH	3.00E+13	0.00	0.	r C2H5		nist	
30	CHF2-CF2 + HO2 = CHF2 + CF2:O+OH	3.00E+13	0.00	0.	r C2H5		nist	
31	CF3-CH2 + HO2 = CF3 + CH2O+ OH	3.00E+13	0.00	0.	r C2H5		nist	
32	CF3-CHF + HO2 = CF3 + CHF:O+OH	3.00E+13	0.00	0.	r C2H5		nist	
33	CF3-CF2 + HO2 = CF3 + CF2:O+OH	3.00E+13	0.00	0.	r C2H5		nist	
34	CH3-CHF + HO2 = CH2:CHF + H2O2	3.00E+11	0.00	0.	r C2H5	2A/3	nist	
35	CH3-CF2 + HO2 = CH2:CF2 + H2O2	3.00E+11	0.00	0.	r C2H5	2A/3	nist	
36	CH2F-CH2 + HO2 = CH2:CHF + H2O2	2.00E+11	0.00	0.	r C2H5	2A/3	nist	
37	CH2F-CHF + HO2 = CHF:CHF-Z + H2O2	2.00E+11	0.00	0.	r C2H5	2A/3	nist	
38	CH2F-CF2 + HO2 = CHF:CF2 + H2O2	2.00E+11	0.00	0.	r C2H5	2A/3	nist	
39	CHF2-CH2 + HO2 = CH2:CF2 + H2O2	1.00E+11	0.00	0.	r C2H5	1A/3	nist	
40	CHF2-CHF + HO2 = CHF:CF2 + H2O2	1.00E+11	0.00	0.	r C2H5	1A/3	nist	
41	CHF2-CF2 + HO2 = CF2:CF2 + H2O2	1.00E+11	0.00	0.	r C2H5	1A/3	nist	
42	CH3-CHF + HO2 = CH3-CH2F + O2	3.00E+11	0.00	0.	r C2H5		nist	
43	CH3-CF2 + HO2 = CH3-CHF2 + O2	3.00E+11	0.00	0.	r C2H5		nist	
44	CH2F-CH2 + HO2 = CH3-CH2F + O2	3.00E+11	0.00	0.	r C2H5		nist	
45	CH2F-CHF + HO2 = CH2F-CH2F + O2	3.00E+11	0.00	0.	r C2H5		nist	
46	CH2F-CF2 + HO2 = CH2F-CHF2 + O2	3.00E+11	0.00	0.	r C2H5		nist	
47	CHF2-CH2 + HO2 = CH3-CHF2 + O2	3.00E+11	0.00	0.	r C2H5		nist	
48	CHF2-CHF + HO2 = CH2F-CHF2 + O2	3.00E+11	0.00	0.	r C2H5		nist	
49	CHF2-CF2 + HO2 = CHF2-CHF2 + O2	3.00E+11	0.00	0.	r C2H5		nist	
50	CF3-CH2 + HO2 = CH3-CF3 + O2	3.00E+11	0.00	0.	r C2H5		nist	
51	CF3-CHF + HO2 = CH2F-CF3 + O2	3.00E+11	0.00	0.	r C2H5		nist	
52	CF3-CF2 + HO2 = CHF2-CF3 + O2	3.00E+11	0.00	0.	r C2H5		nist	

Table 5. NIST HFC Mechanism

JD	Fluoroethylenes: Thermal Decompositions	A	b	E/R	note	ref1	ref2	Hr
1	CH2:CHF = C2H2 + HF	1.00E+14	0.00	35632.	x	70SIM/QUI		
2	CH2:CF2 = C2HF + HF	2.50E+14	0.00	43281.	x	70SIM/TSC		
3	CHF:CHF-Z = C2HF + HF	2.50E+14	0.00	39255.	r +dH		nist	37
4	CHF:CF2 = C2F2 + HF	2.50E+14	0.00	50327.	r +dH		nist	37
	Fluoroethylenes: Activated Decomposition, Methylene Combination (HF elimination)							
5	CH2SING + CHF = C2H2 + HF	1.70E+20	-2.12	1198.	r		nist	
6	CH2SING + CF2 = C2HF + HF	1.70E+20	-2.12	1198.	r		nist	
7	CHF + CHF = C2HF + HF	1.70E+20	-2.12	1198.	r		nist	
8	CHF + CF2 = C2F2 + HF	8.51E+19	-2.12	1198.	k		nist	
	Fluoroethylenes: Activated Decomposition, Methylene Combination (stabilization)							
9	CH2SING + CHF = CH2:CHF	3.10E+24	-3.80	1424.	r		nist	
10	CH2SING + CF2 = CH2:CF2	3.10E+24	-3.80	1424.	r		nist	
11	CHF + CHF = CHF:CHF-Z	1.55E+24	-3.80	1424.	r		nist	
12	CHF + CF2 = CHF:CF2	3.10E+24	-3.80	1424.	k		nist	
13	CF2:CF2 + M = CF2 + CF2 + M	3.96E+50	-9.06	42929.	xk	78SCH/WAG	nist	
	Fluoroethylenes: Activated Decomposition, Methylene Combination (H atom elimination)							
14	CH2SING + CHF = CH2:CF + H	1.64E+07	1.56	2889.	r		nist	
15	CH2SING + CHF = CHF:CH-Z + H	3.28E+07	1.56	2889.	r		nist	
16	CH2SING + CF2 = CF2:CH + H	3.28E+07	1.56	2889.	r		nist	
17	CHF + CHF = CHF:CF-Z + H	3.28E+07	1.56	2889.	r		nist	
18	CHF + CF2 = CF2:CF + H	1.64E+07	1.56	2889.	k		nist	
	Fluoroethylenes: Activated Decomposition, Vinyl + H (HF elimination)							
19	CH2:CF + H = C2H2 + HF	5.98E+20	-2.31	976.	r		nist	
20	CHF:CH-Z + H = C2H2 + HF	5.98E+20	-2.31	976.	r		nist	
21	CF2:CH + H = C2HF + HF	5.98E+20	-2.31	976.	r		nist	
22	CHF:CF-Z + H = C2HF + HF	5.98E+20	-2.31	976.	r		nist	
23	CF2:CF + H = C2F2 + HF	5.98E+20	-2.31	976.	k		nist	
	Fluoroethylenes: Activated Decomposition, Vinyl + H (stabilization)							
24	CH2:CF + H = CH2:CHF	2.40E+34	-7.11	2536.	r		nist	
25	CHF:CH-Z + H = CH2:CHF	2.40E+34	-7.11	2536.	r		nist	
26	CF2:CH + H = CH2:CF2	2.40E+34	-7.11	2536.	r		nist	
27	CHF:CF-Z + H = CHF:CHF-Z	2.40E+34	-7.11	2536.	r		nist	
28	CF2:CF + H = CHF:CF2	2.40E+34	-7.11	2536.	k		nist	

Table 5. NIST HFC Mechanism

JA	Fluoroethylenes: H Atom Addition (stabilization)	A	b	E/R	note	ref1	ref2	Hr
1	CH2:CHF + H (+M) = CH2F-CH2 (+M)	4.20E+08	1.50	498.	r C2H4		nist	
2	CH2:CHF + H (+M) = CH3-CHF (+M)	4.20E+08	1.50	498.	r C2H4		nist	
3	CH2:CF2 + H (+M) = CHF2-CH2 (+M)	4.20E+08	1.50	498.	r C2H4		nist	
4	CH2:CF2 + H (+M) = CH3-CF2 (+M)	4.20E+08	1.50	498.	r C2H4		nist	
	LOW/3.19E27 -2.8 -54./				r C2H4		nist	
	H2/2.0/ CO/2.0/ CO2/3.0 H2O/5.0/				r C2H4		nist	
5	CHF:CHF-Z + H (+M) = CH2F-CHF (+M)	8.40E+08	1.50	498.	r C2H4		nist	
	LOW/6.37E27 -2.8 -54./				r C2H4		nist	
	H2/2.0/ CO/2.0/ CO2/3.0 H2O/5.0/				r C2H4		nist	
6	CHF:CF2 + H (+M) = CHF2-CHF (+M)	4.20E+08	1.50	498.	r C2H4		nist	
7	CHF:CF2 + H (+M) = CH2F-CF2 (+M)	4.20E+08	1.50	498.	r C2H4		nist	
	LOW/3.19E27 -2.8 -54./				r C2H4		nist	
	H2/2.0/ CO/2.0/ CO2/3.0 H2O/5.0/				r C2H4		nist	
8	CF2:CF2 + H (+M) = CHF2-CF2 (+M)	8.40E+08	1.50	498.	r C2H4		nist	
	LOW/6.37E27 -2.8 -54./				r C2H4		nist	
	H2/2.0/ CO/2.0/ CO2/3.0 H2O/5.0/				r C2H4		nist	
	Fluoroethylenes: H Atom Addition (F atom displacement)							
9	C2H4 + F = CH2:CHF + H	2.00E+13	0.00	0.	ref		nist	
10	CH2:CHF + F = CH2:CF2 + H	2.00E+12	0.00	0.	ref		nist	
11	CH2:CHF + F = CHF:CHF-Z + H	5.00E+12	0.00	0.	ref		nist	
12	CHF:CHF-Z + F = CHF:CF2 + H	4.00E+12	0.00	0.	ref		nist	
13	CHF:CF2 + F = CF2:CF2 + H	2.00E+12	0.00	0.	ref		nist	
	Fluoroethylenes: H Atom Abstraction by H							
14	CH2:CHF + H = CHF:CH-Z + H2	3.30E+05	2.53	6161.	rC2H4		nist	
15	CH2:CHF + H = CH2:CF + H2	3.30E+05	2.53	6161.	rC2H4		nist	
16	CH2:CF2 + H = CF2:CH + H2	6.70E+05	2.53	6161.	rC2H4		nist	
17	CHF:CHF-Z + H = CHF:CF-Z + H2	3.30E+05	2.53	6161.	rC2H4		nist	
18	CHF:CF2 + H = CF2:CF + H2	3.30E+05	2.53	6161.	rC2H4		nist	

Table 5. NIST HFC Mechanism

JO	Fluoroethylenes: Oxidation by O	A	b	E/R	note	ref1	ref2	Hr
1	CH2:CHF + O = CH2F + HCO	5.30E+09	1.00	659.	xf	87CVE	nist	
2	CHF:CHF-Z + O = CH2F + CF:O	7.00E+09	1.00	800.	xf	87CVE	nist	
3	CH2:CF2 + O = CHF2 + HCO	4.30E+09	1.00	750.	xf	87CVE	nist	
4	CHF:CF2 + O = CHF2 + CF:O	6.00E+09	1.00	579.	xf	87CVE	nist	
5	CF2:CF2 + O = CF2 + CF2:O	1.90E+09	1.00	0.	xf	87CVE	nist	
6	CH2:CHF + O = CH3 + CF:O	5.30E+09	1.00	1158.	ref E+1	74SLA/GUT	nist	
	Fluoroethylenes: H Atom Abstraction by OH							
7	CH2:CHF + OH = CHF:CH-Z + H2O	2.00E+06	2.00	1434.	xf	88TUL	nist	-6
8	CH2:CHF + OH = CH2:CF + H2O	1.00E+06	2.00	1434.	xf	88TUL	nist	-10
9	CHF:CHF-Z + OH = CHF:CF-Z + H2O	2.00E+06	2.00	1434.	xf	88TUL	nist	-5
10	CH2:CF2 + OH = CF2:CH + H2O	2.00E+06	2.00	1434.	xf	88TUL	nist	
11	CHF:CF2 + OH = CF2:CF + H2O	1.00E+06	2.00	1434.	xf	88TUL	nist	1

Table 5. NIST HFC Mechanism

JO	**Fluorovinyls: Oxidation by O2**					**A**	**b**	**E/R**	**note**	**ref1**	**ref2**	**Hr**
12	CH2:CF	+ O2	=	CH2O	+ CF:O	4.48E+26	-4.55	2758.	r C2H3	direct	nist	
13	CHF:CH-Z	+ O2	=	CHF:O	+ HCO	4.48E+26	-4.55	2758.	r C2H3	direct	nist	
14	CHF:CF-Z	+ O2	=	CHF:O	+ CF:O	4.48E+26	-4.55	2758.	r C2H3	direct	nist	
15	CF2:CH	+ O2	=	CF2:O	+ HCO	4.48E+26	-4.55	2758.	r C2H3	direct	nist	
16	CF2:CF	+ O2	=	CF2:O	+ CF:O	4.48E+26	-4.55	2758.	r C2H3	direct	nist	
17	CH2:CF	+ O2	=	CH2O	+ CF:O	1.05E+38	-8.22	3538.	r C2H3	a/s	nist	
18	CHF:CH-Z	+ O2	=	CHF:O	+ HCO	1.05E+38	-8.22	3538.	r C2H3	a/s	nist	
19	CHF:CF-Z	+ O2	=	CHF:O	+ CF:O	1.05E+38	-8.22	3538.	r C2H3	a/s	nist	
20	CF2:CH	+ O2	=	CF2:O	+ HCO	1.05E+38	-8.22	3538.	r C2H3	a/s	nist	
21	CF2:CF	+ O2	=	CF2:O	+ CF:O	1.05E+38	-8.22	3538.	r C2H3	a/s	nist	
	Fluorovinyls: Oxidation by O											
22	CH2:CF	+ O	=	CH2CO	+ F	3.00E+13	0.00	0.	r C2H3		nist	
23	CHF:CF-Z	+ O	=	CHFCO	+ F	3.00E+13	0.00	0.	r C2H3		nist	
24	CF2:CF	+ O	=	CF2CO	+ F	3.00E+13	0.00	0.	r C2H3		nist	
25	CHF:CH-Z	+ O	=	CHFCO	+ H	3.00E+13	0.00	0.	r C2H3		nist	
26	CF2:CH	+ O	=	CF2CO	+ H	3.00E+13	0.00	0.	r C2H3		nist	
	Fluorovinyls: Oxidation by OH											
27	CH2:CF	+ OH	=	CH2CO	+ HF	3.00E+13	0.00	0.	r C2H3		nist	
28	CHF:CH-Z	+ OH	=	CH2CO	+ HF	3.00E+13	0.00	0.	r C2H3		nist	
29	CHF:CF-Z	+ OH	=	CHFCO	+ HF	2.00E+13	0.00	0.	r C2H3		nist	
30	CF2:CF	+ OH	=	CF2CO	+ HF	1.00E+13	0.00	0.	r C2H3		nist	
31	CH2:CF	+ OH	=	CH3	+ CF:O	3.00E+13	0.00	0.	r C2H3		nist	
32	CHF:CH-Z	+ OH	=	CH2F	+ HCO	3.00E+13	0.00	0.	r C2H3		nist	
33	CHF:CF-Z	+ OH	=	CH2F	+ CF:O	4.00E+13	0.00	0.	r C2H3		nist	
34	CF2:CF	+ OH	=	CHF2	+ CF:O	5.00E+13	0.00	0.	r C2H3		nist	

Table 5. NIST HFC Mechanism

KK	**Fluoroethynes: H Atom Addition/Stabilization**	A	b	E/R	note	refl	ref2	Hr
1	C2HF + H (+M) = CH2:CF (+M)	2.80E+12	0.00	1213.	rC2H2		nist	
2	C2HF + H (+M) = CHF:CH-Z (+M)	1.40E+12	0.00	1213.	rC2H2		nist	
3	LOW/0.67E27 -3.5 2410./							
	H2/2./ CO/2./ CO2/3./ H2O/5./							
4	C2F2 + H (+M) = CHF:CF-Z (+M)	2.80E+12	0.00	1213.	rC2H2		nist	
	LOW/1.33E27 -3.5 2410./							
	H2/2./ CO/2./ CO2/3./ H2O/5./							
	Fluoroethynes: Oxidation							
5	C2HF + O = FCCO-E + H	1.00E+07	2.00	956.	rC2H2 x2	MB A077	nist	
6	C2F2 + O = FCCO-E + F	1.00E+07	2.00	956.	rC2H2 x2	MB A077	nist	
7	C2HF + OH = CHFCO + H	2.18E-04	4.50	-503.	rC2H2 x2	MB A089	nist	
8	C2HF + OH = CH2F + CO	2.50E-04	4.00	-1007.	rC2H2 /2	MB A090	nist	
9	C2HF + OH = HCCO + HF	2.50E-04	4.00	-1007.	rC2H2 /2	MB A090	nist	
10	C2F2 + OH = CF2CO + H	2.18E-04	4.50	-503.	r C2H2	MB A089	nist	
11	C2F2 + OH = FCCO-E + HF	2.50E-04	4.00	-1007.	r C2H2	MB A090	nist	
	Fluoroketenes, Fluoroketyl							
12	CHFCO + H = CH2F + CO	1.13E+13	0.00	1725.	r CH2CO	MB A094	nist	
13	CF2CO + H = CHF2 + CO	1.13E+13	0.00	1725.	r CH2CO	MB A094	nist	
14	CHFCO + H = FCCO-E + H2	5.00E+13	0.00	4026.	r CH2CO	MB A095	nist	
15	CHFCO + O = CHF:O + CO	1.00E+13	0.00	4026.	ul		nist	
16	CF2CO + O = CF2:O + CO	1.00E+13	0.00	4026.	ul		nist	
17	CHFCO + OH = FCCO-E + H2O	7.50E+12	0.00	1007.	r CH2CO	MB A097	nist	
18	FCCO-E + H = CHF + CO	1.00E+14	0.00	0.	r HCCO	MB A101	nist	
19	FCCO-E + O = CF:O + CO	1.00E+14	0.00	0.	r HCCO	MB A102	nist	

Table 5. NIST HFC Mechanism

CF	F Atom Reactions	A	b	E/R	note	ref1	ref2	Hr
1	CH4 + F = CH3 + HF	5.90E+12	0.50	226.	xf	92ATK/BAU	nist	-31
2	CH3F + F = CH2F + HF	1.35E+14	0.00	604.	xf	83MAN/SET	nist	-37
3	CH2F2 + F = CHF2 + HF	9.00E+13	0.00	931.	xf	85CLY/HOD	nist	-36
4	CHF3 + F = CF3 + HF	4.50E+13	0.00	1862.	xf	83CLY/HOD	nist	-27
5	CH3OH + F = CH3O + HF	2.62E+09	1.44	-103.	x	91GLA/KOS		
6	CH3OH + F = CH2OH + HF	4.62E+07	1.97	-151.	x	91GLA/KOS		
7	CH2O + F = HCO + HF	6.00E+13	0.00	1007.	r CHFO		nist	-45
8	CHF:O + F = CF:O + HF	2.65E+13	0.00	906.	x	90FRA/ZHA		-35
9	CH3O + F = CH2O + HF	3.00E+13	0.00	0.	ul		nist	-114
10	HCO + F = CO + HF	1.00E+13	0.00	0.	ul		nist	-120
11	C2H6 + F = C2H5 + HF	8.00E+12	0.00	151.	x	60FET/KNO		
12	CH3-CH2F + F = CH2F-CH2 + HF	9.00E+13	0.00	403.	r C2H6		nist	
13	CH3-CHF2 + F = CHF2-CH2 + HF	1.00E+14	0.00	403.	r C2H6		nist	
14	CH3-CF3 + F = CF3-CH2 + HF	1.00E+14	0.00	2013.	r C2H6		nist	
15	CH3-CH2F + F = CH3-CHF + HF	6.00E+13	0.00	101.	r C2H6		nist	
16	CH2F-CH2F + F = CH2F-CHF + HF	1.30E+14	0.00	403.	r C2H6		nist	
17	CH2F-CHF2 + F = CHF2-CHF + HF	1.30E+14	0.00	403.	r C2H6		nist	
18	CH2F-CF3 + F = CF3-CHF + HF	6.00E+13	0.00	604.	r C2H6		nist	
19	CH3-CHF2 + F = CH3-CF2 + HF	3.00E+13	0.00	403.	r C2H6		nist	
20	CH2F-CHF2 + F = CH2F-CF2 + HF	3.00E+13	0.00	604.	r C2H6		nist	
21	CHF2-CHF2 + F = CHF2-CF2 + HF	6.00E+13	0.00	604.	r C2H6		nist	
22	CHF2-CF3 + F = CF3-CF2 + HF	4.00E+13	0.00	705.	r C2H6		nist	-33
23	C2H4 + F = C2H3 + HF	1.00E+14	0.00	1007.	r CH4		nist	-34
24	CF2:CF2 + F = CF3 + CF2	3.00E+13	0.00	0.	r H		nist	-18
25	C2H3 + F = C2H2 + HF	2.00E+13	0.00	0.	r H		nist	

Table 5. NIST HFC Mechanism

REF	REFERENCE REACTIONS (H,F,O)					A	b	E/R	note	ref1	ref2	Hr
1	HF	+ M	=	H	+ F	3.12E+13	0.00	49985.	x	81BAU/DUX	3000-5000K?	
2	H2	+ F	=	H	+ HF	7.23E+13	0.00	470.	x	89STE/BRU	221-376K	
3	HO2	+ F	=	O2	+ HF	5.00E+13			x	83WAL/WAG	300K	
4	H2O	+ F	=	OH	+ HF	2.53E+13	0.00	400.	x	83WAL/WAG	243-369K	
5	H2O2	+ F	=	HO2	+ HF	3.00E+13			x	83WAL/WAG	300K	
	REFERENCE REACTIONS (Fluoromethane: Decomposition)											
6	CH3F		=	CH2SING	+ HF	1.00E+14	0.00	42778.	x	79SCH/WAG	1150-1570K	
7	CH3F	+ M	=	CH2SING	+ HF	1.00E+16	0.00	33971.	x	79SCH/WAG	1150-1570K	
8	CH2F2		=	CHF	+ HF	8.90E+12	0.00	35380.	x	68POL/SHE	1060-1320K	
9	CHF3	+ M	=	CF2	+ HF	1.30E+16	0.00	29391.	x	91HID/NAK	1500-2500K	
10	CF3	+ F	=	CF4		7.80E+12			x	86PLU/PYA	295K	
11	CF3	+ H	=	CF2	+ HF	5.48E+13			x	89TSA/MCF	298K	
	REFERENCE REACTIONS (Fluoromethane: Abstraction, Metathesis)											
12	CH3F	+ H	=	CH2F	+ H2	1.80E+13	0.00	4731.	x	75WES/DEH	605-871K	
13	CH2F2	+ H	=	CHF2	+ H2	1.32E+13	0.00	4731.	x	72RID/DAV	873-953K	
14	CHF3	+ H	=	CF3	+ H2	3.32E+13	0.00	5536.	xrev	78ART/BEL	350-600K	
15	CF3	+ H2	=	CHF3	+ H	8.90E+11	0.00	4781.	x	78ART/BEL	350-600K	
16	CH3F	+ O	=	CH2F	+ OH	7.83E+12	0.00	4882.	x	67PAR/AZA	858-933K	
17	CH2F2	+ O	=	CHF2	+ OH	2.65E+12	0.00	4429.	x	68PAR/NAL	873-953K	
18	CHF3	+ O	=	CF3	+ OH	5.00E+12	0.00	5385.	x	78JOU/LEB	390-620K	
19	CH4	+ F	=	CH3	+ HF	1.80E+14	0.00	403.	xv	92ATK/BAU	250-450K	
20	CH3F	+ F	=	CH2F	+ HF	0.34 CH4+			x	83MAN/SET	300K	
21	CH2F2	+ F	=	CHF2	+ HF	3.40E+12			x	85CLY/HOD	298K	
22	CHF3	+ F	=	CF3	+ HF	9.00E+10			x	83CLY/HOD	298K	
23	CH3F	+ OH	=	CH2F	+ H2O	4.90E+12	0.00	1887.	x	82JEO/KAU	292-480K	
24	CH2F2	+ OH	=	CHF2	+ H2O	2.65E+12	0.00	1772.	x	82JEO/KAU	250-492K	
25	CHF3	+ OH	=	CF3	+ H2O	1.80E+12	0.00	2914.	x	82JEO/KAU	387-480K	
26	CH3	+ H2O2	=	CH4	+ HO2	1.21E+10	0.00	-300.	xv	86TSA/HAM		
27	CH2O	+ CH3	=	HCO	+ CH4	5.54E+03	2.81	2950.	xv	86TSA/HAM		
28	CH3OH	+ CH3	=	CH3O	+ CH4	1.44E+01	3.10	3490.	xv	86TSA/HAM		
29	CH3OH	+ CH3	=	CH2OH	+ CH4	3.20E+01	3.20	3608.	xv	87TSA		
30	HCO	+ CH3	=	CO	+ CH4	1.20E+14	0.00	0.	xv	86TSA/HAM		

Table 5. NIST HFC Mechanism

REF	REFERENCE REACTIONS (Fluoromethyl Oxidation)	A	b	E/R	note	ref1	ref2	Hr
31	CH3 + O = CH2O + H	8.43E+13	0.00	0.	xv	92BAU/COB		
32	CH3 + OH = Products	3.61E+13	0.00	0.	xv	92BAU/COB		
33	CH3 + HO2 = CH3O + OH	1.81E+13	0.00	0.	v	92BAU/COB		
34	CH3 + HO2 = CH4 + O2	3.61E+12	0.00	0.	v	86TSA/HAM		
35	CF3 + O = CF2:O + F	1.87E+13			x	89TSA/BEL	293K	
36	REFERENCE REACTIONS (Fluoromethylene, Fluoromethylidyne Oxidation, Destruction)							
36	CF2 + F2 = CF3 + F	5.00E+10			x	82SEE/ROT	550K	
37	CF2 + F2 = CF3 + F	1.20E+09			xul	86PLU/RYA	295K	
38	CF2 + O = PRODUCTS	1.21E+13			x	90TSA/MCF	293K	
39	CF2 + OH = CF2:O + H	5.00E+12			x	78BIO/LAZ	1090-1375K	
38	CH + O2 = PRODUCTS	3.30E+13	0.00	0.	xv	92BAU/COB		
39	CH + H2O = PRODUCTS	5.70E+12	0.00	-382.	xv	92BAU/COB		
40	CF + H = PRODUCTS	1.15E+13			x	89TSA/MCF	298K	
41	CF + O = PRODUCTS	7.23E+12			x	90TSA/MCF	293K	
42	CF + O2 = PRODUCTS	9.64E+11			x	92PEE/VAN	294K	
	REFERENCE REACTIONS (Carbonyl Fluorides)							
43	CHF:O + M = CO + HF	2.48E+25	-3.00	21641.	xg	85SAI/KUR	nist	-2
44	CHF:O + H = CF:O + H2	1.10E+08	1.77	1510.	r CH2O	A/2	nist	-4
45	CHF:O + O = CF:O + OH	9.00E+12	0.00	1550.	r CH2O		nist	-2
46	CHF:O + OH = CF:O + H2O	1.72E+09	1.18	-225.	r CH2O		nist	-18
47	CF:O + H2O2 = CHF:O + HO2	1.00E+11	0.00	1963.	r	E*0.56	nist	-13
48	CHF:O + CH3 = CF:O + CH4	2.00E+12	0.00	4529.	rul		nist	-4
49	CF:O + H = CO + HF	1.20E+14	0.00	0.	r HCO		nist	-102
50	CF:O + O = CO2 + F	3.00E+13	0.00	0.	r HCO		nist	-94
51	CF:O + OH = CO2 + HF	3.00E+13	0.00	0.	r HCO		nist	-128
52	CF:O + HO2 = CO2 + F + OH	3.00E+13	0.00	0.	r HCO		nist	-28
	REFERENCE REACTIONS (Fluoroethanes, Fluoroethyls: Carbene Insertion into Fluoromethanes, Fluoromethyls)							
53	CH3F + CH2SING = C2H4 + HF	4.00E+13	0.00	0.	r		nist	-101
54	CH2F + CH2 = CH2:CHF + H	4.00E+13	0.00	0.	r CH3		nist	-66
	REFERENCE REACTIONS (Fluoroethanes: H Atom Abstraction by H, O, OH)							
55	CH3-CH2F + OH = CH2F-CH2 + H2O	5.50E+07	1.60	550.	rxt	91COH/WES	nist	-13
56	CH3-CH2F + OH = CH3-CHF + H2O	3.30E+07	1.60	550.	rxt	91COH/WES	nist	
57	CH3-CHF2 + OH = CHF2-CH2 + H2O	1.54E+07	1.60	570.	rxt	91COH/WES	nist	
58	CH3-CHF2 + OH = CH3-CF2 + H2O	4.40E+06	1.60	670.	rxt	91COH/WES	nist	
59	CH2F-CHF2 + OH = CHF2-CHF + H2O	2.05E+07	1.70	906.	rxt	87COH/BEN	nist	
60	CH2F-CHF2 + OH = CH2F-CF2 + H2O	1.06E+07	1.70	1510.	rxt	87COH/BEN	nist	

Table 5. NIST HFC Mechanism

REF	REFERENCE REACTIONS (Fluoroethanes: H Atom Abstraction by CH3, C2H5, C2H3, HCO)					ref1	ref2	Hr
61	CH3-CH2F + CH3 = CH2F-CH2 + CH4	2.00E+11	0.00	6744.	r		nist	1
62	CH3-CHF + CH2O = CH3-CH2F + HCO	5.50E+03	2.80	2969.	r C2H5		nist	
	REFERENCE REACTIONS (Fluoroethanes, Fluoroethyls: Association with O2, O, HO2)							
63	CH3-CHF + H2O2 = CH3-CH2F + HO2	9.00E+09	0.00	503.	r C2H5		nist	
64	CH3-CHF + O2 = CH2:CHF + HO2	2.56E+19	-2.77	995.	r C2H5		nist	
65	CH2F-CH2 + O = CH2O + CH2F	6.60E+13	0.00	0.	r C2H5	3A/3	nist	
66	CH3-CHF + HO2 = CH2:CHF + H2O2	3.00E+11	0.00	0.	r C2H5	2A/3	nist	
	REFERENCE REACTIONS (Fluoroethylenes: H Atom Addition/Stabilization, F Atom Displacement, H Atom Abstraction)							
67	CH2:CF2 + H (+M) = CH3-CF2 (+M)	4.20E+08	1.50	498.	r C2H4		nist	
	LOW/3.19E27 -2.8 -54./				r C2H4		nist	
	C2H4 + F = CH2:CHF + H	2.00E+13	0.00	0.	ref		nist	
68	CH2:CHF + H = CHF:CH-Z + H2	3.30E+05	2.53	6161.	rC2H4		nist	
	REFERENCE REACTIONS (Fluoroethylenes: Oxidation by O)							
69	CH2:CHF + O = CH2F + HCO	5.30E+09	1.00	659.	xf	87CVE	nist	
70	CHF:CHF-Z + O = CH2F + CF:O	7.00E+09	1.00	800.	xf	87CVE	nist	
71	CH2:CF2 + O = CHF2 + HCO	4.30E+09	1.00	750.	xf	87CVE	nist	
72	CHF:CF2 + O = CHF2 + CF:O	6.00E+09	1.00	579.	xf	87CVE	nist	
73	CF2:CF2 + O = CF2 + CF2:O	1.90E+09	1.00	0.	xf	87CVE	nist	
	REFERENCE REACTIONS (Fluoroethylenes: H Atom Abstraction by OH)							
74	CH2:CHF + OH = CHF:CH-Z + H2O	2.00E+06	2.00	1434.	xf	88TUL	nist	-6
	REFERENCE REACTIONS (Fluorovinyls)							
75	CH2:CF + O2 = CH2O + CF:O	4.48E+26	-4.55	2758.	r C2H3	direct	nist	
76	CH2:CF + O2 = CH2O + CF:O	1.05E+38	-8.22	3538.	r C2H3	a/s	nist	
77	CH2:CF + O = CH2CO + F	3.00E+13	0.00	0.	r C2H3		nist	
78	CH2:CF + OH = CH2CO + HF	3.00E+13	0.00	0.	r C2H3		nist	
	REFERENCE REACTIONS (Fluoroethynes)							
79	C2HF + H (+M) = CHF:CH-Z (+M)	1.40E+12	0.00	1213.	rC2H2		nist	
	LOW/0.67E27 -3.5 2410./							
	H2/2./ CO/2./ CO2/3./ H2O/5./							
80	C2HF + O = FCCO-E + H	1.00E+07	2.00	956.	rC2H2 x2	MB A077	nist	
81	C2HF + OH = CHFCO + H	2.18E-04	4.50	-503.	rC2H2 x2	MB A089	nist	
82	C2HF + OH = CH2F + CO	2.50E-04	4.00	-1007.	rC2H2 /2	MB A090	nist	

Table 5. NIST HFC Mechanism

REF	REFERENCE REACTIONS (Fluoroketenes, Fluoroketyl)	A	b	E/R	note	ref1	ref2	Hr
83	CHFCO + H = CH2F + CO	1.13E+13	0.00	1725.	r CH2CO	MB A094	nist	
84	CHFCO + H = FCCO-E + H2	5.00E+13	0.00	4026.	r CH2CO	MB A095	nist	
85	CHFCO + OH = FCCO-E + H2O	7.50E+12	0.00	1007.	r CH2CO	MB A097	nist	
86	FCCO-E + H = CHF + CO	1.00E+14	0.00	0.	r HCCO	MB A101	nist	
87	FCCO-E + O = CF:O + CO	1.00E+14	0.00	0.	r HCCO	MB A102	nist	
	REFERENCE REACTIONS(F Atom Reactions)							
88	CH2O + F = HCO + HF	6.00E+13	0.00	1007.	r CHFO		nist	-45
89	C2H3 + F = C2H2 + HF	2.00E+13	0.00	0.	r C2H3		nist	
90	CHF:CF-Z + F = CHF + CF2	1.00E+13	0.00	0.	r C2H3		nist	
91	CF2:CF2 + F = CF3 + CF2	3.00E+13	0.00	0.	r C2H3		nist	-18

Table 5. NIST HFC Mechanism

NOTE	EXPLANATION
k	$AT^b e^{-E/RT}$
A	prefactor (mol, cm^3, s^{-1})
b	temperature dependence (dimensionless)
E/R	activation energy (K)
Hr	heat of reaction (kcal/mol)
x	experimental data
xh	experimental data measured at high temperatures
xf	experimental data fit with reasonable temperature dependence (b)
xg	experimental data fit with temperature dependence
xt	experimental data fit with TST temperature dependence
xk	RRKM benchmarked to experimental data
xv	evaluated recommendation based on experimental data
xrev	based on experimental data for reverse reaction
r	relative to reference reaction (e.g., r CH3 - referenced to analogous reaction for CH3)
rul	relative to reference reaction, upper limit estimate
ul	upper limit estimate
k	RRKM
a	calculated with ab initio transition state partition functions
ak	RRKM with ab initio thermodynamics

Table 5. NIST HFC Mechanism

NOTATION	REFERENCE
65PRI/BRY	Pritchard et al., 1965
65TSC	Tschuikow-Roux, 1965
67PAR/AZA	Parsamyan et al., 1970
68PAR/NAL	Parsamyan and Nalbanddyan, 1968
70CAD/DAY	Cadman et al., 1970
70SIM/QUI	Simmie et al., 1970
70TSC/QUI	Tschuikow-Roux and Quiring, 1970
71BRA/BEL	Brabbs et al., 1971
71JAC/HOU	Jachimowski and Houghton, 1971
71KER/TIM	Kerr and Timlin, 1971
71KOC/MOI	Kochubei and Moin, 1971
71MIL/HAR	Millward et al., 1971
71TSC/MIL	Tschuikow-Roux et al., 1971a
71TSC/QUI	Tschuikow-Roux et al., 1971b
71WAG/WAR	Wagner et al., 1971
72KER/PAR	Kerr and Parsonage, 1972
72MIL/TSC	Millward and Tschuikow-Roux, 1972
72RID/DAV	Ridley et al., 1972
72SKI/LIF	Skinner et al., 1972
73CLA/DOV	Clark and Dove, 1973
73PEE/MAH	Peeters and Mahnen, 1973
73SCH/WAG	Schug and Wagner, 1973
74SEK/TSC	Sekhar and Tschuikow-Roux, 1974
74SLA/GUT	Slagle et al., 1974
75BOW	Bowman, 1975
75WES/DEH	Westenberg and deHaas, 1975
76PAY/STI	Payne and Stief, 1976
77ATR/BAL	Atri et al.. 1977
77KEA/MAT	Keating and Matula, 1977
78ART/BEL	Arthur and Bell, 1978
78BIO/LAZ	Biordi et al., 1978
78JOU/LEB	Jourdain et al., 1978
79COH/WES	Cohen and Westberg, 1979
79MIC/NAV	Michael et al., 1979
79SCH/WAG	Schug et al., 1979

Table 5. NIST HFC Mechanism

NOTATION	REFERENCE
80BUT/FLE	Butler et al., 1980
80DEA/JOH	Dean et al., 1980
80KLE/SKO	Klemm et al., 1980
81BAU/DUX	Baulch et al., 1981
81HOW/SMI	Howard and Smith, 1981
81MES/FIL	Messing et al., 1981
81VEY/LES	Veyret and Lesclaus, 1981
82BER/FLE	Berman et al., 1982
83BAU/CRA	Baulch et al., 1983
83KIE/KAP	Kiefer et al., 1983
83TUL/RAV	Tully et al., 1983
83WAL/WAG	Walther and Wagner, 1983
83WAS/HAT	Washida et al., 1983
84RYA/PLU	Ryan and Plumb, 1984
84TEM/WAG	Temps and Wagner, 1984
84WAR	Warnatz, 1984
85SAI/KUR	Saito et al., 1985
86PLU/RYA	Plumb and Ryan, 1986a, 1986b
86SUT/MIC	Sutherland et al., 1986
86TSA/HAM	Tsang and Hampson, 1986
87COH/BEN	Cohen and Benson, 1987a, 1987b
87CVE	Cvetanovic, 1987
87DEA/WES	Dean and Westmoreland, 1987
88SUT/MIC	Sutherlan et al., 1988
88WAG/WAR	Wagner and Wardlaw, 1988
88ZAB/FLE	Zabarnick et al., 1988
89STE/BRU	Stevens et al., 1989
89STE/SMI	Steward, P.H.
89TSA/BEL	Tsai et al., 1989
89TSA/MCF	Tsai and McFadden, 1989

Table 5. NIST HFC Mechanism

NOTATION	REFERENCE
90BOZ/DEA	Bozzelli and Dean, 1990
90NOR	Norton, 1990
90TSA/MCF	Tsai and McFadden, 1990a, 1990b
91COH/WES	Cohen and Westberg, 1991
91HID/NAK	Hidaka et al., 1991
92BAU/COB	Baulch et al., 1992
92MAR/SZE	Maricq and Szente, 1992
92WES	Westmoreland, 1992
RRKM	this work, RRKM calculations
QRRK	this work, QRRK calculations
BAC	this work, BAC-MP4 & RRKM calculations
ref	this work, by analogy to other reactions

Table 5. NIST HFC Mechanism

6. Bibliography

6.1. Overview

A list of references is given below that was compiled and reviewed as part of this work. The list of references is divided into a number of different sections:

(6.2) General Thermochemistry and Kinetics,
(6.3) Hydrocarbon Chemistry,
(6.4) Fluorine Chemistry,
(6.5) Fluorocarbon Thermochemistry,
(6.6) Oxidized Fluorocarbon Thermochemistry,
(6.7) Fluorocarbon Kinetics (Decompositions),
(6.8) Fluorocarbon Kinetics (Abstractions),
(6.9) Fluorocarbon Kinetics (Oxidations),
(6.10) Oxidized Fluorocarbon Kinetics,
(6.11) Fluorocarbon Kinetics (Other),
(6.12) Flame Inhibition (Halogens), and
(6.13) Flame Inhibition (non-Halogens).

The references for "Hydrocarbon Kinetics" are not meant to be comprehensive, but rather documentation of those rate constants used in this work. The references for "Flame Inhibition" are also not meant to be comprehensive, but rather representative of flame inhibition chemistry as related to this work. In the other reference sections, all relevant references are included, both those references for which thermochemical or kinetic data were utilized in the reaction set, as well as other related sources of relevant data.

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