NIST Technical Note 2170

Modeling of Combustion of Fluorine-Containing Refrigerants

Valeri I. Babushok
Donald R. Burgess, Jr
Dennis K. Kim
Michael J. Hegetschweiler
Gregory T. Linteris

This publication is available free of charge from:
https://doi.org/10.6028/NIST.TN.2170

National Institute of Standards and Technology
U.S. Department of Commerce

NIST Technical Note 2170

Modeling of Combustion of Fluorine-Containing Refrigerants

Valeri I. Babushok
Donald R. Burgess, Jr
Dennis K. Kim
Michael J. Hegetschweiler
Gregory T. Linteris
National Institute of Standards and Technology

This publication is available free of charge from:
https://doi.org/10.6028/NIST.TN.2170

November 2021

U.S. Department of Commerce
Gina M. Raimondo, Secretary

National Institute of Standards and Technology
James K. Olthoff, Performing the Non-Exclusive Functions and Duties of the Under Secretary of Commerce for Standards and Technology & Director, National Institute of Standards and Technology

National Institute of Standards and Technology Technical Note 2170
Natl. Inst. Stand. Technol. Tech. Note 2170, 93 pages (November 2021)
CODEN: NTNOEF

This publication is available free of charge from:
https://doi.org/10.6028/NIST.TN.2170

Abstract

A gas-phase chemical kinetic model for the combustion of C_1-C_3 fluorine-containing refrigerants is presented, including a list of relevant species, their thermodynamic and transport properties, and the Arrhenius parameters for their reactions. Also included are tables of available experimental data in the literature for the laminar burning velocities for these HFC refrigerants and their mixtures. A comparison is made between the experimental data and predicted burning velocities as a function of the fuel-air equivalence ratio for the refrigerants. The model has been developed for the refrigerants: R-32, R-125, R-134a, R-152a, R-143, R-143a, R-1234yf, R-1234ze(E), R-1243zf and their mixtures. Agreement between predicted and measured burning velocity is very good for most of the refrigerant mixtures, and reasonably good agreement for a few.

Key words

Burning velocity; flame speed; GWP; enthalpy of formation; global warming potential; hydrofluorocarbons; chemical kinetic model; low-GWP refrigerants; refrigerant flammability; R-1234yf; R-1234ze(E); R-1243yf; R-134a; R-152a; R-125, R-32; R-143; R-143a; fluoropropenes.

Table of Contents

List of Tables

List of Figures

1. Introduction

Hydrofluorocarbons (HFCs) that are currently used as refrigerants have high global warming potentials (GWPs). They are projected to be major contributors to increases in radiative forcing in the Earth's atmosphere [1]. Their production and use are being phased down as stipulated in the Kigali Agreement to the Montreal Protocol [2]. New low-GWP replacements have been developed such as fluorinated propenes, which are being adopted by the heating, ventilating, air conditioning and refrigeration (HVAC&R) industry. Unfortunately, the modifications to reduce their tropospheric lifetimes (such as adding double bonds and hydrogen atoms) also makes these compounds have higher reactivities, and makes them slightly flammable.

The unstretched laminar burning velocity S_u^0 is a useful metric for flammability since it is a fundamental combustion parameter related to flammability limits, turbulent burning velocity and rate of pressure rise in explosions, and it also used in fire safety standards. For example, ASHRAE Standard 34, Designation and Safety Classification of Refrigerants [3] and ISO 817, Refrigerants - Designation and safety classification [4], use the burning velocity of hydrofluorocarbon/air mixtures for safety classification. Mixtures with peak burning velocity (over all values of the equivalence ratio, ϕ) less than 10 cm/s receive the less-flammable 2L classification, while those above 10 cm/s are designated class 2.

The burning velocity can be calculated using detailed kinetic models, and the ability to accurately calculate and predict burning velocities is useful to the industry. New refrigerants will be blends that are optimized for the simultaneous requirements of cycle efficiency, volumetric capacity, material compatibility, low toxicity, low-GWP, and low flammability. All these properties, except flammability, can presently be calculated or estimated fairly well for most refrigerants and their blends. The ability to predict burning velocity will allow more complete discovery and then optimization of new refrigerant blends, since it is faster and easier to predict burning velocities than to measure them, once a good kinetic mechanism has been developed and validated.

The proposed kinetic mechanism has been developed and validated, and consists of kinetic, thermodynamic, and transport data for the relevant fluorine-containing species and includes a hydrocarbon sub-mechanism. Using this mechanism with its associated data, the planar, 1-D, adiabatic laminar burning velocities have been calculated for a range of equivalence ratios ϕ. The model has been optimized by matching the calculated burning velocity with available experimental data from the literature. Note that although stretch, radiation heat losses, buoyancy and other secondary effects may affect the experiments, the published experimental data are adopted without alteration for comparison to the laminar, planar, adiabatic calculations presented here. This is necessary since the raw experimental data are not available for more sophisticated post-processing that could, to some extent, account for these effects. Hence, the experimental burning velocities presently compared to the model are suspected to have variable secondary deviations, and the present mechanism, while a useful first step, is an approximation that can serve until more accurate experimental data become available.

The mechanism has been developed for the refrigerant-air flames of: R-32, R-125, R-134a, R-152a, R-1234yf, R-1234ze(E), R-1243zf, R-227ea and their mixtures. In addition, the fluoropropene refrigerants have been examined for oxidizers with different O_2/N_2 ratios. Table

1 contains the list of HFC compounds and their mixtures considered in the present kinetic model (marked by asterisk after the name of compounds). That is, comparisons have also been made for the additional compounds: R-41, R-161, R-143, R143a, R152, and R116. As shown in the figures following, the model predictions are generally good, except for the compounds: R-41, R152, and R-161. For these compounds, the kinetic model overpredicts the burning velocity up to 2-5 cm/s depending on the equivalence ratio. While these compounds are included in the model (for completeness, and because experimental data are available), the lack of good agreement is not a major constraint since they are not widely-used refrigerants. Hence, the model is presently described as applying only to the compounds R-32, R-152a, R-134a, R-125, R-227ea, R-1234yf, R-1234ze(E), and R-1243zf.

2. Available experimental data on burning velocities of HFC refrigerants

Table 1 lists the HFC refrigerants along with the references for the experimental burning velocities available in literature. As it was indicated above, HFC compounds and their mixtures marked by asterisk were studied in this work.

Table 1. List of HFC refrigerants with experimental data on burning velocities.

HFC refrigerant	CAS number	References
C_1-hydrofluorocarbons		
R-32, CH_2F_2, difluoromethane,*	75-10-5	[5-16]
R-41, CH_3F, fluoromethane, *	593-53-3	[11, 17]
C_2- hydrofluorocarbons		
R-134a, CH_2FCF_3, 1,1,1,2-tetrafluoroethane, *	811-97-2	[18]
R-143, CH_2FCHF_2, 1,1,3-trifluoroethane, *	430-66-0	[10]
R-143a, CH_3CF_3, 1,1,1-trifluoroethane, *	420-46-2	[6, 10, 11]
R-152, CH_2FCH_2F, 1,2-difluroethane, *	624-72-6	[17]
R-152a, CH_3CHF_2, 1,1-difluoroethane, *	75-37-6	[6, 10-12, 14, 16, 18, 19]
R-161, C_2H_5F, fluoroethane, *	353-36-6	[11, 17]
C_3-hydrofluorocarbons		
R-1234yf, CH_2=$CFCF_3$, 1-propene, 2,3,3,3-tetrafluoro, *	754-12-1	[7, 11, 20, 21]
R-1234ze(E), E-CHF=$CHCF_3$, E-1-propene, 1,3,3,3-tetrafluoro	29118-24-9, 1645-83-6	[20, 21]
R-1243zf, CH_2=$CHCF_3$, propene, 3,3,3-trifluoro, *	677-21-4	[11]
R-1243yf, CH_2=$CFCHF_2$, 1-propene, 2,3,3-trifluoro, *	158664-13-2	[11]
HFCs mixtures		
R-32/R-1234yf, *		[7, 22]
R-152a/R-134a, *		[16, 19]

R-152a/R-125, *		[19]
R-152a/R-116, *		[19]
R-152a/R-1234yf, *		[16]
R-32/R-134a		[8, 9]
R-32/R-1234ze(E)		[23]
R-1234yf/C_3H_8, *		[7]
R-134a/CH_4, *		[24]

3. Thermodynamic data

Table 2 lists the fluorine-containing hydrocarbon and oxidized-hydrocarbon species considered in the kinetic model with their standard enthalpies of formation $\Delta_f H^o$, standard entropies S_o, and heat capacities at constant pressure $C_{p,}^o$ (all at 298.15 K). Thermochemical data for the species CF_3CCF, $CF{=}CHCF_3$, $CHF{=}CCF_3$ and $CH{=}CFCF_3$ were estimated using group additivity approaches, using several sources [7, 25-31]. Data for the other species were taken from the literature [27-29, 32]. Note that the thermodynamic data for fluorine-containing species were updated from a previous set of data [33] using two main sources [32, 34]. Thermodynamic polynomials in Chemkin format are presented in Appendix A.

Table 2. Thermodynamic properties of fluorine-containing species considered in the kinetic model.

Species	**$\Delta_f H^0$(298 K) kJ/mol**	***U*** **kJ/mol**	***S*^{o}(298 K) J/mol/K**	**C_p^o (298 K) J/mol/K**	**Reference**
Fluoromethanes					
CH_3F	−235.55	0.70	259.375	37.505	[34]*
CH_2F_2	−451.66	0.68	246.347	42.869	[34]*
CHF_3	−697.45	0.65	222.826	51.139	[34]*
CF4	-933.4 -933.47	 0.25	261.459	61.052	[32]* [35]
Fluoromethyls					
CH_2F	−30.39	0.50	229.665	42.869	[34]*
CHF_2	−243.45	0.51	258.000	43.062	[34]*
CF_3	−469.06	0.52	264.521	49.642	[34]*
Fluoromethylenes					
CHF	148.614 148.66	0.45 0.43	223.342	34.588	[32]* [35]
CF_2	−194.06	0.41	240.831	38.915	[34]*
CF	246.932 246.74	0.7 0.13	213.034	30.056	[32]* [35]
Oxidized C1 Fluorocarbons					
CHFO	-382.529	0.47	246.727	40.019	[32]*

	382.23	0.31			[35]
CF_2O	-606.65	0.50	258.971	47.365	[32]*
CFO	-176.305 176.04	0.50 0.37	248.992	38.880	[32]* [35]
CF_3O	-630.696	n/a	283.750	64.550	[32]*
Fluoroethanes					
CH_3-CH_2F	-272.54 -272.07	0.94 0.36	270.630	59.575	[32]* [35]
CH_2F-CH_2F	−447.97	0.98	286.321	66.868	[34]*
CH_3-CHF_2	−503.00 -502.72	 0.56	282.502	67.266	[34]* [35]
CH_2F-CHF_2	−668.37	0.97	72.609	17.996	[34]*
CH_3-CF_3	−753.94	0.89	287.652	78.074	[34]*
CHF_2-CHF_2	−880.86	1.05	313.143	84.129	[34]*
CH_2F-CF_3	−909.70	0.95	315.752	86.273	[34]*
CHF_2-CF_3	−1114.81	1.04	334.635	95.808	[34]*
CF_3-CF_3	−1345.51	1.00	341.033	106.294	[34]*
Fluoroethyls					
CH_2F-CH_2	−59.77	0.85	278.832	60.737	[34]*
CH_3-CHF	−74.06	0.84	273.994	58.671	[34]*
CH_2F-CHF	−247.94	0.85	293.335	69.307	[34]*
CHF_2-CH_2	−282.72	0.80	297.938	66.752	[34]*
CH_3-CF_2	−298.20	0.79	290.406	67.075	[34]*
CH_2F-CF_2	-446.0	10	311.329	73.757	[33]*
CHF_2-CHF	-451.9	10	310.91	75.822	[33]*
CF_3-CH_2	−527.95	0.91	302.541	77.046	[34]*
CHF_2-CF_2	-664.921	10	328.485	84.011	[33]*
CF_3-CHF	−699.45	1.07	326.393	85.544	[34]*
CF_3-CF_2	−898.77	0.97	340.995	94.231	[34]*
Fluoroethylenes					
CH_2CHF	−142.93	0.84	252.674	50.407	[34]*
CHFCHF[Z]	-306.5 -309.66	 0.9	268.723	58.349	[32]* [35]
CH_2CF_2	−351.07	0.84	266.054	60.237	[34]*
$CHFCF_2$	-487.84 -495.98	8.21 0.41	292.665	69.191	[32]* [35]
CF_2CF_2	−674.30	0.78	300.128	80.459	[34]*
Fluoroethenyls					
CHFCH[Z]	123.025	10	256.93	50.531	[33]*
CH_2CF	109.216	10	256.9	50.031	[33]*
CHFCF[Z]	-41.008	10	279.526	57.3	[33]*

CF_2CH	-67.8	10	277.016	58.984	[33]*
CF_2CF	-228.175	10	297.643	66.178	[32]*
Fluoroethynes					
C_2HF	104.419 105.66	0.93 0.41	231.573	52.268	[32]* [35]
C_2F_2	5.59 5.69	0.66 0.65	256.504	61.987	[36]* [35]
C_2F	353.847 453.9 460.2 449.8 455.8	 10 10 1.6 8.0	231.036	42.6	[32]* [33] [33] [35] [37]
Fluoroketenes					
CHFCO	-147.2	10	270.739	56.538	[33]*
CF_2CO	-290.4	10	288.732	67.692	[33]*
CFCO	69.0	10	276.179	56.702	[33]*
C3-fluorinated, etc					
C_3F_7H	-1564.816		399.058	136.690	[32]*
C_3F_7	-1347.122 -1346.9 -1349.0	 n/a 8.0	416.386	135.964	[32]* [37]
C_3F_6	-1157.253 -1157.05 -1154.95	 n/a	373.675	121.759	[32]* [37]
CF_3COF	-1028.43	5.9	340.28	88.79	[38]*
CF_3CHO	-775.71	2.1	318.28	80.42	[38]*
CF_3CO	-602.08	3.8	264.35	72.59	[38]*
$C_2F_5COC_3F_7$	-2723.	n/a	676.0	588.69	[39]
CF_3COCH_3	-837.3 -831.1	 4.4	357	108.5	[40]* [41]
CH_2CFO	-250.6 -251.46	 2.9	274.5	62.9	[29]* [35]
Fluoropropenes					
CF_3CHCH_2 (R-1243zf)	-631.131	6.0	319.468	90.704	[32]*
CH_2CFCF_3 (R-1234yf)	-813.261	8.4	327.768	101.255	[32]*
$CHFCHCF_3$ (R-1234ze(E))	-830.0		342.7	98.4	[27, 42]*

Fluoropropenyls					
CF_3CCH_2	-374.941	7.9	325.439	91.100	[32]*
CF_3CHCH	-376.895	n/a	323.105	90.727	[32]*
$CFCHCF_3$	-564.4		346.885	96.439	[42, 43]*
$CHCFCF_3$	-567.6	n/a	332.1	99.9	[44]*
$CHFCCF_3$	-548.2		347.7	96.0	[42, 43]*
Fluoropropynes					
CF_3CCH	-428.5 -419.0	5.7	314	88.3	[41]* [35]
$CFCCF_3$	-531.2	n/a	333.4	96.6	[44]*

* Data used in the current work.
U – expanded uncertainty (2σ), kJ/mol

4. Kinetic model

Four sub-mechanisms form the framework for the kinetic model: 1) GRI-Mech 3.0 [45], which includes reactions important for high-temperature oxidation of hydrocarbons up to C_3 species; 2) the NIST C_1-C_2 hydrofluorocarbon model [46] with modifications [47, 48], developed to describe hydrocarbon flames with added HFC fire suppressants; 3) the C_3-hydrofluorocarbon reactions developed for flame inhibition by heptafluoropropane (R-227ea, FM-200) [49] and 2-bromo-3,3,3-trifluoropropene (2-BTP) [40, 41], which is a bromo-substituted fluoropropene; and 4) the model for the decomposition of 2,3,3,3-tetrafluoropropene, 1,3,3,3-tetrafluoropropene, 3,3,3-trifluoropropene [43,44]. Several rate constants of the model were adjusted, based on reaction pathway and sensitivity analyses, to obtain agreement with experimental data for the burning velocities for the set of HFC refrigerants.

Note that in this version of the kinetic model we used GRI-Mech 3.0 model as the hydrocarbon part of the model. Since it was found that there are shifts in the predicted burning velocity with changes in the hydrocarbon oxidation model (particularly for the mono-fluorinated HFCs (R-41 and R-161), the hydrocarbon part of the model will eventually be modified. In the interim, we have modified several termolecular reactions of GRI-Mech 3.0 including third body efficiencies for some HFC compounds, and we changed the reaction channel for reaction $HCCO+O_2$ (below). Due to the relatively large sensitivity of the results to the rate constants of hydrocarbon/hydrogen reaction system, like $H+O_2=OH+O$, $CO+O+M=CO_2+M$, $HCO+M=CO+H+M$, $CO+O+M=CO_2+M$ etc., some shift in the results was observed. The experiments with the replacement of the hydrocarbon part of the model (propane model [50], C_1-C_3 block of reactions from JetSurF-2.0 [51]) demonstrated the difference in the results from 1 cm/s to 4 cm/s depending on the HFC refrigerant and on the equivalence ratio (R-134a, R-152a, R-1234yf and R-1243zf).

Appendix B provides a table of the Arrhenius rate parameters for the kinetic model (Chemkin format). The main assumption during construction of the fluoropropene part of the model was that intermediate species formed by the addition of radicals to the double bond decompose very quickly to the presumed set of products. Rate constants were estimated by analogy with similar reactions and using empirical structure-reactivity relationships. For consumption of

CF_3CHCH_2 (R-1243zf) by radicals it was assumed that the major pathway is the radical addition with further elimination of the CF_3 radical ($CF_3CHCH_2+H=CF_3+C_2H_4$, $CF_3CHCH_2+OH=CF_3+CH_3CHO$). It is of interest that the reaction proceeding in the flame zone of R-1234yf, R-1243zf and R-1234ze(E) is sensitive to the channel for the reaction of the HCCO radical with oxygen molecule. It was necessary to change the channel in the GRI-Mech model (OH+CO+CO) to the channel with the products $H+CO+CO_2$ with the same rate constant. The mechanism of this reaction was discussed in [52, 53]. Appendix C provides the transport parameters (in CHEMKIN format) for all of the species in the model.

Flame equilibrium calculations and preliminary burning velocity simulations provided rough estimates of the intermediate species concentrations, which were used to evaluate the possible reactions. The complete model contains 1064 reactions with 113 species. Numerous changes to both the rates and the reactions may be made once a variety of experimental data and theoretical results are available for testing the mechanism.

5. Modeling procedure

The Chemkin set of programs [54-56] and the open-source software package Cantera [57] were used for combustion equilibrium calculations and for laminar flame calculations. For burning velocity calculations, the equations of mass, species, and energy conservation are solved numerically for the initial gas compositions, temperature, and pressure corresponding to those in the experiments. The solution assumes isobaric, adiabatic, steady, planar, one-dimensional, laminar flow and neglects radiation and the Dufour effect, but includes thermal diffusion. Molecular diffusion is modeled using the Hirschfelder approximation and the multi-component transport. The boundary conditions, corresponding to a freely propagating flame, are inlet mass fractions, velocity and temperature, and vanishing gradients downstream from the flame.

6. Comparison of simulation results with experimental data

The results of model validation are presented for HFC refrigerants and their mixtures in the figures below. Experimental results are presented as symbols, modeling data as a line. The burning velocity data in the original publications were typically manually extracted from plots using a digitizer program, and the determined numerical values are provided in tables in Appendix E. All experiments were performed at standard initial conditions: 1 bar and 298 K. Mixture compositions are provided as molar fractions.

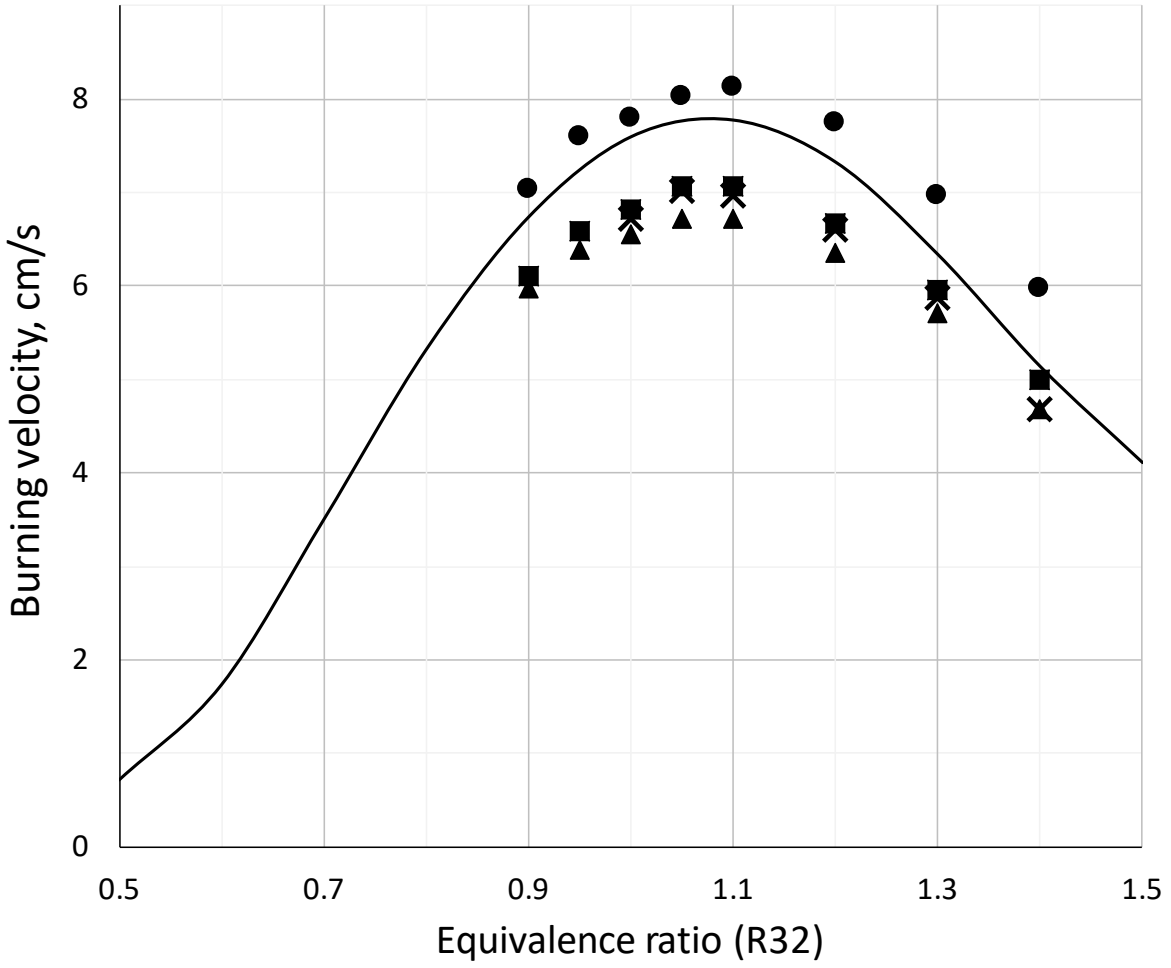

Figure 1. Burning velocity dependence on the equivalence ratio (R-32/air, ■ – OTL,[5]; ● – ADI, [5]; x –[16]; ▲ - [10])

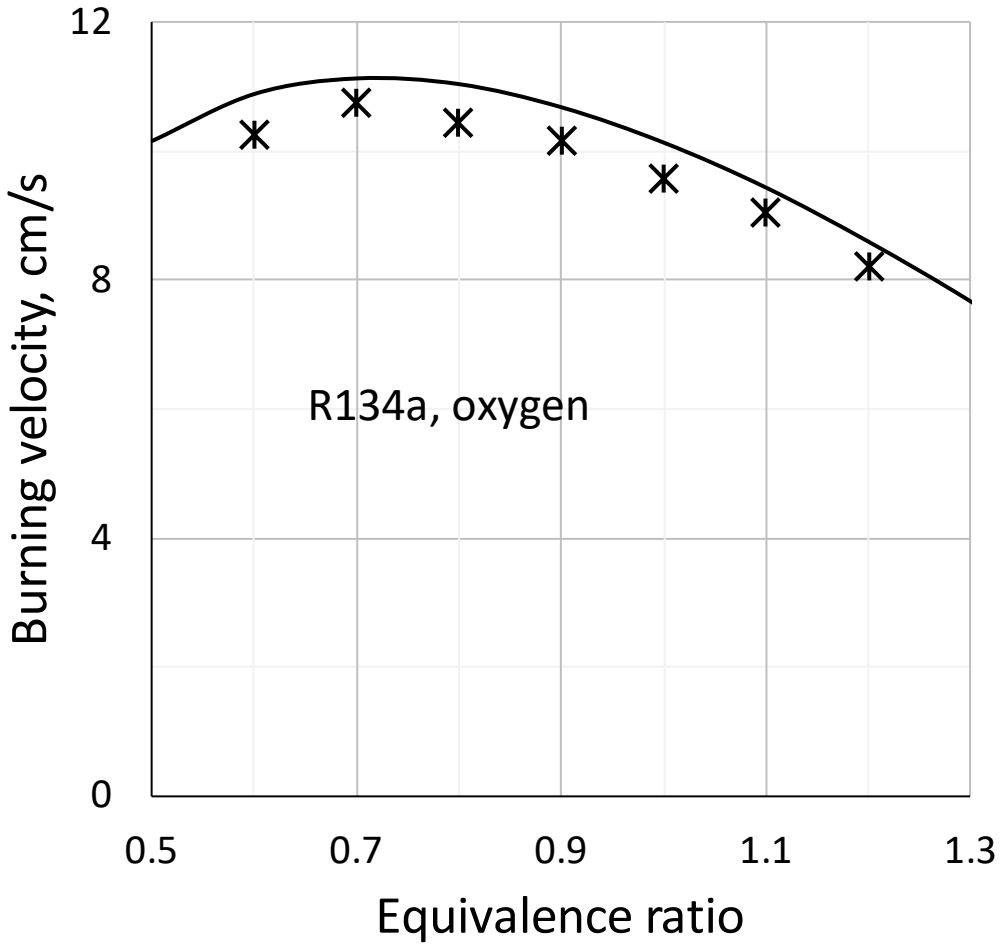

Figure 2. Burning velocity dependence on the equivalence ratio for R-134a/Oxygen mixture (experimental data of Burrell et al. [18]).

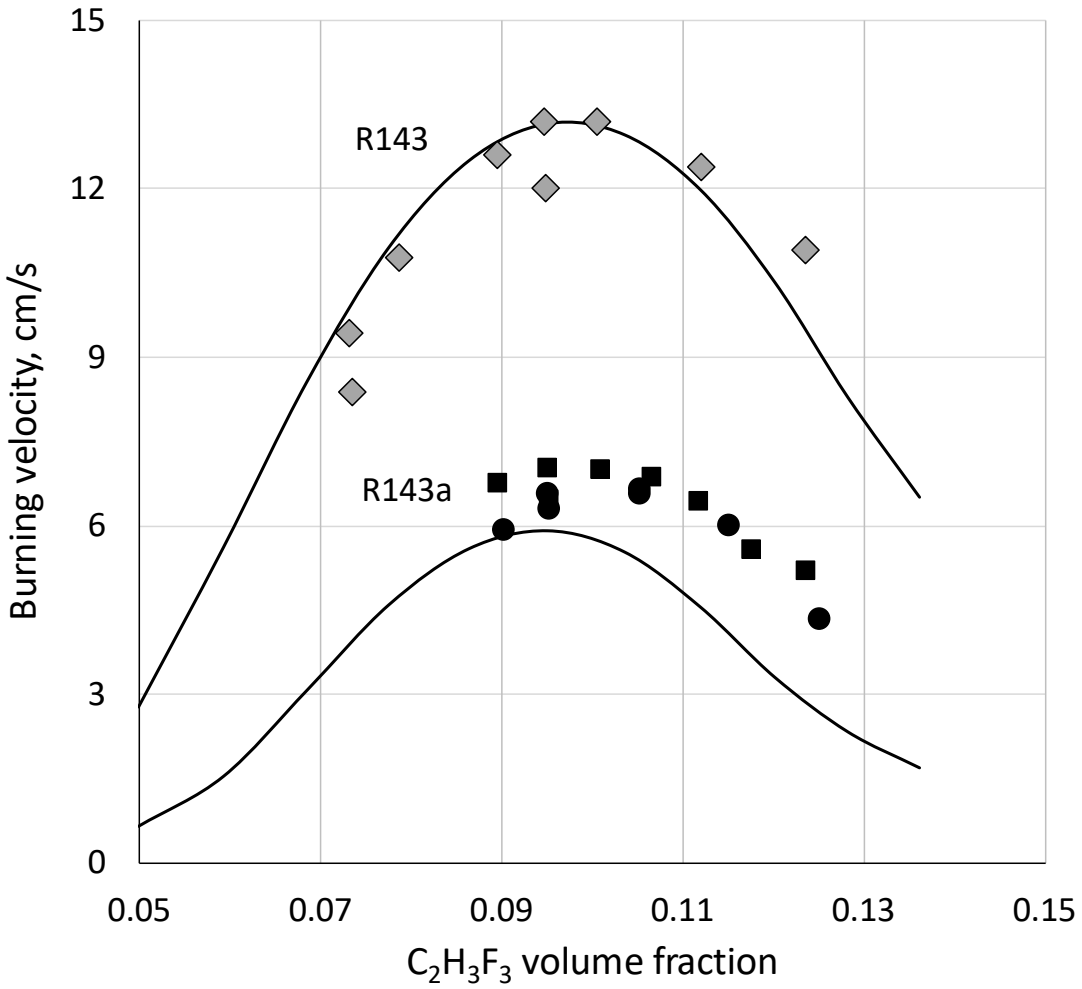

Figure 3. Dependence of burning velocity on the volume fraction of R-143 and of R-143a (298 K, 1 bar, ♦ - [10], ■ - [10], ● - [6])

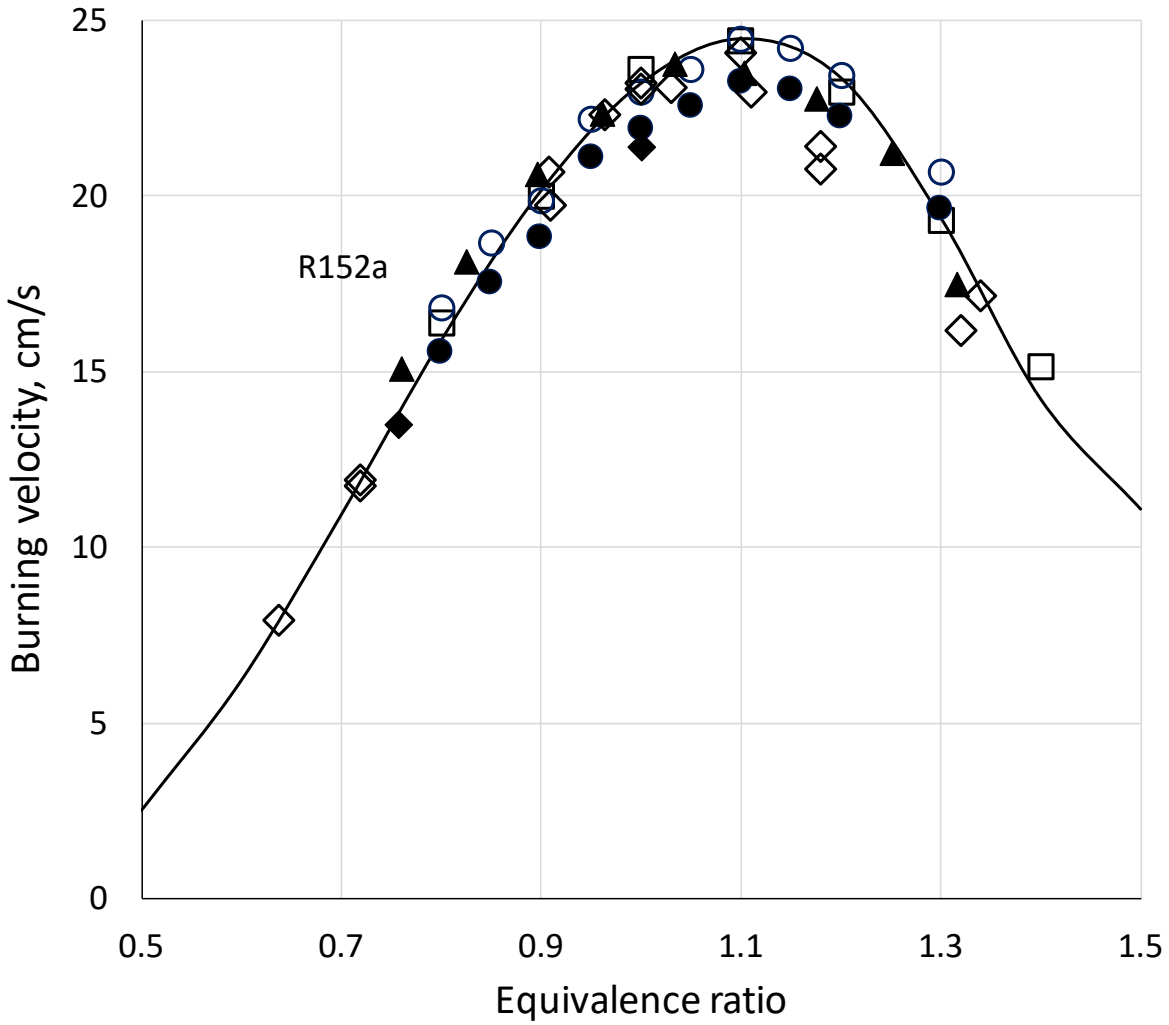

Figure 4. Dependence of burning velocity on the equivalence ratio for R-152a (◊ - tube method [10], ♦ - Schlieren method [10], ▲ – SV method [10], ● - [18], □ – [16], ○ - [18]).

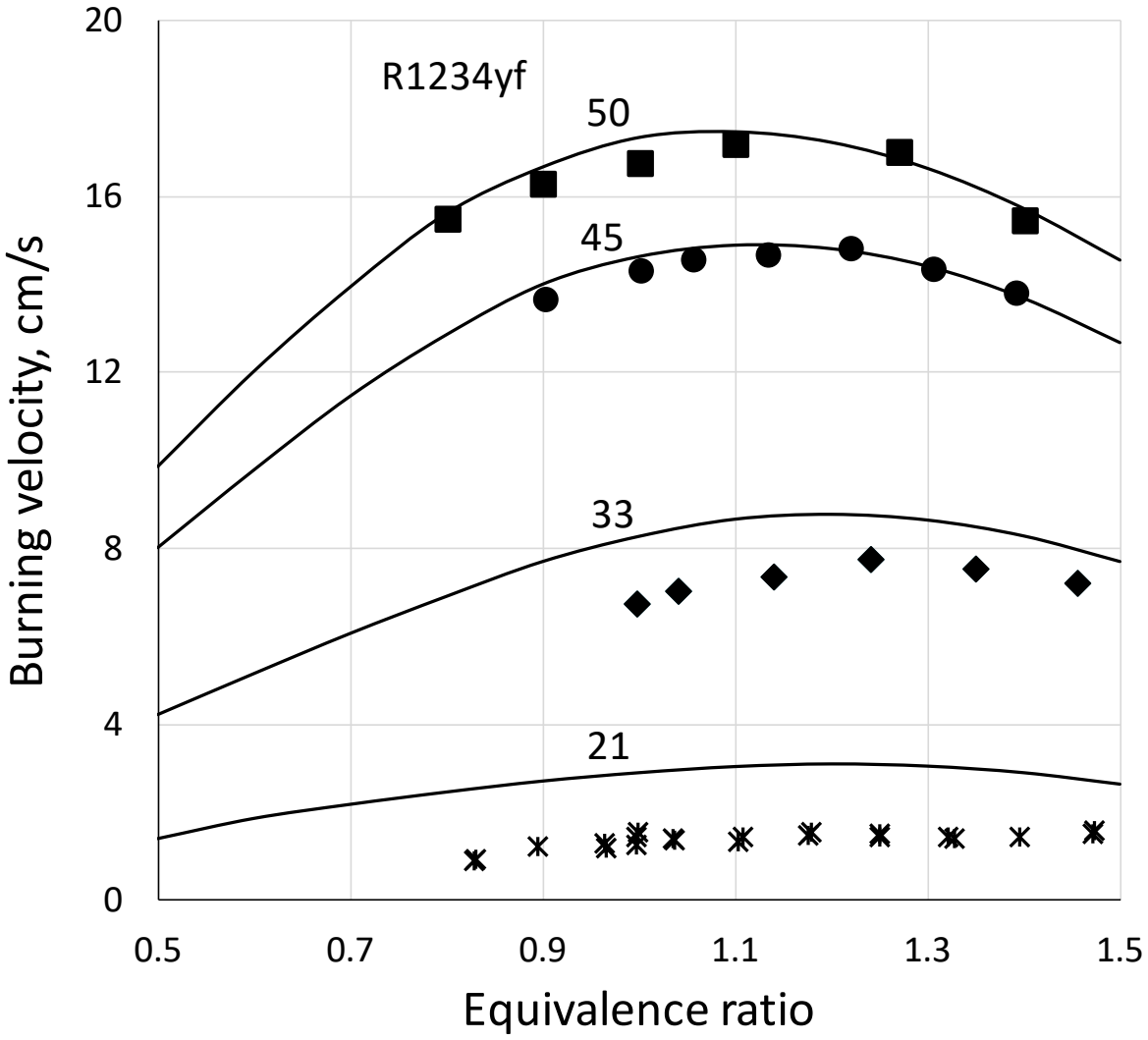

Figure 5. Burning velocity dependence on the equivalence ratio for R-1234yf at different volume fractions of oxygen in air ($X_{O_2,ox}$ = 21, 33, 45 and 50 % of O_2 in air, experimental data of Takizawa et al. [11]).

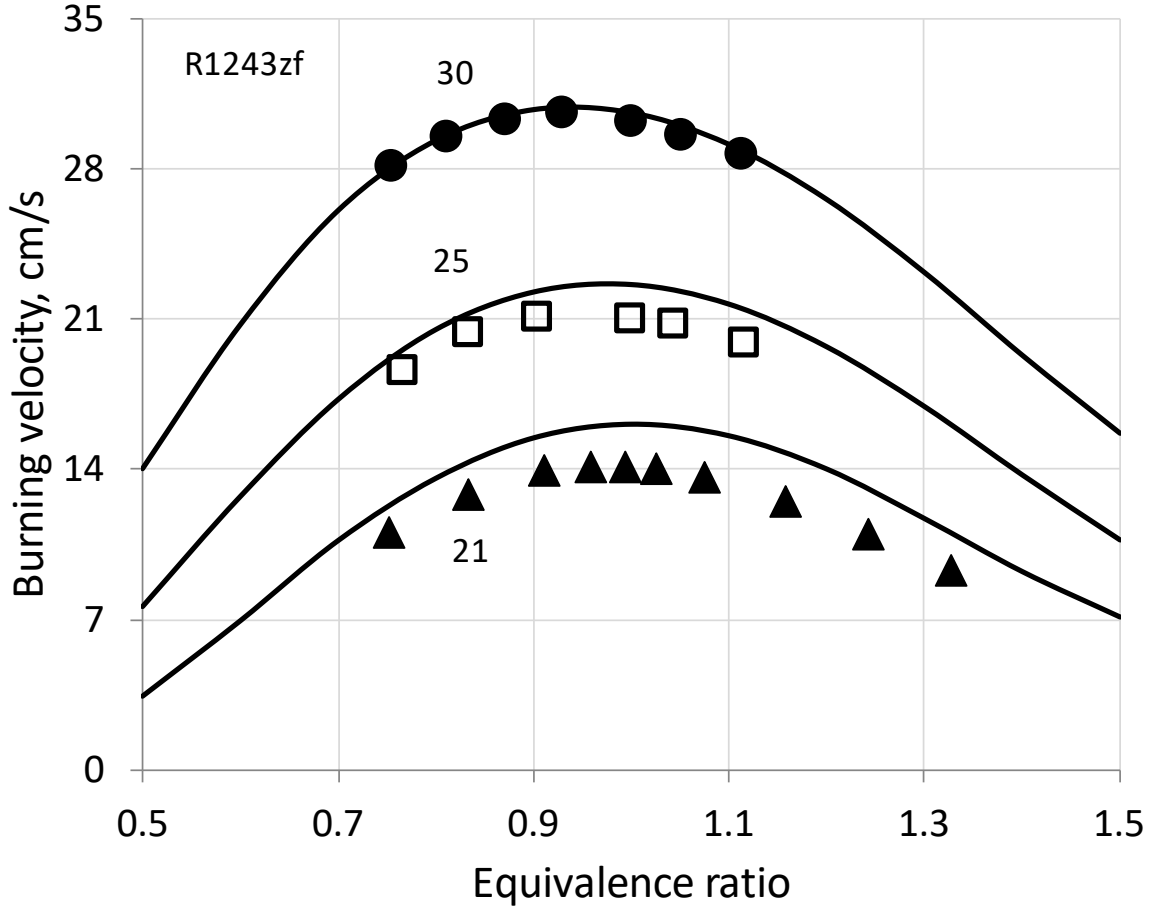

Figure 6. Burning velocity dependence for R-1243zf at different volume fractions of oxygen in air ($X_{O_2,ox}$ = 21, 25, and 30 % of O_2 in air). All points are measurements of Takizawa et al. [11].

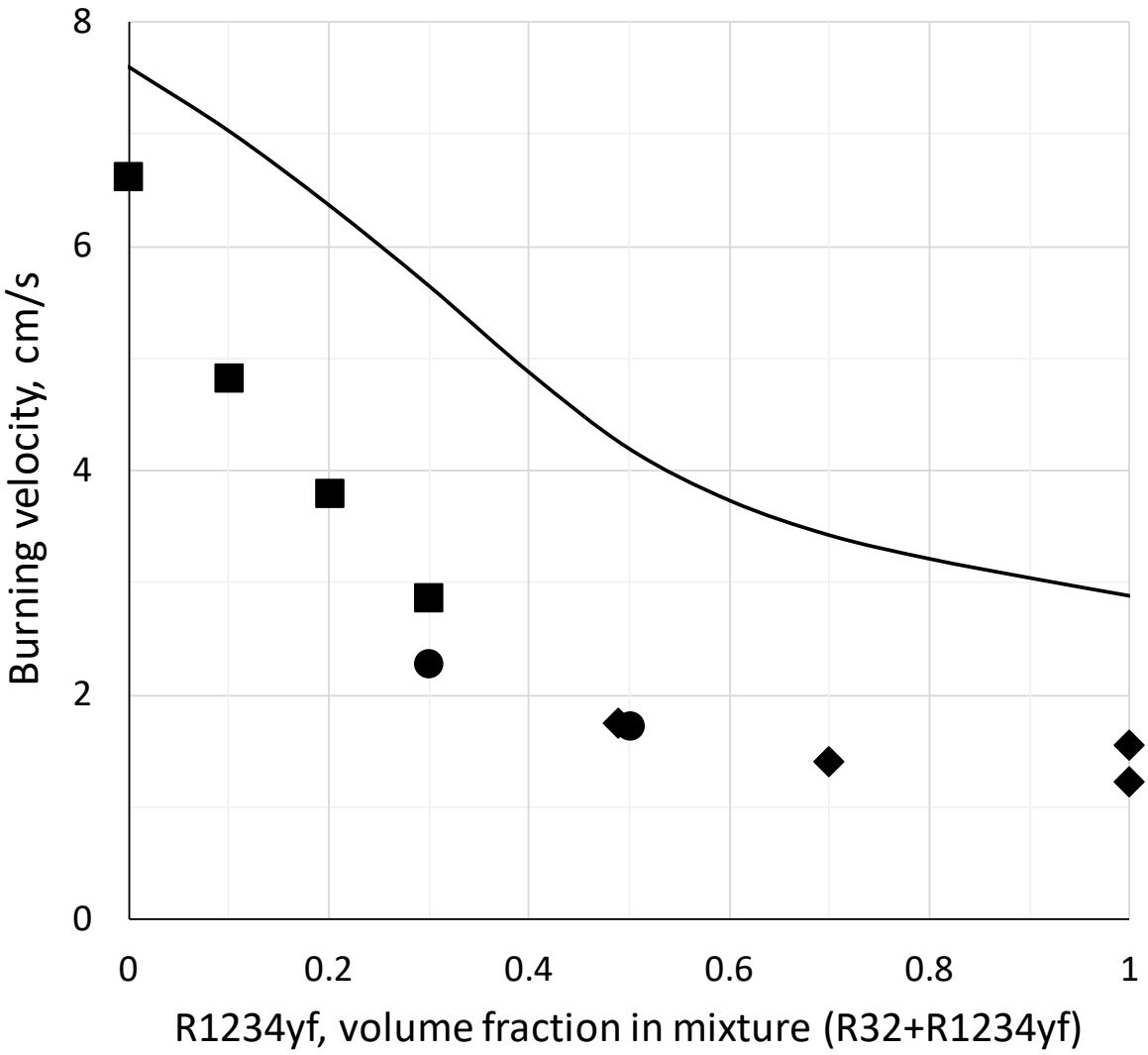

Figure 7. Dependence of burning velocity on volume fraction of R-1234yf in mixture of R-1234yf/R-32 (♦ - [22], ● - [22], ■ - [7]). Experimental data of [7,22] were taken from Fig.4 of [7].

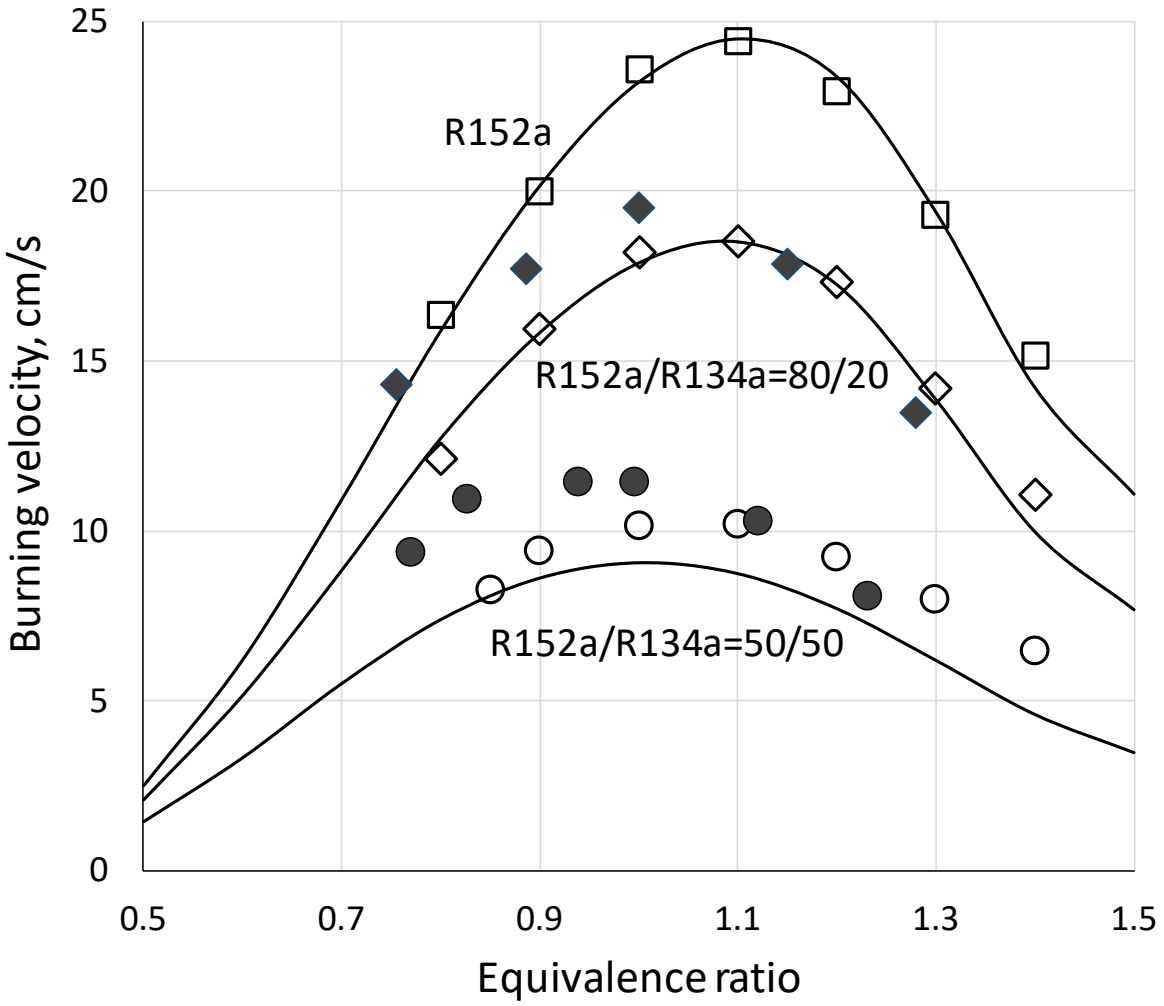

Figure 8. Burning velocity dependence of R-152a and of mixtures of R-152a/R-134a on the equivalence ratio (□ – NIST[16], ♦,● -[19], ◊,○ – NIST [16]).

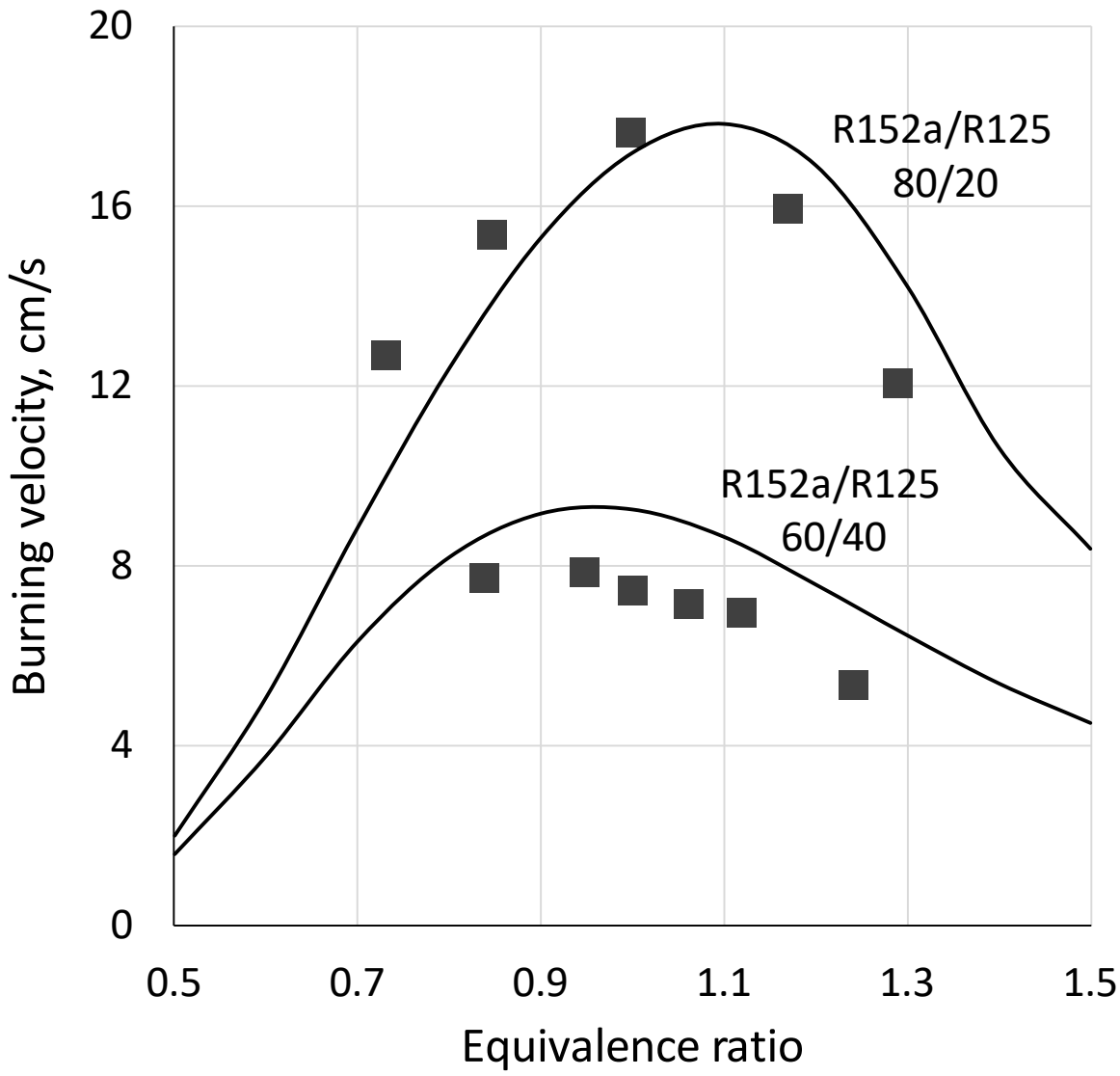

Figure 9. Burning velocity dependence on the equivalence ratio for mixtures R-152a/R-125 (experimental data of Takizawa et al. [19]).

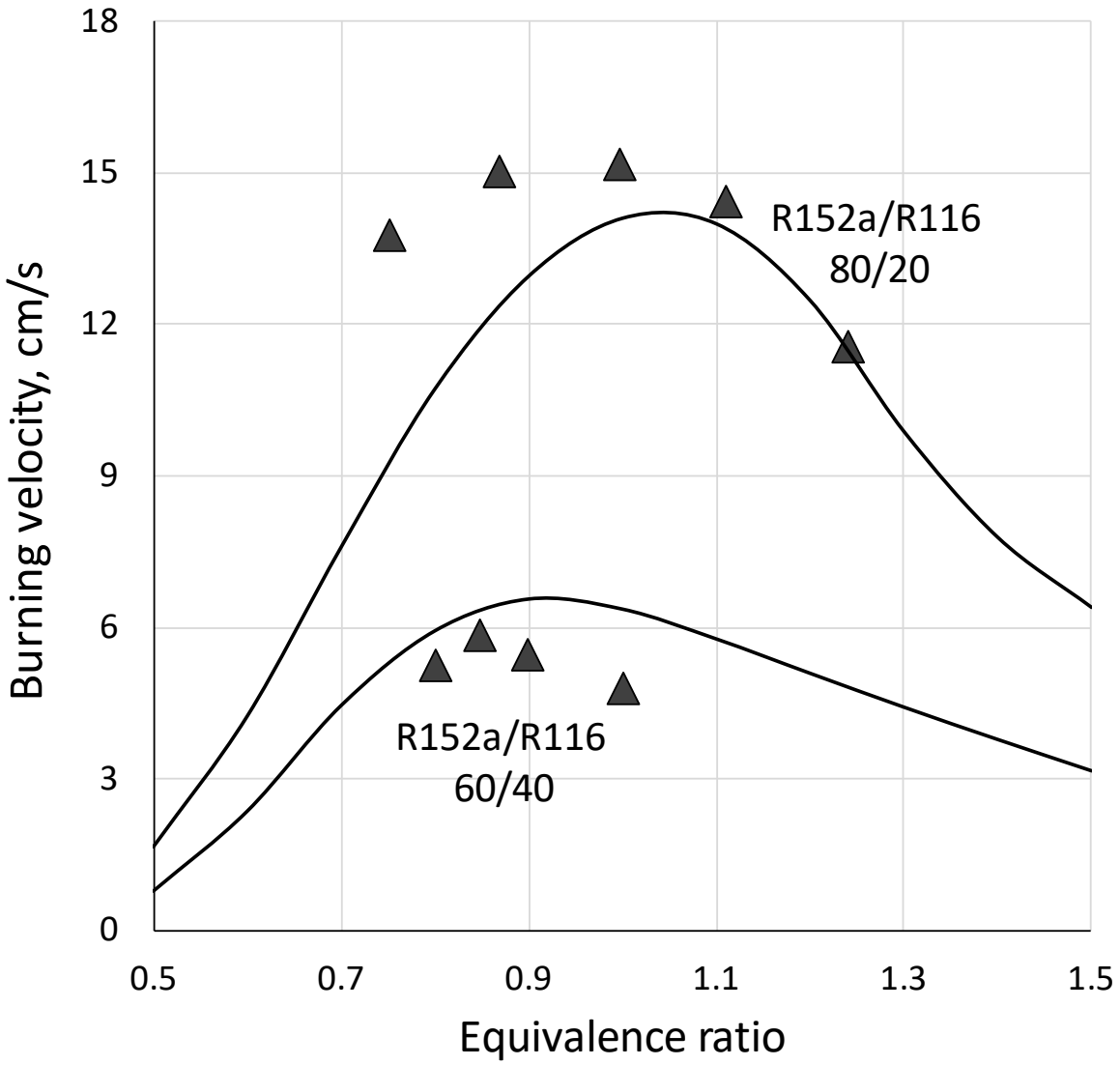

Figure 10. Burning velocity dependence on the equivalence ratio for mixtures R-152a/R-116 (experimental data of Takizawa et al. [19]).

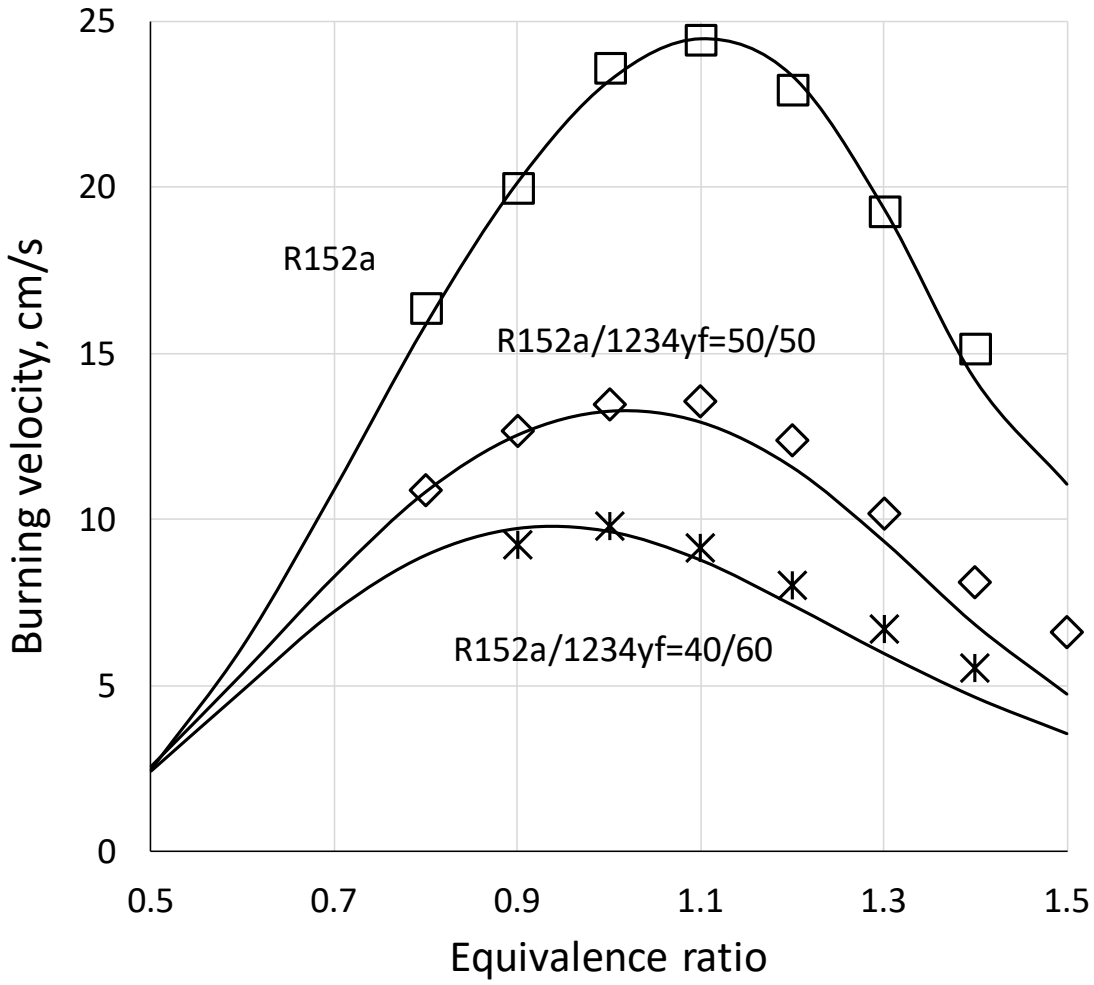

Figure 11. Burning velocity dependence on the equivalence ratio for R-152a and mixtures R-152a/R-1234yf (experimental data of Kim et al. [16]).

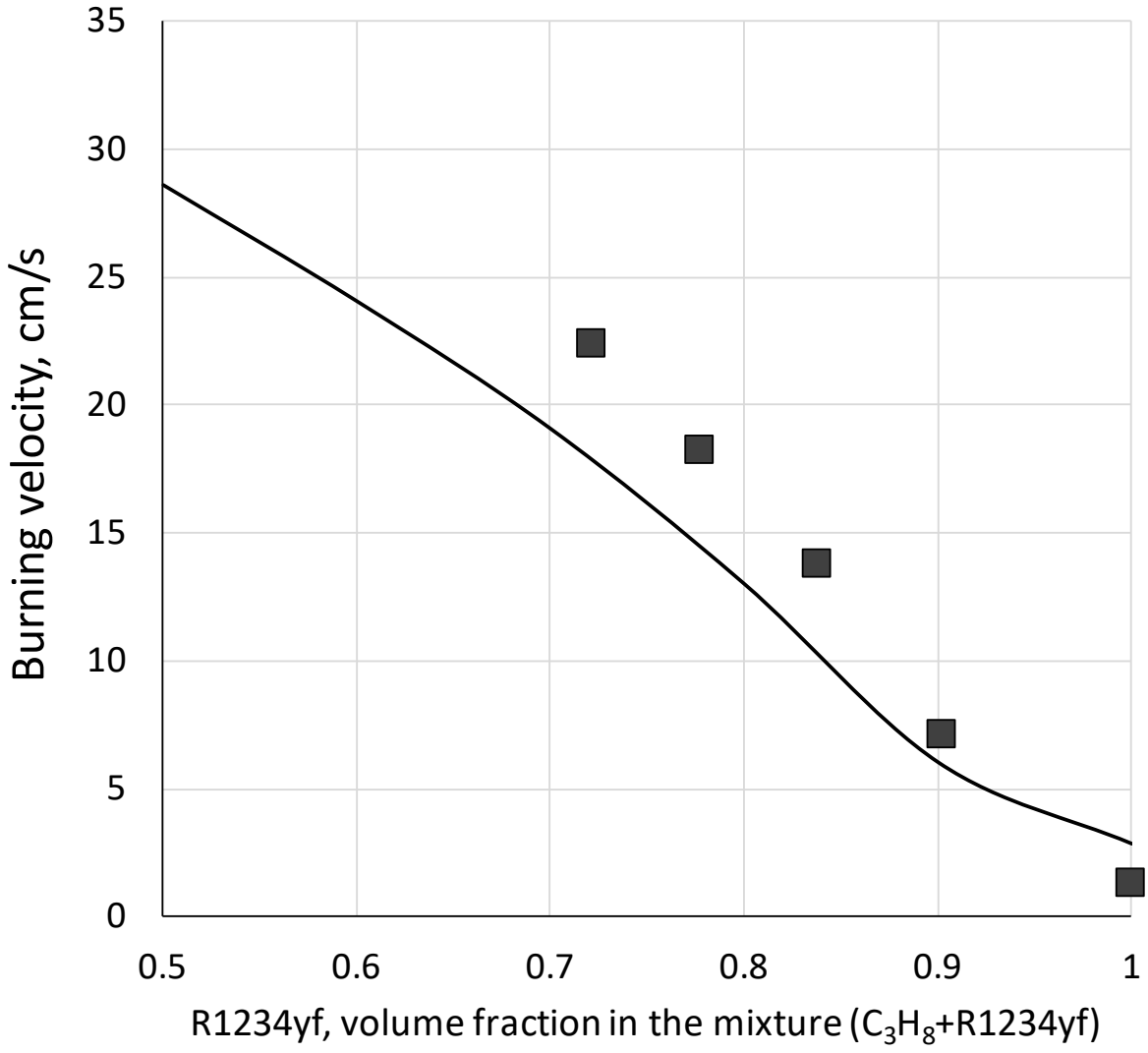

Figure 12. Burning velocity dependence on the R-1234yf volume fraction in the mixture C_3H_8/R-1234yf (experimental data of Papas et al. [7]).

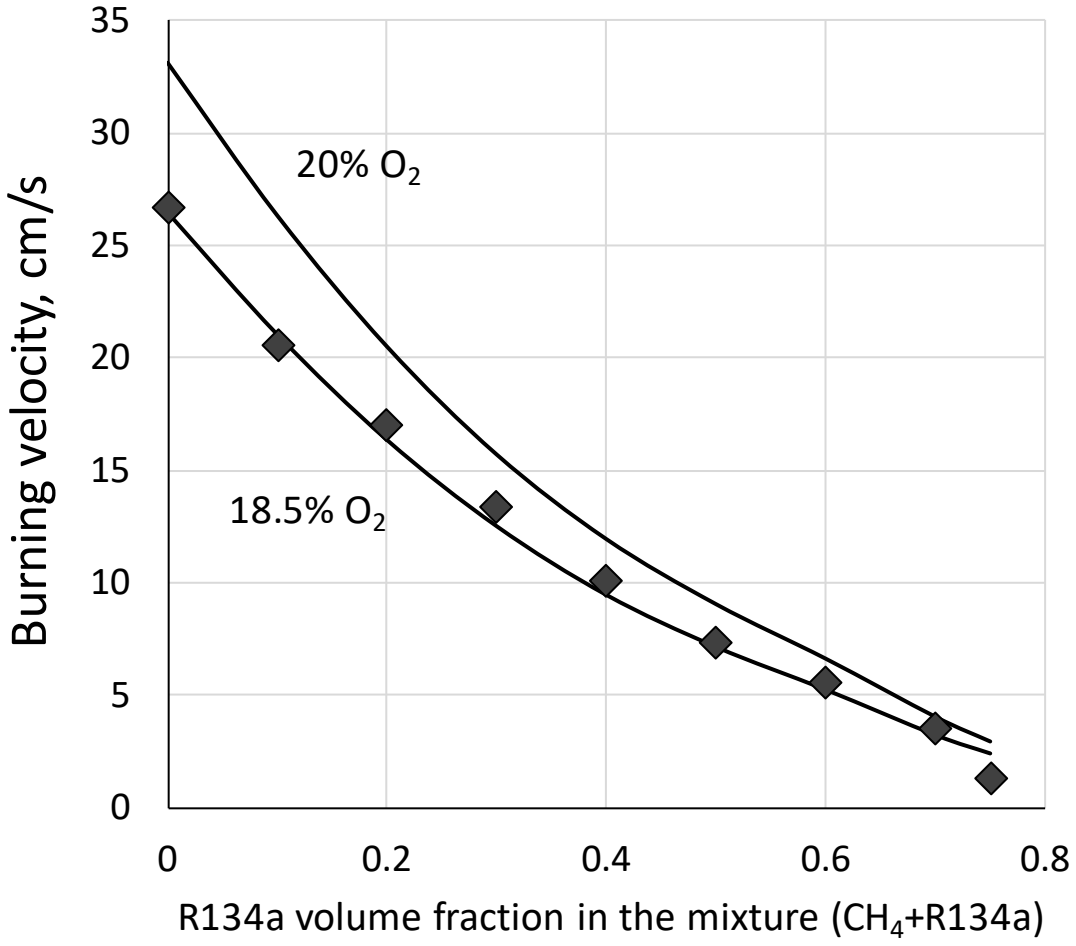

Figure 13. Burning velocity dependence on the volume fraction of R-134a in the mixture R-134a/CH_4 for 18.5 % of oxygen in air (experimental measurements if Choi et al. [24])*.

*Note: Ref. [24] also includes data for $X_{O_2,ox}$=0.20; however, it was found that these experimental data do not agree with either data for pure methane/air flames at $X_{O_2,ox}$=0.20 in the literature [45,58,59] or the present modeling results. Since the results for $CH_4/O_2/N_2$ flames at $X_{O_2,ox}$=0.185 from these authors do agree with literature values, we use that data with added R134a for our comparisons.

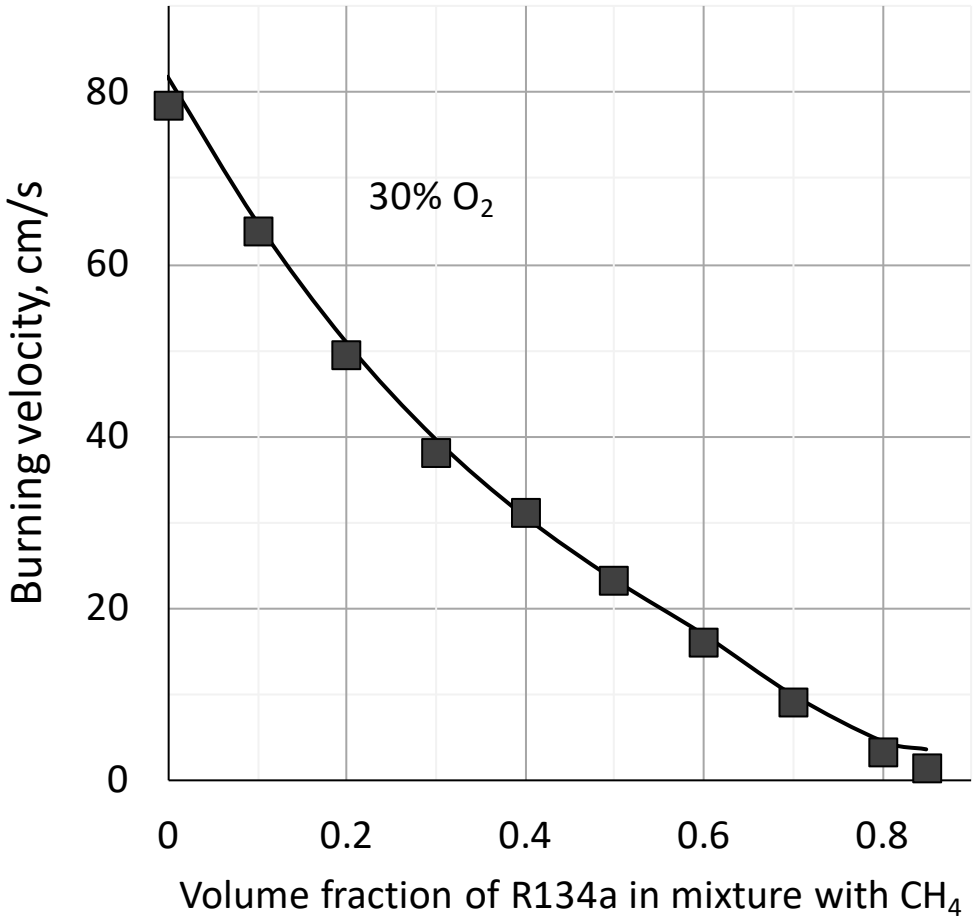

Figure 14. Burning velocity dependence on the volume fraction of R-134a in the mixture R-134a/CH_4 for 30 % of oxygen in air (experimental measurements if Choi et al. [24]).

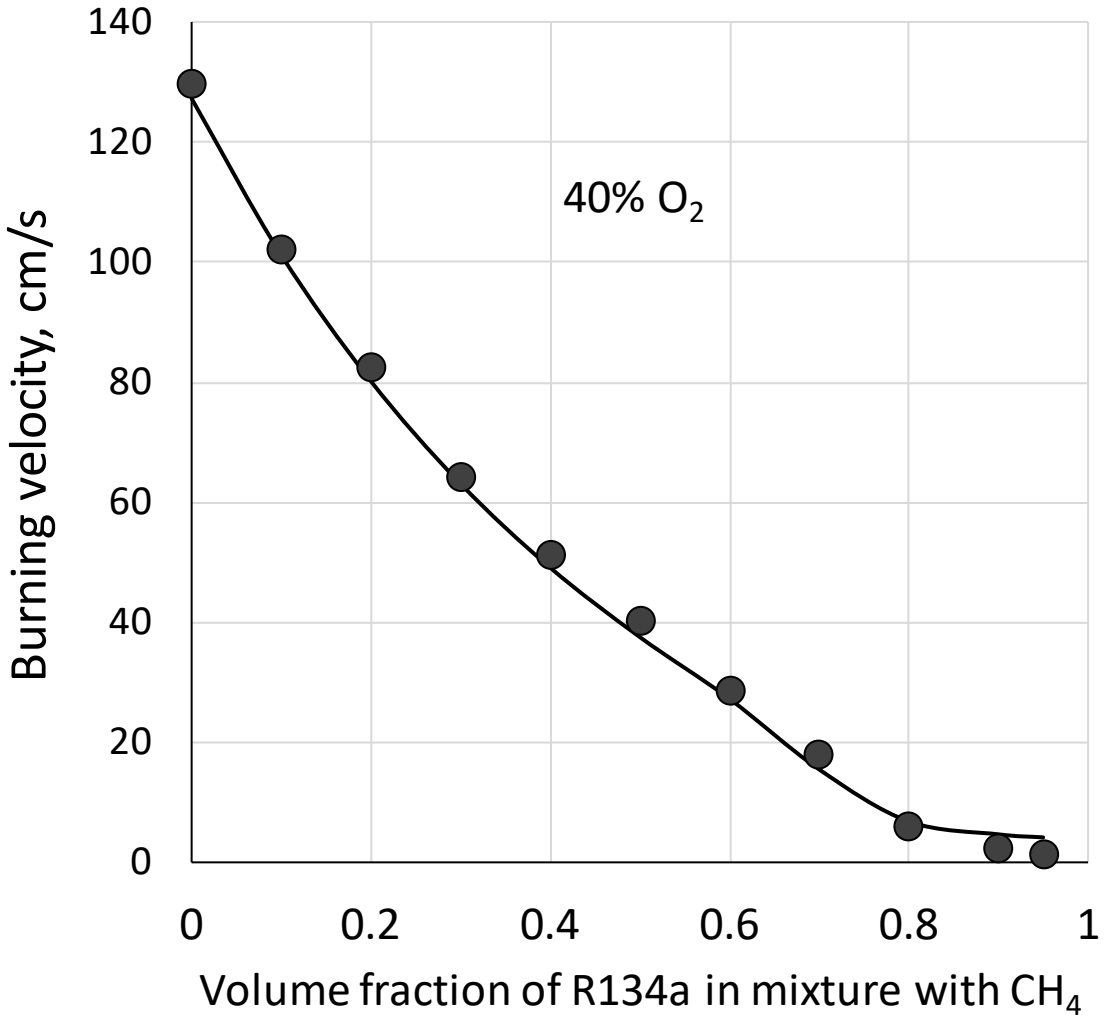

Figure 15. Burning velocity dependence on the volume fraction of R-134a in the mixture R-134a/CH_4 for 40 % of oxygen (experimental measurements if Choi et al. [24]).

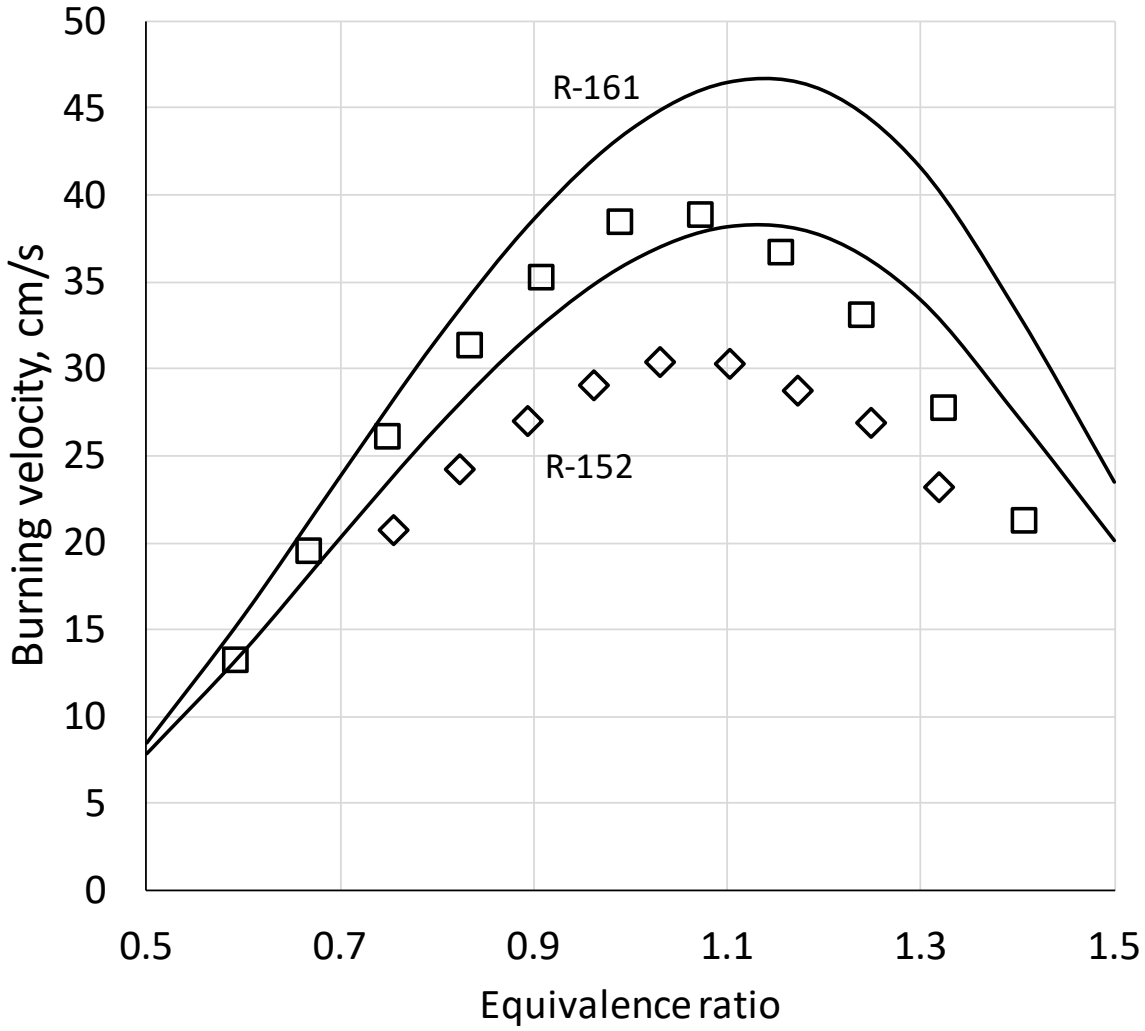

Figure 16. Burning velocity dependence on the equivalence ratio for R-161 and R-152 (experimental data of Takizawa et al. [17]).

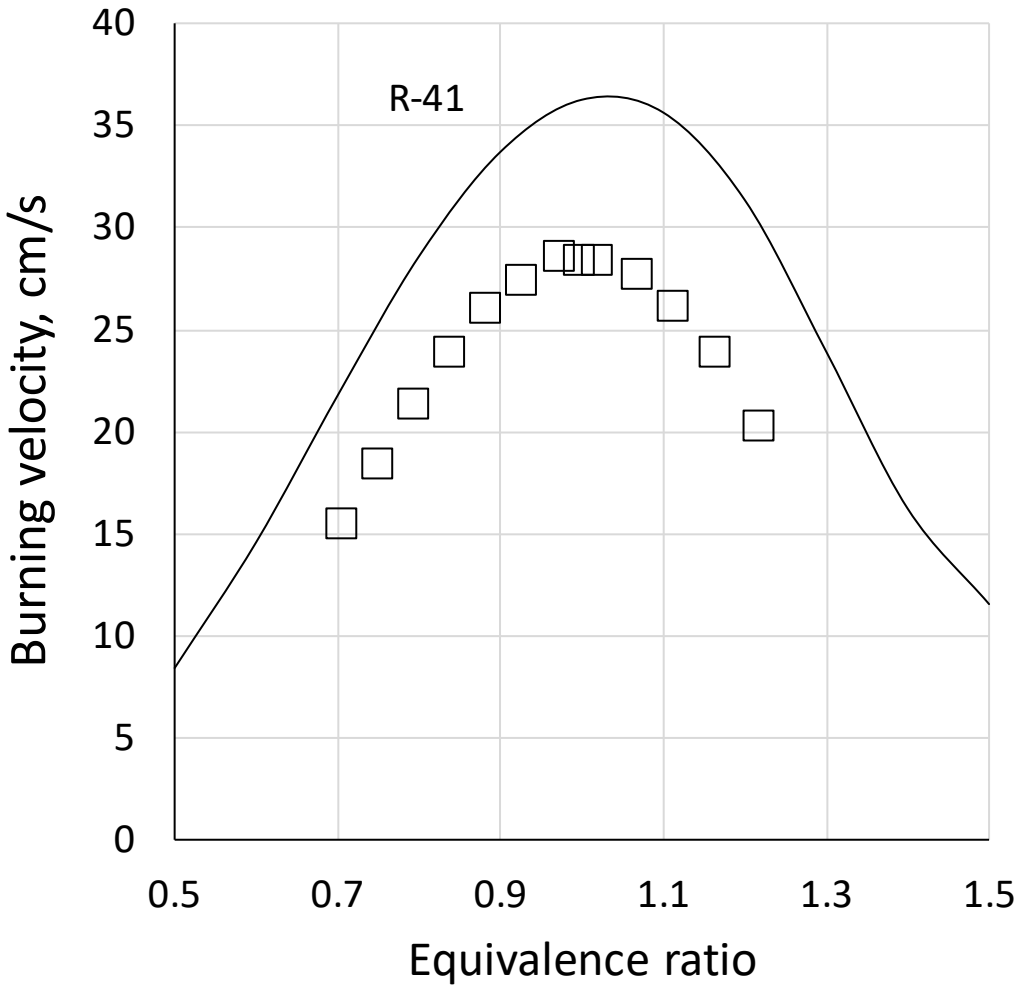

Figure 17. Burning velocity dependence on the equivalence ratio for R-41 (experimental data of Takizawa et al. [17]).

Table 3 describes the accuracy of the predicted burning velocity data as compared to the experimental results.

Table 3. Summary of differences between modeled and experimental burning velocities

R-32/air		Model 3 % lower than AD, 10 % higher than OTL
R-134a/O_2	100 % O_2	Model agrees with data to within (3 to 5) %
R-143/air		Model agrees with data to within (3 to 5) %
R-152a/air		Model agrees with data to within (3 to 5) %
R-134a/CH_4/air	18.5, 30, 40% O_2	Model agrees with data to within about 5%
R-152a/R-134a/air	80/20 ratio	Model agrees with data to within 5%
	50/50 ratio	Model is low by about 20 %
R-1234yf/air	45 %, 50 % O_2	Model agrees to within about 3 %
R-1234yf/air	33 % O_2	Model is high by about 15%
R-1234yf/air	21 % O_2	Model is high by a factor of two. 3 cm/s versus 1.5 cm/s
R-1243zf/air	18 %, 21 % O_2	Model agrees to within about 5 %
R-1243zf/air	25 % O_2	Model is low by about 10 %
R-152a/R-1234yf/air	100/0 ratio	Model agrees to within about 5 %
	50/50 ratio	Model is low by about 10 %
	40/60 ratio	Model is low by about 10 %
R-152a/R-116/air	80/20 ratio	Model is low by about 7 %
	60/40 ratio	Model is low by about 15 %
R-161/air		Model is high by about (10 to 15) %
R-142a/air		Model is high by about 15 %
R-152a/R-125/air	80/20 ratio	Model is high by about 10 %
	60/40 ratio	Model is high by about 20 %
R-41		Model is high by about (20 to 25) %

Comparison of modeling results obtained with the developed model with the experimental data of different authors demonstrate good agreement except the monofluorinated compounds: R-41 and R-161, for which differences up to 25% can be observed depending on the equivalence ratio. The comparisons demonstrate a tendency of the model to overpredict burning velocities below (7 to 10) cm/s, which is the result of radiation heat losses, and which were not considered in the present simulations. For some refrigerants, the equivalence ratio of peak burning velocity is shifted slightly as compared to the experimental results; however, even in those cases the model predicts the maximum values of burning velocity reasonably well.

7. Summary

A kinetic mechanism is proposed for the combustion of the C_1-C_3 hydrofluorocarbon refrigerants: difluoromethane (R-32), fluoroethanes (R-125, R134a, R-143, R-143a, and R-

152a,), and fluoropropenes (R-1234yf, R-1234ze(E), R-1243zf) and their mixtures/blends (R-152a/R-134a, R-152a/R-116, R-152a/R-125, R-152a/R-1234yf, R-134a/CH_4, R-32/R-1234yf, R-1234yf/C_3H_8). The thermodynamic and transport data for fluorine-containing species considered in the model, are provided in Chemkin format. The overall kinetic model includes 1064 reactions with 113 species. The kinetic model was validated against experimental burning velocities as a function of the equivalence ratios of the blend in air. Additionally, for some cases, the experimental data and modeling were performed for different oxygen loadings in the oxidizer. Comparison of modeling results with available experimental measurements demonstrates reasonably good agreement. The largest disagreement occurs for burning velocities below about 5 cm/s (e.g., R1234yf with air) for which the prediction is about factor of two higher than the experiment, likely due to radiation heat losses not accounted for in the experiments.

Acknowledgements

This work was supported by the Buildings Technologies Office of the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy under contract no. DE-EE0007615 with Antonio Bouza serving as Project Manager. This work was also supported by the U.S. Department of Defense, Strategic Environmental Research and Development Program (SERDP), project WP19-1385.

References

[1] Velders GJ, Ravishankara AR, Miller MK, Molina MJ, Alcamo J, Daniel JS, Fahey DW, Montzka SA, Reimann S (2012) Preserving Montreal Protocol climate benefits by limiting HFCs. *Science* 335(6071):922-923.

[2] United Nations Environment Programme (2016) *Further Amendment of the Montreal Protocol*, United Nations Environment Programme, Kigali, Rwanda, UNEP/OzLPro28/CRP/10.

[3] ASHRAE (2010) *Designation and Safety Classification of Refrigerants*, ANSI/ASHRAE Addendum to ANSI/ASHRAE Standard 34-2016, ASHRAE, Atlanta, GA, USA.

[4] ISO (2017) International Organization for Standarization (ISO-817): Refrigerants—Designation and safety classification. Geneva, Switzerland.

[5] Burrell RR, Pagliaro JL, Linteris GT (2019) Effects of stretch and thermal radiation on difluoromethane/air burning velocity measurements in constant volume spherically expanding flames. *Proceedings of Combustion Institute* 37:4231-4238.

[6] Clodic D , Jabbour T (2011) Method of test for burning velocity measurement of flammable gases and results. *HVAC&R Research* 17(1):51-75. https://doi.org/10.1080/10789669.2011.543252

[7] Papas P, Zhang S, Kim W, Zeppieri SP, Colket MB, Verma P (2017) Laminar flame speed of 2,3,3,3-tetrafluoropropene mixtures. *Proceedings of Combustion Institute* 36(1):1145-1154.

[8] Takizawa K, Igarashi N, Tokuhashi K, Kondo S, Mamiya M, Nagai H (2013) Assessment of Burning Velocity Test Methods for Mildly Flammable Refrigerants,

Part 2: Vertical-Tube Method. *ASHRAE Transactions 2013, Vol 119, Pt 2* 119:255-264.

[9] Takizawa K, Takagi S, Tokuhashi K, Kondo S, Mamiya M, Nagai H (2013) Assessment of Burning Velocity Test Methods for Mildly Flammable Refrigerants, Part 1: Closed-Vessel Method. *ASHRAE Transactions 2013, Vol 119, Pt 2,* 119:243-254.

[10] Takizawa K, Takahashi A, Tokuhashi K, Kondo S, Sekiya A (2005) Burning velocity measurement of fluorinated compounds by the spherical-vessel method. *Combust Flame* 141(3):298-307. https://doi.org/DOI 10.1016/j.combustflame.2005.01.009

[11] Takizawa K, Tokuhashi K, Kondo S (2009) Flammability assessment of CH2=CFCF3: Comparison with fluoroalkenes and fluoroalkanes. *Journal of Hazardous Materials* 172(2-3):1329-1338. https://doi.org/10.1016/j.jhazmat.2009.08.001

[12] Davis SG, Pagliaro JL, Debold TF, van Wingerden M, van Wingerden K (2017) Flammability and explosion characteristics of mildly flammable refrigerants. *Journal of Loss Prevention in the Process Industries* 49:662-674. https://doi.org/10.1016/j.jlp.2017.05.019

[13] Jabbour T (2004) *Flammable Refrigerant Classification Based on the Burning Velocity*, Ph.D. Thesis, L'Ecole des Mines de Paris, Paris, France.

[14] Moghaddas A, Bennett C, Rokni E, Metghalchi H (2014) Laminar burning speeds and flame structures of mixtures of difluoromethane (HFC-32) and 1,1-difluoroethane (HFC-152a) with air at elevated temperatures and pressures. *HVAC&R Research* 20(1):42-50. https://doi.org/10.1080/10789669.2013.822252

[15] Burgess Jr DR, Burrell RR, Babushok VI, Manion JA, Hegetschweiler MJ, Linteris GT (2020) Burning Velocities of R-32/O2/N2 Mixtures: Experimental Measurements and Development of a Validated Detailed Chemical Kinetic Model. Submitted. *Combustion and Flame*.

[16] Kim DK , Linteris GT (2021) Study of Flame Propagation in R-152a/air Mixtures and in the Blends of R-152a with R-134a and R-1234yf, to be submitted. *Combustion Science and Technology*.

[17] Takizawa K, Takahashi A, Tokuhashi K, Kondo S, Sekiya A (2006) Burning velocity measurement of HFC-41, HFC-152, and HFC-161 by the spherical-vessel method. *Journal of Fluorine Chemistry* 127(12):1547-1553. https://doi.org/10.1016/j.jfluchem.2006.07.013

[18] Burrell RR, Hegetschwiler MJ, Burgess Jr DR, Manion JA, Babushok VI, Linteris GT (2019) R-152a/air and R-134a/oxygen constant volume spherical flame burning velocity measurements. *11th US National Combustion Meeting*, Pasadena, CA.

[19] Takizawa K, Takahashi A, Tokuhashi K, Kondo S, Sekiya A (2006) Reaction stoichiometry for combustion of fluoroethane blends. *ASHRAE Transactions* 112(2):459-468.

[20] Takizawa K (2015) Fundamental Flammability (Section 2). *Risk Assesssment of Mildly Flammable Refrigerants. Technical report,* JSRAE, Tokyo, Japan.

[21] Takizawa K, Hihara E, Dang C, Ito M (2017) 2. Fundamental flammibility. 2.3.1. Effect of humidity on burning velocity. *Risk Assessment of Mildly Flammable Refrigerants Final Report 2016*, The Japan Society of Refrigerating and Air Conditioning Engineers, Tokyo, Japan, pp 22-67.

[22] Takizawa K, Tokuhashi K, Kondo S, Mamiya M, Nagai H (2010) Flammability assesment of CH2=CFCF3 (R-1234yf) and its mixtures with CH2F2 (R-32). 2010 International Symposium on Next-generation Air Conditioning and Refrigeration Technology Tokyo, Japan 2010.

[23] Liu Q, Li Y, Gao W, Zhang K, Huang L, Bi M (2020) Hazard evaluation of R32/R1234ze(E) cloud explosion. *International Journal of Refrigeration-Revue Internationale Du Froid* 111:159-167. https://doi.org/10.1016/j.ijrefrig.2019.11.025

[24] Choi BC, Park JS, Ghoniem AF (2016) Characteristics of outwardly propagating spherical flames of R134a(C2H2F4)/CH4/O-2/N-2 mixtures in a constant volume combustion chamber. *Energy* 95:517-527. https://doi.org/10.1016/j.energy.2015.11.043

[25] Holmes JL , Aubry C (2012) Group Additivity Values for Estimating the Enthalpy of Formation of Organic Compounds: An Update and Reappraisal. 2. C, H, N, O, S, and Halogens. *Journal of Physical Chemistry A* 116(26):7196-7209. https://doi.org/10.1021/jp303780m

[26] Luo Y-R (2003) *Handbook of Dissociation Energies in Organic Compounds,* CRC Press, Boca Raton, FL.

[27] Matsugi A , Shiina H (2014) Kinetics of Hydrogen Abstraction Reactions from Fluoromethanes and Fluoroethanes. *Bulletin of the Chemical Society of Japan* 87(8):890-901. https://doi.org/10.1246/bcsj.20140101

[28] Matsugi A , Takahashi K (2017) Thermal Decomposition of 2,3,3,3-and trans-1,33,3-Tetrafluoropropenes. *Journal of Physical Chemistry A* 121(26):4881-4890. https://doi.org/10.1021/acs.jpca.7b04086

[29] Needham CD , Westmoreland PR (2017) Combustion and flammability chemistry for the refrigerant HFO-1234yf (2,3,3,3-tetrafluroropropene). *Combustion and Flame* 184:176-185. https://doi.org/10.1016/j.combustflame.2017.06.004

[30] Orlov YD, Zaripov RK, Lebedev YA (1998) Determination of enthalpies of formation of organic free radicals from bond dissociation energies - 2. Halosubstituted radicals. *Russian Chemical Bulletin* 47(4):621-624. https://doi.org/10.1007/bf02495965

[31] Stein SE , Brown RL (2019) Structures and Properties Group Additivity Model. in *NIST Chemistry WebBook,* National Institute of Standards and Technology, Gaithersburg, MD, retrieved 2019 .

[32] Goos E, Burcat A, Ruscic B (2012) *Extended Third Millennium Thermodynamic Database for Combustion and Air-Pollution Use with updates from Active Thermochemical Tables,* Technion-IIT, Haifa, Israel. Available at: ftp://ftp.technion.ac.il/pub/supported/aetdd/thermodynamics/BURCAT.THR.

[33] Burgess DR, Zachariah MR, Tsang W, Westmoreland PR (1995) Thermochemical and chemical kinetic data for fluorinated hydrocarbons. *Progress in Energy and Combustion Science* 21(6):453-529. https://doi.org/10.1016/0360-1285(95)00009-7

[34] Ganyecz A, Kallay M, Csontos J (2018) High Accuracy Quantum Chemical and Thermochemical Network Data for the Heats of Formation of Fluorinated and Chlorinated Methanes and Ethanes. *Journal of Physical Chemistry A* 122(28):5993-6006. https://doi.org/10.1021/acs.jpca.8b00614

[35] Ruscic B , Bross DH (2020) *Active thermochemical tables (ATcT), version 1.122p* (Argonne National Laboratory). Available at: https://atct.anl.gov/Thermochemical%20Data/version%201.122p/.

[36] Ruscic B , Bross DH (2019) *Active thermochemical tables (ATcT), version 1.122d* (Argonne National Laboratory). Available at: https://atct.anl.gov/Thermochemical%20Data/version%201.122d/index.php.
[37] Bauschlicher CW , Ricca A (2000) Heats of formation for CnFm, CnFm+, CHFm, and CHFm+. *Journal of Physical Chemistry A* 104(19):4581-4585. https://doi.org/10.1021/jp9942771
[38] Purnell DL, Jr. , Bozzelli JW (2019) Thermochemical Properties: Enthalpy, Entropy, and Heat Capacity of C2-C3 Fluorinated Aldehydes. Radicals and Fluorocarbon Group Additivity. *Journal of Physical Chemistry A* 123(3):650-665. https://doi.org/10.1021/acs.jpca.8b09065
[39] Linteris GT, Babushok VI, Sunderland PB, Takahashi F, Katta VR, Meier O (2013) Unwanted combustion enhancement by C6F12O fire suppressant. *Proceedings of the Combustion Institute* 34:2683-2690. https://doi.org/10.1016/j.proci.2012.06.050
[40] Babushok VI, Linteris GT, Burgess DR, Baker PT (2015) Hydrocarbon flame inhibition by C3H2F3Br (2-BTP). *Combustion and Flame* 162(4):1104-1112. https://doi.org/10.1016/j.combustflame.2014.10.002
[41] Burgess DR, Babushok VI, Linteris GT, Manion JA (2015) A Chemical Kinetic Mechanism for 2-Bromo-3,3,3-trifluoropropene (2-BTP) Flame Inhibition. *International Journal of Chemical Kinetics* 47(9):533-563. https://doi.org/10.1002/kin.20923
[42] Balaganesh M , Rajakumar B (2012) Rate Coefficients and Reaction Mechanism for the Reaction of OH Radicals with (E)-CF3CH═CHF, (Z)-CF3CH═CHF, (E)-CF3CF═CHF, and (Z)-CF3CF═CHF between 200 and 400 K: Hybrid Density Functional Theory and Canonical Variational Transition State Theory Calculations. *The Journal of Physical Chemistry A* 116(40):9832-9842. https://doi.org/10.1021/jp3077276
[43] Babushok VI, Burgess DR, Jr., Hegetschweiler MJ, Linteris GT (2020) Flame propagation in the mixtures of O-2/N-2 oxidizer with fluorinated propene refrigerants (CH2CFCF3, CHFCHCF3, CH2CHCF3). *Combustion Science and Technology*. https://doi.org/10.1080/00102202.2020.1720663
[44] Babushok VI , Linteris GT (2017) Kinetic mechanism of 2,3,3,3-tetrafluoropropene (HFO-1234yf) combustion. *Journal of Fluorine Chemistry* 201:15-18. https://doi.org/10.1016/j.jfluchem.2017.07.005
[45] Smith GP, Golden DM, Frenklach M, Moriarty NW, Eiteneer B, Goldenberg M, Bowman CT, Hanson RK, Song S, Gardiner JWC, Lissianski VV, Qin Z (2000) *GRI Mech 3.0,* University of California, Berkeley, Berkeley, CA). Available at: http://www.me.berkeley.edu/gri_mech.
[46] Burgess Jr DR, Zachariah MR, Tsang W, Westmoreland PR (1995) Thermochemical and chemical kinetic data for fluorinated hydrocarbons. *Prog Energy Combust Sci* 21(6):453-529. https://doi.org/10.1016/0360-1285(95)00009-7
[47] Babushok VI, Linteris GT, Meier O (2012) Combustion properties of halogenated fire suppressants. *Combust Flame* 159:3569-3575.
[48] Linteris GT, Burgess DR, Takahashi F, Katta VR, Chelliah HK, Meier O (2012) Stirred reactor calculations to understand unwanted combustion enhancement by potential halon replacements. *Combustion and Flame* 159(3):1016-1025. https://doi.org/10.1016/j.combustflame.2011.09.011

[49] Williams BA, L'Esperance DM, Fleming JW (2000) Intermediate species profiles in low-pressure methane/oxygen flames inhibited by 2-H heptafluoropropane: Comparison of experimental data with kinetic modeling. *Combust Flame* 120(1-2):160-172.

[50] Qin ZW, Lissianski VV, Yang HX, Gardiner WC, Davis SG, Wang H (2000) Combustion chemistry of propane: A case study of detailed reaction mechanism optimization. *Proceedings of the Combustion Institute* 28:1663-1669. https://doi.org/10.1016/s0082-0784(00)80565-2

[51] Wang H, Dames E, Sirjean B, Sheen DA, Tango R, Violi A, Lai JYW, Egolfopoulos FN, Davidson DF, Hanson RK, Bowman CT, Law CK, Tsang W, Cernansky NP, Miller DL, Lindsted RP (2010) *A high-temperature chemical kinetic model of n-alkane (up to n-dodecane), cyclohexane, and methyl-, ethyl-, n-propyl and n-butyl-cyclohexane oxidation at high temperatures, JetSurF version 2.0*. Available at: http://melchior.usc.edu/JetSurF/JetSurF2.0.

[52] Klippenstein SJ, Miller JA, Harding LB (2003) Resolving the mystery of prompt CO2: The HCCO+O-2 reaction. *Proceedings of the Combustion Institute* 29:1209-1217. https://doi.org/10.1016/s1540-7489(02)80150-x

[53] Zou P , Osborn DL (2004) On the mechanism of the HCCO+O-2 reaction: Probing multiple pathways to a single product channel. *Physical Chemistry Chemical Physics* 6(8):1697-1705. https://doi.org/10.1039/b400183d

[54] Kee RJ, Rupley FM, Miller JA (1989) CHEMKIN-II: A fortran chemical kinetics package for the analysis of gas phase chemical kinetics. Report SAND89-8009B, Sandia National Laboratories, Livermore, CA, USA.

[55] Kee RJ, Rupley FM, Miller JA (1990) The Chemkin Thermodynamic Data Base. Report SAND87-8215B, Sandia National Laboratories, Livermore, CA, USA.

[56] Kee RJ, Grcar JF, Smooke MD, Miller JA (1991) A fortran computer program for modeling steady laminar one-dimensional premixed flames. Report SAND85-8240, Sandia National Laboratories, Livermore, CA, USA.

[57] Goodwin DG, Moffat HK, Speth RL (2016) Cantera: An object-oriented software toolkit for chemical kinetics, thermodynamics, and transport processes. http:/www.cantera.org, Version 2.1.1. (California Institute of Technology, Pasedena, CA).

[58] Dyakov IV, Konnov AA, De Ruyck J, Bosschaart KJ, Brock ECM, De Goey LPH (2001) Measurement of adiabatic burning velocity in methane-oxygen-nitrogen mixtures. *Combustion Science and Technology* 172:81-96. https://doi.org/10.1080/00102200108935839

[59] Stone R, Clarke A, Beckwith P (1998) Correlations for the laminar-burning velocity of methane/diluent/air mixtures obtained in free-fall experiments. *Combustion and Flame* 114(3-4):546-555. https://doi.org/10.1016/s0010-2180(97)00329-5

[60] Kee RJ, Dixon-Lewis G, Warnatz J, Coltrin RE, Miller JA (1986) A Fortran Computer Code Package for the Evaluation of Gas-Phase, Multicomponent Transport Properties. Report SAND86-8246, Sandia National Laboratory, Livermore, CA.

[61] Reid RC, Prausnitz JM, Sherwood TK (1977) *The Properties of Gases and Liquids* (McGraw-Hill).

[62] Avendano C, Lafitte T, Adjiman CS, Galindo A, Mueller EA, Jackson G (2013) SAFT-gamma Force Field for the Simulation of Molecular Fluids: 2. Coarse-Grained Models

of Greenhouse Gases, Refrigerants, and Long Alkanes. *Journal of Physical Chemistry B* 117(9):2717-2733. https://doi.org/10.1021/jp306442b

[63] Teja AS, Smith RL, King RK, Sun TF (1999) Correlation and prediction of the transport properties of refrigerants using two modified rough hard-sphere models. *Int J Thermophys* 20(1):149-161. https://doi.org/10.1023/a:1021438516081

[64] Setokuchi O, Kutsuna S, Sato M (2006) A theoretical study of thermal decomposition of CF3CO, C2F5CO and C3F7CO. *Chemical Physics Letters* 429(4-6):360-364. https://doi.org/10.1016/j.cplett.2006.08.040

[65] Wang H , Frenklach M (1994) Transport-properties of polycyclic aromatic-hydrocarbons for flame modeling. *Combustion and Flame* 96(1-2):163-170. https://doi.org/10.1016/0010-2180(94)90167-8

Appendix A: Thermodynamic data for fluorine-containing species (Chemkin format).

```
F                 J 6/82F   1    0    0    0G   200.000  6000.000 1000.        1
burcat,2013
 0.26716339E+01-0.17461853E-03 0.69066504E-07-0.11953478E-10 0.75236739E-15    2
 0.87874123E+04 0.39842568E+01 0.24196743E+01 0.29392909E-02-0.89212228E-05    3
 0.99118537E-08-0.37947152E-11 0.87573220E+04 0.47468987E+01 0.95483679E+04    4
HF                T 2/11F  1.H  1.   0.   0.G   200.000  6000.000 1000.        1
burcat,2013
 2.92491143E+00 8.50523032E-04-1.58179777E-07 1.17507204E-11-1.43309132E-16    2
-3.36352481E+04 4.19018883E+00 3.48137108E+00 2.12245717E-04-6.86359044E-07    3
 8.56185857E-10-2.34581508E-13-3.38607305E+04 1.02579990E+00-3.28178089E+04    4
F2  REF ELEMENT   RUS 89F   2    0    0    0G   200.000  6000.000 1000.        1
burcat,2013
 3.86166219E+00 7.88367679E-04-1.81982940E-07-9.17436560E-12 2.65193472E-15    2
-1.23238655E+03 2.04119869E+00 3.20832415E+00 1.25919179E-03 3.89747979E-06    3
-7.22184984E-09 3.31837862E-12-1.03425794E+03 5.61903603E+00 0.00000000E+00    4
HOF               T 5/11H  1.O  1.F  1.   0.G   200.000  6000.000 1000.        1
burcat,2013
 4.12528386E+00 2.31519777E-03-7.76666333E-07 1.19549024E-10-6.91728055E-15    2
-1.19136862E+04 2.89862207E+00 3.92035391E+00-1.39927977E-03 1.39115337E-05    3
-1.79018174E-08 7.24565658E-12-1.16927573E+04 4.87858424E+00-1.04951464E+04    4
F2O               71STU/F   2O   1    0    0G   300.00   3000.00  1245.00      1
 0.60502237E+01 0.11801203E-02-0.62998049E-06 0.16265308E-09-0.16630594E-13    2
 0.86796609E+03-0.55559173E+01 0.23117985E+01 0.14403418E-01-0.18975198E-04    3
 0.11788725E-07-0.28156285E-11 0.17661785E+04 0.13044809E+02                   4
FO                ATcT/AF  1.O  1.   0.   0.G   200.000  6000.000 1000.        1
burcat,2013
 4.10435161E+00 3.22444815E-04-6.01630664E-08-1.10998596E-11 1.61567239E-15    2
 1.20593514E+04 2.35480534E+00 4.34438108E+00-5.37168023E-03 1.77166504E-05    3
-2.00073120E-08 7.67510992E-12 1.22051341E+04 2.24948929E+00 1.33822679E+04    4
FO2               71STU/F   1O   2    0    0G   300.00   3000.00  1360.00      1
 0.56242097E+01 0.17066411E-02-0.89995239E-06 0.22561211E-09-0.22048285E-13    2
-0.40013089E+03-0.17257001E+01 0.36727894E+01 0.76317941E-02-0.79426701E-05    3
 0.40752038E-08-0.83001063E-12 0.13887520E+03 0.82723509E+01                   4
!***********************
```

```
!*** C1 Fluorocarbons ***
!**********************
CH3F  FC-41 -236  T05/11C  1.H  3.F  1.   0.G   200.000  6000.000 1000.       1
2018GAN/KAL(burcat,2013)
 3.31348457E+00 8.59183430E-03-3.07886159E-06 4.96069542E-10-2.96514660E-14    2
-3.00122760E+04 4.75257452E+00 5.03514272E+00-1.46119198E-02 6.06479225E-05    3
-6.60649862E-08 2.42867162E-11-2.95973280E+04 3.08070101E-01-2.84535108E+04    4
CH2F2   FC-32     T 9/99C   1H   2F   2    0G   200.000  6000.000 1000.       1
2018GAN/KAL(burcat,2013)
 5.06948195E+00 7.23193135E-03-2.64021025E-06 4.30854708E-10-2.59873096E-14    2
-5.65991527E+04-2.34590394E+00 4.25023157E+00-6.84861262E-03 4.85583334E-05    3
-5.83442752E-08 2.24503933E-11-5.56073052E+04 5.76716418E+00-5.44480432E+04    4
CHF3  FLUOROFORM  T 9/99C   1H   1F   3    0G   200.000  6000.000 1000.       1
2018GAN/KAL(burcat,2013)
 7.24609031E+00 5.42386441E-03-2.02314394E-06 3.34946402E-10-2.04067524E-14    2
-8.68239019E+04-1.28982398E+01 2.73539203E+00 8.72478957E-03 1.74821510E-05    3
-3.21504750E-08 1.41694928E-11-8.51820557E+04 1.24879863E+01-8.33830015E+04    4
CF4    FC-14      g 7/99C  1.F  4.   0.   0.G   200.000  6000.000 1000.       1
burcat,2013
 9.47336526E+00 3.59407743E-03-1.40334012E-06 2.39113889E-10-1.48513407E-14    2
-1.15816621E+05-2.49736848E+01 1.05119594E+00 2.78318369E-02-2.46683439E-05    3
 6.75882532E-09 9.14850873E-13-1.13574198E+05 1.81936795E+01-1.12227900E+05    4
CH2F              T 8/09C  1.H  2.F  1.   0.G   200.000  6000.000 1000.       1
2018GAN/KAL(burcat,2013)
 4.11283513E+00 5.00104452E-03-1.74095833E-06 2.75007611E-10-1.62099637E-14    2
-5.25924503E+03 2.38852694E+00 3.78123930E+00-4.49840351E-04 1.88358140E-05    3
-2.40702692E-08 9.53477519E-12-4.88500871E+03 5.56895443E+00-3.85801124E+03    4
CHF2              g 6/88C  1.H  1.F  2.   0.G   200.000  6000.000 1000.       1
2018GAN/KAL(burcat,2013)
 5.52321120E+00 4.21970092E-03-1.58435294E-06 2.63969157E-10-1.61337618E-14    2
-3.14404682E+04-2.40335469E+00 4.12220872E+00-2.33706659E-03 2.99282606E-05    3
-3.88422961E-08 1.55352879E-11-3.05990045E+04 7.22245467E+00-2.87329019E+04    4
CF3               ATcT/AC  1.F  3.   0.   0.G   200.000  6000.000 1000.       1
2018GAN/KAL(burcat,2013)
 7.42981696E+00 2.61728694E-03-1.02141596E-06 1.73975666E-10-1.08028191E-14    2
-5.91795501E+04-1.22816891E+01 2.38179059E+00 1.37269527E-02-3.47674937E-06    3
-9.01697393E-09 5.57384083E-12-5.76871035E+04 1.43743316E+01-5.62149784E+04    4
CHF  singlet      T 7/11C  1.H  1.F  1.   0.G   200.000  6000.000 1000.       1
burcat,2013
 2.09415280E+00 5.34934017E-03-1.69762943E-06 2.19446141E-10-1.00205977E-14    2
 1.72042147E+04 1.37860960E+01 4.42272584E+00-5.60196198E-03 2.21848969E-05    3
-2.39634368E-08 8.91306513E-12 1.66515542E+04 2.54111183E+00 1.78740539E+04    4
CF2               ATcT/AC  1.F  2.   0.   0.G   200.000  6000.000 1000.       1
2018GAN/KAL(burcat,2013)
 5.35787718E+00 1.80622418E-03-7.80465045E-07 1.47642691E-10-9.44754424E-15    2
-2.52559006E+04-2.63410779E+00 3.56435487E+00 1.23021056E-03 1.39909866E-05    3
-2.13708286E-08 9.10710807E-12-2.45418819E+04 7.83907808E+00-2.30031595E+04    4
CF                ATcT/AC  1.F  1.   0.   0.G   200.000  6000.000 1000.       1
burcat,2013
 3.74644062E+00 8.01632001E-04-2.95064248E-07 5.03803598E-11-3.08738254E-15    2
 2.84554882E+04 3.84191679E+00 3.99598712E+00-4.62546013E-03 1.58270762E-05    3
-1.73528410E-08 6.45553921E-12 2.86045210E+04 3.67054970E+00 2.96989239E+04    4
!*******************************
!*** Oxidized C1 Fluorocarbons ***
!*******************************
```

```
CHFO              T07/11C  1.O  1.F  1.H  1.G   200.000  6000.000 1000.       1
burcat,2013
 4.78813214E+00 4.76650220E-03-1.74367126E-06 2.84956025E-10-1.72050907E-14    2
-4.79424476E+04 3.51967468E-01 3.74246307E+00-1.31011108E-03 2.46792673E-05    3
-3.12953787E-08 1.22624735E-11-4.72269701E+04 7.89719615E+00-4.60074015E+04    4
CF2O              T 5/11C  1.O  1.F  2.   0.G   200.000  6000.000 1000.       1
burcat,2013
 6.81631709E+00 3.16473302E-03-1.21776278E-06 2.05582278E-10-1.26893138E-14    2
-7.55374518E+04-9.52865117E+00 2.12979433E+00 1.41019782E-02-5.94383395E-06    3
-5.30542094E-09 3.97366263E-12-7.41637142E+04 1.51109046E+01-7.29630489E+04    4
CFO  (CFO/COF)    T 9/11F  1.C  1.O  1.   0.G   200.000  6000.000 1000.       1
burcat,2013
 5.01565891E+00 1.95763376E-03-7.49685297E-07 1.25610155E-10-7.59885072E-15    2
-2.29785255E+04 3.69669039E-01 3.37992233E+00 4.19050548E-03 2.12353533E-06    3
-6.20586665E-09 2.85352218E-12-2.24063200E+04 9.39466699E+00-2.12044967E+04    4
CF3O Radical      T07/04C  1.F  3.O  1.   0.G   200.000  6000.000 1000.       1
burcat,2013
 9.76423201E+00 3.30092424E-03-1.28961521E-06 2.19815579E-10-1.36560199E-14    2
-7.94771282E+04-2.37694198E+01 1.82041152E+00 2.65327204E-02-2.45066904E-05    3
 7.86171828E-09 2.73540764E-13-7.73780958E+04 1.68621895E+01-7.58568931E+04    4
!*********************
!*** Fluoroethanes ***
!*********************
CH3-CH2F          T 6/11C  2.H  5.F  1.   0.G   200.000  6000.000 1000.       1
burcat,2013
 6.18081698E+00 1.35890229E-02-4.87040213E-06 7.84862029E-10-4.69209214E-14    2
-3.58341343E+04-7.96594699E+00 4.00577312E+00-3.11043983E-04 5.57188865E-05    3
-7.28404563E-08 2.90642195E-11-3.43213851E+04 7.92813391E+00-3.27788408E+04    4
CH2F-CH2F  HFC-152T 9/10C  2.H  4.F  2.   0.G   200.000  6000.000 1000.       1
2018GAN/KAL(burcat,2013)
 1.00315710E+01 1.11994308E-02-4.26519119E-06 7.11447245E-10-4.35028559E-14    2
-5.85296182E+04-2.85864919E+01 5.58943786E+00-1.13537115E-02 9.78443079E-05    3
-1.22110880E-07 4.76646013E-11-5.56834525E+04 2.61081947E+00-5.41655491E+04    4
CH3-CHF2  HFC-152aT 6/11C  2.F  2.H  4.   0.G   200.000  6000.000 1000.       1
2018GAN/KAL(burcat,2013)
 7.67995887E+00 1.22243125E-02-4.37573530E-06 7.04756402E-10-4.21223621E-14    2
-6.40850702E+04-1.47344376E+01 3.25212905E+00 1.18717590E-02 2.57923969E-05    3
-4.29488908E-08 1.82237758E-11-6.22767756E+04 1.11051557E+01-6.01899571E+04    4
CH2F-CHF2 68LACSKI96ZAC C   2H   3F   3    0G   300.00   3000.00  1100.00     1
2018GAN/KAL
 0.92726485E+01 0.12040181E-01-0.48605999E-05 0.88656689E-09-0.59650602E-13    2
-8.43982994E+04-0.21387996E+02 0.64737590E+00 0.36292494E-01-0.31143200E-04    3
 0.14464592E-07-0.30120967E-11-8.19413424E+04 0.23295333E+02                   4
CH3-CF3 FC-143A   T11/03C  2.H  3.F  3.   0.G   200.000  6000.000 1000.       1
2018GAN/KAL(burcat,2013)
 1.00540918E+01 1.02515900E-02-3.70172133E-06 5.99863654E-10-3.60117460E-14    2
-9.48129775E+04-2.72330585E+01 1.75260632E+00 3.04395701E-02-1.49788607E-05    3
-5.70775683E-09 5.66225345E-12-9.24091835E+04 1.62401353E+01-9.08838885E+04    4
CHF2-CHF2         T 5/03C  2.H  2.F  4.   0.G   200.000  6000.000 1000.       1
2018GAN/KAL(burcat,2013)
 1.19960865E+01 8.98721146E-03-3.36363101E-06 5.54000254E-10-3.35654907E-14    2
-1.10809976E+05-3.53416069E+01 3.98924014E+00 1.72571738E-02 2.36853869E-05    3
-4.89142700E-08 2.21225708E-11-1.08018610E+05 9.12364634E+00-1.06235966E+05    4
CH2F-CF3          T 5/03C  2.H  2.F  4.   0.G   200.000  6000.000 1000.       1
2018GAN/KAL(burcat,2013)
```

```
 1.25551115E+01 8.40186071E-03-3.12077291E-06 5.12284572E-10-3.10110291E-14    2
-1.14409890E+05-3.80374329E+01 2.29239681E+00 3.03108483E-02-5.33713985E-06    3
-2.19456612E-08 1.29970288E-11-1.11354002E+05 1.62830568E+01-1.09844116E+05    4
CHF2-CF3          A 4/05C  2.H  1.F  5.   0.G   200.000  6000.000 1000.        1
2018GAN/KAL(burcat,2013)
 1.45281312E+01 6.80984691E-03-2.67132939E-06 4.54433791E-10-2.81433657E-14    2
-1.39668599E+05-4.67174252E+01 2.56680624E+00 3.63877723E-02-1.93606756E-05    3
-9.02362714E-09 8.52266342E-12-1.36273767E+05 1.56968804E+01-1.34704270E+05    4
CF3-CF3           T 6/11C  2.F  6.   0.   0.G   200.000  6000.000 1000.        1
2018GAN/KAL(burcat,2013)
 1.70284831E+01 4.64174937E-03-1.92155485E-06 3.37538839E-10-2.13452416E-14    2
-1.68162295E+05-5.98112608E+01 1.56503771E+00 5.10909623E-02-5.07167534E-05    3
 1.88993955E-08-7.73770882E-13-1.64148368E+05 1.89556430E+01-1.62429295E+05    4
!********************
!*** Fluoroethyls ***
!********************
CH2F-CH2 beta-Flu T 4/10C  2.H  4.F  1.   0.G   200.000  6000.000 1000.        1
2018GAN/KAL(burcat,2013)
 6.17560952E+00 1.07042948E-02-3.78369889E-06 6.04072338E-10-3.58779020E-14    2
-9.89977825E+03-5.63727120E+00 4.38588734E+00 4.44184913E-03 2.81593156E-05    3
-3.89282386E-08 1.56055864E-11-8.87171985E+03 6.28370097E+00-7.34746654E+03    4
CH3-CHF alfa-Flu  T 4/10C  2.H  4.F  1.   0.G   200.000  6000.000 1000.        1
2018GAN/KAL(burcat,2013)
 5.75331333E+00 1.11537753E-02-3.96206053E-06 6.34664198E-10-3.77832181E-14    2
-1.15237093E+04-3.95888581E+00 4.74843909E+00 5.09114984E-04 3.62637445E-05    3
-4.54978044E-08 1.75184149E-11-1.05832291E+04 4.50273732E+00-9.09966697E+03    4
CH2F-CHF  95BURZAC91CHE C   2H   3F   2    0G   300.00   3000.00  1250.00      1
2018GAN/KAL (NIST)
 0.87214510E+01 0.86815505E-02-0.35422910E-05 0.66313495E-09-0.44742292E-13    2
-3.34060307E+04-0.18251835E+02 0.22898344E+01 0.25577305E-01-0.19912795E-04    3
 0.75880439E-08-0.11237829E-11-3.14764727E+04 0.15431326E+02                   4
CHF2-CH2  90CHERAU      C   2H   3F   2    0G   300.00   3000.00  1100.00      1
2018GAN/KAL (NIST)
 0.67982556E+01 0.12130852E-01-0.52871420E-05 0.10362364E-08-0.74087387E-13    2
-3.69269815E+04-0.72160920E+01 0.12123746E+01 0.29952820E-01-0.27809679E-04    3
 0.14586627E-07-0.33536338E-11-3.54757375E+04 0.21112708E+02                   4
CH3-CF2   78ROD90CHERAU C   2H   3F   2    0G   300.00   3000.00  1150.00      1
2018GAN/KAL (NIST)
 0.64772061E+01 0.12487615E-01-0.53578191E-05 0.10304861E-08-0.72450865E-13    2
-3.86798594E+04-0.63195346E+01 0.23142186E+01 0.23701830E-01-0.16389184E-04    3
 0.57257237E-08-0.80729590E-12-3.74727734E+04 0.15358357E+02                   4
CH2F-CF2  91CHERAU      C   2H   2F   3    0G   300.00   3000.00  1150.00      1
 0.88702445E+01 0.10089497E-01-0.43915564E-05 0.85758186E-09-0.61164127E-13    2
-0.57295496E+05-0.17248955E+02 0.20900802E+01 0.29390131E-01-0.25553336E-04    3
 0.11710794E-07-0.23112930E-11-0.55373132E+05 0.17813614E+02                   4
CHF2-CHF  91CHERAU      C   2H   2F   3    0G   300.00   3000.00  1250.00      1
 0.94245630E+01 0.93845534E-02-0.40694952E-05 0.79548881E-09-0.56874376E-13    2
-0.58166030E+05-0.20313155E+02 0.18136794E+01 0.32776675E-01-0.32420504E-04    3
 0.16831319E-07-0.36002411E-11-0.56094627E+05 0.18591066E+02                   4
CF3-CH2   78ROD90CHERAU C   2H   2F   3    0G   300.00   3000.00  1150.00      1
2018GAN/KAL (NIST)
 0.95879571E+01 0.92998799E-02-0.40774688E-05 0.80571741E-09-0.58185489E-13    2
-6.72872509E+04-0.22107686E+02 0.71700835E+00 0.40531459E-01-0.47864066E-04    3
 0.29440811E-07-0.73125849E-11-6.51420629E+04 0.22103248E+02                   4
CHF2-CF2  95BURZAC91CHE C   2H   1F   4    0G   300.00   3000.00  1250.00      1
```

```
 0.11627462E+02 0.71020241E-02-0.30321751E-05 0.58031013E-09-0.40595926E-13    2
-0.84517281E+05-0.30486515E+02 0.30303759E+01 0.31363562E-01-0.29518978E-04    3
 0.13983874E-07-0.27124342E-11-0.82031363E+05 0.14088813E+02                   4
CF3-CHF   95BURZAC91CHE C   2H   1F   4    0G   300.00   3000.00  1250.00      1
2018GAN/KAL (NIST)
 0.11753063E+02 0.71311773E-02-0.31225055E-05 0.61530080E-09-0.44414594E-13    2
-8.86441929E+04-0.31333337E+02 0.21777569E+01 0.37699208E-01-0.41607296E-04    3
 0.23110573E-07-0.51391529E-11-8.61215759E+04 0.17267626E+02                   4
CF3-CF2           T03/10C  2.F  5.   0.   0.G   200.000  6000.000 1000.       1
2018GAN/KAL (burcat,2013)
 1.45575510E+01 4.16794014E-03-1.72789494E-06 3.02375137E-10-1.90423730E-14    2
-1.13453173E+05-4.50857249E+01 2.35961717E+00 4.06759536E-02-3.97029086E-05    3
 1.42583579E-08-3.10091084E-13-1.10281694E+05 1.70748780E+01-1.08475901E+05    4
!**********************
!*** Fluoroethylenes ***
!**********************
CH2CHF            RUS 91C  2.H  3.F  1.   0.G   200.000  6000.000 1000.       1
2018GAN/KAL (burcat,2013)
 5.92787061E+00 8.89384427E-03-3.17971566E-06 5.11681548E-10-3.05632459E-14    2
-1.98276668E+04-7.04448245E+00 2.61149895E+00 6.68683582E-03 2.76818258E-05    3
-4.33824699E-08 1.85254269E-11-1.84326315E+04 1.26328255E+01-1.68500609E+04    4
CHFCHF[E]         RUS 91C  2.H  2.F  2.   0.G   200.000  6000.000 1000.       1
burcat,2013
 7.73658780E+00 7.46809856E-03-2.71232867E-06 4.41227895E-10-2.65588270E-14    2
-3.96779496E+04-1.52286382E+01 2.82321391E+00 1.39737055E-02 8.79179901E-06    3
-2.39558133E-08 1.12741216E-11-3.80129641E+04 1.17612525E+01-3.65144789E+04    4
CHFCHF[Z]         RUS 91C  2.H  2.F  2.   0.G   200.000  6000.000 1000.       1
burcat,2013
 7.64662972E+00 7.55622756E-03-2.74600447E-06 4.46890910E-10-2.69075698E-14    2
-4.00302113E+04-1.46982798E+01 2.69825023E+00 1.23878271E-02 1.53768601E-05    3
-3.23557844E-08 1.47696831E-11-3.82972358E+04 1.28259603E+01-3.68632667E+04    4
CHFCHF(Z)         RUS 91C  2.H  2.F  2.   0.G   200.000  6000.000 1000.       1
burcat,2013
 7.64662972E+00 7.55622756E-03-2.74600447E-06 4.46890910E-10-2.69075698E-14    2
-4.00302113E+04-1.46982798E+01 2.69825023E+00 1.23878271E-02 1.53768601E-05    3
-3.23557844E-08 1.47696831E-11-3.82972358E+04 1.28259603E+01-3.68632667E+04    4
CH2CF2  FC-1132A  T 6/11C  2.H  2.F  2.   0.G   200.000  6000.000 1000.       1
2018GAN/KAL (burcat,2013)
 8.95189658E+00 7.14641061E-03-2.79505418E-06 4.77439020E-10-2.97191427E-14    2
-4.60294637E+04-2.29204220E+01 1.28301801E+00 2.31903824E-02-9.70095198E-06    3
-4.40973912E-09 3.38826355E-12-4.35424071E+04 1.82378552E+01-4.00420470E+04    4
CHFCF2            T 6/11C  2.H  1.F  3.   0.G   200.000  6000.000 1000.       1
burcat,2013
 9.56303811E+00 6.03922396E-03-2.24656246E-06 3.71316848E-10-2.25981353E-14    2
-6.23666082E+04-2.23573620E+01 2.00354119E+00 2.74140646E-02-2.30032301E-05    3
 7.09389407E-09 1.96148641E-13-6.03000360E+04 1.65697402E+01-5.86733313E+04    4
CF2CF2            ATcT/AC  2.F  4.   0.   0.G   200.000  6000.000 1000.       1
2018GAN/KAL;burcat,2013
 1.14178412E+01 4.59161071E-03-1.77520928E-06 3.00598731E-10-1.85921260E-14    2
-8.52927617E+04-3.16445526E+01 1.99308667E+00 3.84734406E-02-5.32322754E-05    3
 3.92122720E-08-1.19302747E-11-8.30021485E+04 1.53134111E+01-8.12242694E+04    4
!********************
!*** Fluorovinyls ***
!********************
CHFCH[E]  96ZACWES      C   2H   2F   1    0G   300.00   3000.00  1050.00      1
```

```
 0.58993136E+01 0.70760772E-02-0.28887543E-05 0.53085830E-09-0.35873561E-13    2
 0.12541439E+05-0.53585386E+01 0.26848631E+00 0.27945434E-01-0.35411860E-04    3
 0.25148746E-07-0.73773052E-11 0.13892575E+05 0.22559566E+02                   4
CHFCH[Z]  96ZACWES      C   2H   2F   1    0G   300.00   3000.00  1050.00     1
 0.52720505E+01 0.81754708E-02-0.34673780E-05 0.64788558E-09-0.43922904E-13    2
 0.12647789E+05-0.19972542E+01 0.44420192E+00 0.26606878E-01-0.31480981E-04    3
 0.20535551E-07-0.55252516E-11 0.13722215E+05 0.21668910E+02                   4
CH2CF     96ZACWES      C   2H   2F   1    0G   300.00   3000.00  1050.00     1
 0.59366687E+01 0.65440923E-02-0.23741343E-05 0.38223533E-09-0.22535997E-13    2
 0.10745181E+05-0.55730445E+01 0.93664567E+00 0.23455005E-01-0.26099122E-04    3
 0.16833431E-07-0.46658292E-11 0.12014041E+05 0.19594667E+02                   4
CHFCF[E]          T 6/02C  2.H  1.F  2.   0.G   200.000  6000.000 1000.       1
burcat,2013
 7.87499232E+00 4.77134517E-03-1.76600789E-06 2.90903847E-10-1.76623863E-14    2
-8.08846630E+03-1.36036843E+01 3.08690083E+00 1.60213261E-02-7.49407266E-06    3
-3.65234768E-09 3.19176449E-12-6.67208283E+03 1.15973919E+01-5.11154596E+03    4
CHFCF[Z]  96ZACWES      C   2H   1F   2    0G   300.00   3000.00  1050.00     1
 0.77264612E+01 0.50029540E-02-0.18613080E-05 0.31199442E-09-0.19536071E-13    2
-0.79003013E+04-0.12864265E+02 0.14830603E+01 0.25289629E-01-0.28989928E-04    3
 0.18356855E-07-0.49865919E-11-0.62750421E+04 0.18768190E+02                   4
CF2CH     96ZACWES      C   2H   1F   2    0G   300.00   3000.00  1050.00     1
 0.74110309E+01 0.64817026E-02-0.30631409E-05 0.62562526E-09-0.45512604E-13    2
-0.11017369E+05-0.11617089E+02 0.64712617E+00 0.31659599E-01-0.41452904E-04    3
 0.28609364E-07-0.80609769E-11-0.94385390E+04 0.21799374E+02                   4
CF2CF             tpis91C  2.F  3.   0.   0.G   200.000  6000.000 1000.       1
burcat,2013
 9.28002368E+00 3.72628116E-03-1.44027826E-06 2.43838247E-10-1.50793717E-14    2
-3.08448687E+04-1.92329718E+01 2.41464240E+00 2.68291562E-02-3.39283388E-05    3
 2.31906358E-08-6.71131007E-12-2.90990246E+04 1.53576825E+01-2.74437210E+04    4
!************************
!*** Fluoroacetylenes ***
!************************
C2HF              T 7/11C  2.H  1.F  1.   0.G   200.000  6000.000 1000.       1
burcat,2013
 6.20949775E+00 3.69584855E-03-1.29973578E-06 2.06830940E-10-1.22578311E-14    2
 1.04017383E+04-8.93525071E+00 1.30649331E+00 2.77924488E-02-4.86268691E-05    3
 4.25956865E-08-1.42675759E-11 1.12860035E+04 1.39346815E+01 1.25586475E+04    4
C2F               tpis91C  2.F  1.   0.   0.G   200.000  6000.000 1000.       1
burcat,2013
 5.26094396E+00 2.14579712E-03-8.07509859E-07 1.34379596E-10-8.21353206E-15    2
 4.07468230E+04-3.14254580E+00 2.70218031E+00 1.27931571E-02-2.04432188E-05    3
 1.78526199E-08-6.17934124E-12 4.13318085E+04 9.33996365E+00 4.25578275E+04    4
C2F2              T 7/11C  2.F  2.   0.   0.G   200.000  6000.000 1000.       1
ATcT,2019 (burcat,2013)
 7.53993696E+00 2.75655100E-03-1.01925304E-06 1.67696082E-10-1.01706808E-14    2
-1.85733725E+03-1.32743125E+01 4.21917369E+00 1.74654857E-02-2.90187341E-05    3
 2.55812733E-08-8.81243821E-12-1.15082175E+03 2.68488791E+00 3.43976975E+02    4
!**********************
!*** Fluoroketenes ***
!**********************
CHFCO     96ZACWES      C   2H   1F   1O   1G   300.00   3000.00  1050.00     1
 0.67776435E+01 0.62335944E-02-0.25595800E-05 0.47531383E-09-0.32595082E-13    2
-0.20336925E+05-0.85911299E+01 0.19623675E+01 0.22507519E-01-0.25638947E-04    3
 0.16791690E-07-0.47348234E-11-0.19104027E+05 0.15674252E+02                   4
CF2CO     96ZACWES      C   2F   2O   1    0G   300.00   3000.00  1050.00     1
```

```
 0.88684122E+01 0.42627717E-02-0.17381349E-05 0.31228667E-09-0.20426586E-13    2
-0.38145628E+05-0.17907486E+02 0.34054339E+01 0.22694311E-01-0.28035260E-04    3
 0.19124705E-07-0.55121984E-11-0.36737327E+05 0.96487236E+01                   4
CFCO      96ZACWES      C   2F   1O   1    0G   300.00   3000.00  1050.00     1
 0.73033099E+01 0.29793943E-02-0.13058250E-05 0.25407405E-09-0.18103465E-13    2
 0.57355650E+04-0.98434103E+01 0.37594179E+01 0.14231997E-01-0.16010254E-04    3
 0.98885732E-08-0.26613184E-11 0.66747250E+04 0.81859183E+01                   4
CF3OF             71STU/C   1O   1F   4    0G   300.00   3000.00  1440.00     1
 0.12399629E+02 0.32529590E-02-0.14291450E-05 0.29960628E-09-0.25133306E-13    2
-0.96721165E+05-0.34715971E+02 0.24959868E+01 0.32773790E-01-0.35901194E-04    3
 0.18734756E-07-0.37862643E-11-0.93915478E+05 0.16231910E+02                   4
!****************
!***C3-fluorinated,etc***
!************************
C3F7H  FC227EA    T12/99C   3H   1F   7    0G   200.000  6000.000 1000.       1
burcat,2013
 2.03195617E+01 1.04618873E-02-3.99351610E-06 6.70976809E-10-4.12886922E-14    2
-1.96070480E+05-7.39087817E+01 3.19381844E+00 5.64358210E-02-4.24435538E-05    3
 6.01422805E-09 4.21730731E-12-1.91302556E+05 1.47970140E+01-1.88203033E+05    4
C3F7 CF3CF*CF3 M  T12/99C   3F   7    0    0G   200.000  6000.000 1000.       1
burcat,2013
 2.05301132E+01 7.60062764E-03-2.96491015E-06 5.04882378E-10-3.13452721E-14    2
-1.69702083E+05-7.19281430E+01 3.14241614E+00 6.03443070E-02-6.17598017E-05    3
 2.79379580E-08-4.02551172E-12-1.65147364E+05 1.66897624E+01-1.62020670E+05    4
C3F6  CF2=CF-CF3  A11/04C  3.F  6.   0.   0.G   200.000  6000.000 1000.       1
burcat,2013
 1.87296098E+01 5.74055067E-03-2.31302367E-06 4.01017749E-10-2.51741915E-14    2
-1.46123551E+05-6.59853551E+01 2.35781302E+00 5.80498289E-02-6.67557556E-05    3
 3.68109988E-08-7.92990472E-12-1.41947032E+05 1.68586208E+01-1.39184698E+05    4
CF3O2             NIST  C   1F   3O   2    0G   300.000  5000.000             1
  0.1005499E+02  0.8205633E-02 -0.5062363E-05  0.1433123E-08 -0.1534602E-12    2
 -0.1015453E+06 -0.2260937E+02  0.4379631E+00  0.4555659E-01 -0.6176471E-04    3
  0.4131473E-07 -0.1106784E-10 -0.8164120E+05  0.2413379E+02                   4
C3F7O             Hynes C   3F   7O   1    0G   300.000  5000.000             1
  0.2287185E+02  0.7640052E-02 -0.1657346E-05 -0.2941549E-09  0.1035168E-12    2
 -0.1880432E+06 -0.8666051E+02  0.1136218E+01  0.7336590E-01 -0.7413762E-04    3
  0.3256982E-07 -0.4255755E-11 -0.1823545E+06  0.2413339E+02                   4
C3F7O2            Hynes C   3F   7O   2    0G   300.000  5000.000             1
  0.1787408E+02  0.2373510E-01 -0.1367114E-04  0.3718392E-08 -0.3930683E-12    2
 -0.1860711E+06 -0.5607585E+02  0.1641474E+01  0.8751624E-01 -0.1100224E-03    3
  0.7251820E-07 -0.2041578E-10 -0.1828074E+06  0.2252190E+02                   4
CF3COF                 C   2F   4O   1    0G   300.000  5000.000             1
Purnell/Bozzelli,2019
  0.1006273E+02  0.1214340E-01 -0.7263414E-05  0.2011440E-08 -0.2118963E-12    2
-1.27589631E+05 -0.2073074E+02  0.1769974E+01  0.4245083E-01 -0.5069665E-04    3
  0.3111379E-07 -0.7895977E-11-1.25711631E+05  0.2018299E+02                   4
C3F6O             hynes C   3F   6O   1    0G   300.000  5000.000             1
  0.1704561E+02  0.1455861E-01 -0.8812300E-05  0.2462951E-08 -0.2613377E-12    2
 -0.1744044E+06 -0.5524056E+02  0.2606280E+01  0.7231953E-01 -0.1005112E-03    3
  0.7052793E-07 -0.1995183E-10 -0.1713574E+06  0.1482562E+02                   4
CF3CHO            NIST  C   2F   3H   1O   1G   300.000  5000.000             1
Purnell/Bozzelli,2019 (NIST)
  0.8047711E+01  0.1377502E-01 -0.7751215E-05  0.2053101E-08 -0.2090976E-12    2
-9.65904246E+04 -0.1217682E+02  0.2986401E+01  0.2819500E-01 -0.2091598E-04    3
  0.5048025E-08  0.6025630E-12-9.52619146E+04  0.1374664E+02                   4
```

```
CF3CO             NIST  C   2F   3O   1    0G   300.000  5000.000             1
Purnell/Bozzelli,2019 (NIST)
  0.8273660E+01  0.9456556E-02 -0.5544948E-05  0.1509502E-08 -0.1566714E-12    2
-7.56835411E+04 -0.1889926E+02 -0.7058443E+01  0.1041643E+00 -0.2377523E-03    3
  0.2500676E-06 -0.9594719E-10-7.32842611E+04  0.4950205E+02                   4
C3F7OH            hynes C   3F   7O   1H   1G   300.000  5000.000             1
  0.1696278E+02  0.2565773E-01 -0.1513042E-04  0.4192663E-08 -0.4490027E-12    2
 -0.2188921E+06 -0.5534448E+02  0.1429132E+01  0.8909125E-01 -0.1141049E-03    3
  0.7694099E-07 -0.2212097E-10 -0.2159364E+06  0.1918044E+02                   4
C2F5COC3F7             0C   6F  12O   1     G   300.000  3000.000 1000.00     1
Hf -650.8;Cp,S-Smith KD data
 0.30630959E+02 0.38184828E-01-0.24308864E-04 0.70308675E-08-0.76600556E-12    2
-0.33931382E+06-0.11703101E+03 0.47864609E+01 0.12945436E+00-0.14305048E-03    3
 0.74083490E-07-0.14502047E-10-0.33353949E+06 0.10680870E+02                   4
C2F5CO                 0C   3F   5O   1H   0G   300.000  2500.000 1000.00     1
 0.10993560E+02 0.22635009E-01-0.16215860E-04 0.53906966E-08-0.68205687E-12    2
-0.12892516E+06-0.29543968E+02 0.58825005E+01 0.31427282E-01-0.11926324E-04    3
-0.91209576E-08 0.58588476E-11-0.12732035E+06-0.19730690E+01                   4
C2F5CHO                0C   3F   5O   1H   1G   300.000  2500.000 1000.00     1
 0.70011481E+01 0.36515406E-01-0.27132992E-04 0.93304054E-08-0.12151653E-11    2
-0.14764381E+06-0.28355041E+01 0.23841549E+01 0.57546395E-01-0.62523998E-04    3
 0.35487425E-07-0.83951742E-11-0.14684857E+06 0.18798064E+02                   4
C3F7CO                 0C   4F   7O   1     G   300.000  2500.000 1000.00     1
 0.49092940E+01 0.56218006E-01-0.44870281E-04 0.16215609E-07-0.21904541E-11    2
-0.18448922E+06 0.12881551E+02 0.45819062E+01 0.62040688E-01-0.60374001E-04    3
 0.31064553E-07-0.70309731E-11-0.18464940E+06 0.13332725E+02                   4
C3F7CHO                0C   4F   7O   1H   1G   300.000  2500.000 1000.00     1
 0.10618414E+02 0.46140362E-01-0.34401925E-04 0.11943552E-07-0.15745340E-11    2
-0.20345971E+06-0.11769315E+02 0.45903305E+01 0.62406189E-01-0.47030908E-04    3
 0.12516368E-07 0.24388842E-12-0.20186177E+06 0.19274330E+02                   4
!
CF3CHCH2               H   3C   3F   3    0g    200.00   6000.00 1000.00     1
Burcat
 1.22166309E+01 1.11177411E-02-4.07566929E-06 6.63454514E-10-3.98729557E-14    2
-8.08780489E+04-3.63340348E+01 1.56834820E+00 3.70715693E-02-1.66534622E-05    3
-1.15669918E-08 9.46282072E-12-7.78570098E+04 1.92579065E+01-7.59072147E+04    4
CF3CCH2                H   2C   3F   3    0g    200.00   6000.00 1000.00     1
Burcat
 1.25859962E+01 8.12317961E-03-2.95982852E-06 4.80631726E-10-2.89086264E-14    2
-4.99277916E+04-3.65971752E+01 1.34293581E+00 4.37082126E-02-4.41291023E-05    3
 1.98066011E-08-2.52757681E-12-4.70859152E+04 2.02494155E+01-4.50947551E+04    4
CF3CHCH CF3-CH=CH A10/04C   3H   2F   3    0G   200.000   6000.00 1000.00     1
Burcat
 1.27774168E+01 7.93163451E-03-2.88750413E-06 4.67651599E-10-2.80481227E-14    2
-5.02306417E+04-3.79660841E+01 6.81987133E-01 4.69264463E-02-4.86400872E-05    3
 2.20469507E-08-2.75414626E-12-4.72313621E+04 2.29560885E+01-4.53297573E+04    4
CF3CCH                 H   1C   3F   3    0g    300.00   5000.00 1000.00     1
 1.20875571E+01 6.73607631E-03-2.69300970E-06 4.89991898E-10-3.33727293E-14    2
-5.60204633E+04-3.43479861E+01 2.81616474E-01 5.25169846E-02-7.44406106E-05    3
 5.35249568E-08-1.53175885E-11-5.33966440E+04 2.34333278E+01                   4
!
CF3COCH3               H   3C   3O   1F   3g    300.00   5000.00 1000.00     1
 1.37707128E+01 1.39114007E-02-5.56646243E-06 1.01277226E-09-6.89535233E-14    2
-1.06311755E+05-4.15671452E+01 2.31183560E+00 4.62931613E-02-3.86726491E-05    3
 1.45780128E-08-1.48757320E-12-1.03127581E+05 1.75781936E+01                   4
```

```
CH2CFCF3  2,3,3,3-T 1/10C   3H   2F   4    0G   200.000  6000.000 1000.00     1
Burcat
 1.43109945E+01 9.44785369E-03-3.52268169E-06 5.79391979E-10-3.50621207E-14    2
-1.03384074E+05-4.69130460E+01 1.00153498E+00 4.98007666E-02-4.61878165E-05    3
 1.64791672E-08-3.13155879E-13-9.99486839E+04 2.07746963E+01-9.78122362E+04    4
CH-CFCF3               H   1C   3F   4    0g    200.00   6000.00 1000.00     1
est
 1.43232063E+01 6.55666899E-03-2.43587955E-06 3.98836047E-10-2.40439148E-14    2
-7.35563379E+04-4.52117067E+01 4.99663120E-01 5.71202270E-02-7.49546439E-05    3
 4.83897613E-08-1.22362197E-11-7.03969480E+04 2.30298398E+01                   4
CFCCF3                 H   0C   3F   4    0g    300.00   5000.00 1000.00     1
est,Dixon/Smart,1989
 1.38905011E+01 5.04274517E-03-2.01504138E-06 3.33703287E-10-1.85455570E-14    2
-6.89349055E+04-4.23902350E+01 1.66216798E+00 5.04259227E-02-7.06032551E-05    3
 4.96669771E-08-1.39443207E-11-6.60891537E+04 1.80212557E+01                   4

CHFCHCF3               0F   4C   3H   2     G   300.000  3000.000 1000.00     1
matsugi,2017/balaganesh,2012
 0.94812168E+01 0.20003084E-01-0.11232250E-04 0.29986969E-08-0.30926159E-12    2
-0.10389801E+06-0.19385037E+02 0.94199275E+00 0.48232398E-01-0.44684845E-04    3
 0.19372845E-07-0.29209028E-11-0.10189379E+06 0.23293679E+02                   4
CFCHCF3                0F   4C   3H   1     G   300.000  3000.000 1000.00     1
est/balaganesh,2012
 0.97942485E+01 0.16627541E-01-0.96960143E-05 0.26570454E-08-0.27915513E-12    2
-0.71851659E+05-0.19584352E+02 0.22137780E+01 0.41937544E-01-0.40143199E-04    3
 0.17943289E-07-0.28477463E-11-0.70084971E+05 0.18240006E+02                   4
CHFCCF3                0F   4C   3H   1     G   300.000  3000.000 1000.00     1
est/balaganesh,2012
 0.97242171E+01 0.16694442E-01-0.97176099E-05 0.26585199E-08-0.27889692E-12    2
-0.69892141E+05-0.19116208E+02 0.23285801E+01 0.40806304E-01-0.37679375E-04    3
 0.15829011E-07-0.22038484E-11-0.68139480E+05 0.17931137E+02                   4
CH2CFO                 H   2C   2O   1F   1g    300.00   5000.00 1000.00     1
Needham et.al,CNF,2017
 8.36520592E+00 7.20529018E-03-2.94164587E-06 5.42254381E-10-3.72494180E-14    2
-3.34931011E+04-1.79788801E+01 8.07509260E-01 3.06961531E-02-3.16571339E-05    3
 1.70422410E-08-3.77730061E-12-3.14927535E+04 2.05215635E+01                   4
```

Appendix B: Kinetic model, Chemkin format.

($AT^ne^{-E/RT}$, units: mole, K, cm, cal, s)

```
ELEMENTS
O  H  C  N  F AR
end
species
H2      H       O       O2      OH      H2O     HO2     H2O2
C       CH      CH2     CH2(S)  CH3     CH4     CO      CO2
HCO     CH2O    CH2OH   CH3O    CH3OH   C2H     C2H2    C2H3
C2H4    C2H5    C2H6    HCCO    CH2CO   HCCOH
AR      C3H7    C3H8    CH2CHO  CH3CHO  N2
CH3CO   C3H6    CH3CCH2
!*******************************
!*** Hydrogen/Oxygen/Fluorine ***
!*******************************
HF        F         F2
!************************
!*** C1 Fluorocarbons ***
!************************
CH3F      CH2F2     CHF3      CF4 CH2F      CHF2      CF3
                    CHF       CF2 CF
!*********************************
!*** Oxidized C1 Fluorocarbons ***
!*********************************
CF3O CF2O CHFO CFO
!*********************
!*** Fluoroethanes ***
!*********************
CH3-CH2F  CH3-CHF2  CH3-CF3
CH2F-CH2F CH2F-CHF2 CH2F-CF3
          CHF2-CHF2 CHF2-CF3
                    CF3-CF3
!*********************
!***  Fluoroethyls ***
!*********************
          CH3-CHF   CH3-CF2
CH2F-CH2  CH2F-CHF  CH2F-CF2
CHF2-CH2  CHF2-CHF  CHF2-CF2
CF3-CH2   CF3-CHF   CF3-CF2
!*********************
!***  Fluoroethenes ***
!*********************
CH2CHF    CH2CF2
CHFCHF[Z] CHFCF2
CF2CF2
!*********************
!***  Fluorovinyls ***
!*********************
          CH2CF
CHFCH[Z] CHFCF[Z]
CF2CH    CF2CF
!*********************
```

```
!***  Fluoroethynes ***
!*********************
C2HF      C2F2
!*********************
!*** Fluoroketenes ***
!*********************
CHFCO      CF2CO     CFCO
!*********************
!** FM-200 species **
!*********************
C3F7H C3F7 C3F6 C3F7O2
C3F7O C3F6O     C3F7OH
CF3COF CF3CO   CF3CHO
!***************************
!*** 2BTP ****
!***************************
CF3CHCH2 CF3CCH2
CF3CHCH  CF3CCH
CF3COCH3
!***************************
!*** HFO1234yf***************
!***************************
CH2CFCF3  CH-CFCF3  CFCCF3
!***************************
!*** HFO1234zee *************
!***************************
CHFCHCF3        !1234zee
CFCHCF3  CHFCCF3  CH2CFO
end

THERMO
END

REACTIONS
2O+M<=>O2+M                                1.200E+17   -1.000        .00
H2/ 2.40/ H2O/15.40/ CH4/ 2.00/ CO/ 1.75/ CO2/ 3.60/ C2H6/ 3.00/ AR/  .83/
 CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./
O+H+M<=>OH+M                               5.000E+17   -1.000        .00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./
O+H2<=>H+OH                                3.870E+04    2.700    6260.00
O+HO2<=>OH+O2                              2.000E+13     .000        .00
O+H2O2<=>OH+HO2                            9.630E+06    2.000    4000.00
O+CH<=>H+CO                                5.700E+13     .000        .00
O+CH2<=>H+HCO                              8.000E+13     .000        .00
O+CH2(S)<=>H2+CO                           1.500E+13     .000        .00
O+CH2(S)<=>H+HCO                           1.500E+13     .000        .00
O+CH3<=>H+CH2O                             5.060E+13     .000        .00
O+CH4<=>OH+CH3                             1.020E+09    1.500    8600.00
O+CO(+M)<=>CO2(+M)                         1.800E+10     .000    2385.00
   LOW/ 6.020E+14     .000    3000.00/
H2/2.00/ O2/6.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/3.50/ C2H6/3.00/ AR/ .50/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./
O+HCO<=>OH+CO                              3.000E+13     .000        .00
O+HCO<=>H+CO2                              3.000E+13     .000        .00
```

```
O+CH2O<=>OH+HCO                          3.900E+13     .000    3540.00
O+CH2OH<=>OH+CH2O                        1.000E+13     .000        .00
O+CH3O<=>OH+CH2O                         1.000E+13     .000        .00
O+CH3OH<=>OH+CH2OH                       3.880E+05    2.500    3100.00
O+CH3OH<=>OH+CH3O                        1.300E+05    2.500    5000.00
O+C2H<=>CH+CO                            5.000E+13     .000        .00
O+C2H2<=>H+HCCO                          1.350E+07    2.000    1900.00
O+C2H2<=>OH+C2H                          4.600E+19   -1.410   28950.00
O+C2H2<=>CO+CH2                          6.940E+06    2.000    1900.00
O+C2H3<=>H+CH2CO                         3.000E+13     .000        .00
O+C2H4<=>CH3+HCO                         1.250E+07    1.830     220.00
O+C2H5<=>CH3+CH2O                        2.240E+13     .000        .00
O+C2H6<=>OH+C2H5                         8.980E+07    1.920    5690.00
O+HCCO<=>H+2CO                           1.000E+14     .000        .00
O+CH2CO<=>OH+HCCO                        1.000E+13     .000    8000.00
O+CH2CO<=>CH2+CO2                        1.750E+12     .000    1350.00
O2+CO<=>O+CO2                            2.500E+12     .000   47800.00
O2+CH2O<=>HO2+HCO                        1.000E+14     .000   40000.00
H+O2+M<=>HO2+M                           2.800E+18    -.860        .00
O2/ .00/ H2O/ .00/ CO/ .75/ CO2/1.50/ C2H6/1.50/ N2/ .00/ AR/ .00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./  CH3-CHF2 /6./
H+2O2<=>HO2+O2                           2.080E+19   -1.240        .00
H+O2+H2O<=>HO2+H2O                       11.26E+18    -.760        .00
H+O2+N2<=>HO2+N2                         2.600E+19   -1.240        .00
H+O2+AR<=>HO2+AR                         7.000E+17    -.800        .00
H+O2<=>O+OH                              2.650E+16    -.6707  17041.00
2H+M<=>H2+M                              1.000E+18   -1.000        .00
H2/ .00/ H2O/ .00/ CH4/2.00/ CO2/ .00/ C2H6/3.00/ AR/ .63/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./
2H+H2<=>2H2                              9.000E+16    -.600        .00
2H+H2O<=>H2+H2O                          6.000E+19   -1.250        .00
2H+CO2<=>H2+CO2                          5.500E+20   -2.000        .00
H+OH+M<=>H2O+M                           2.200E+22   -2.000        .00
H2/ .73/ H2O/3.65/ CH4/2.00/ C2H6/3.00/ AR/ .38/
H+HO2<=>O+H2O                            3.970E+12     .000     671.00
H+HO2<=>O2+H2                            4.480E+13     .000    1068.00
H+HO2<=>2OH                              0.840E+14     .000     635.00
H+H2O2<=>HO2+H2                          1.210E+07    2.000    5200.00
H+H2O2<=>OH+H2O                          1.000E+13     .000    3600.00
H+CH<=>C+H2                              1.650E+14     .000        .00
H+CH2(+M)<=>CH3(+M)                      6.000E+14     .000        .00
     LOW  /  1.040E+26   -2.760   1600.00/
     TROE/   .5620  91.00  5836.00  8552.00/
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+CH2(S)<=>CH+H2                         3.000E+13     .000        .00
H+CH3(+M)<=>CH4(+M)                      13.90E+15    -.534     536.00
     LOW  /  2.620E+33   -4.760   2440.00/
     TROE/   .7830   74.00  2941.00  6964.00 /
H2/2.00/ H2O/6.00/ CH4/3.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+CH4<=>CH3+H2                           6.600E+08    1.620   10840.00
H+HCO(+M)<=>CH2O(+M)                     1.090E+12     .480    -260.00
     LOW  /  2.470E+24   -2.570    425.00/
     TROE/   .7824  271.00  2755.00  6570.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+HCO<=>H2+CO                            7.340E+13     .000        .00
```

```
H+CH2O(+M)<=>CH2OH(+M)                    5.400E+11     .454    3600.00
     LOW  /  1.270E+32   -4.820   6530.00/
     TROE/   .7187  103.00  1291.00  4160.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH2O(+M)<=>CH3O(+M)                     5.400E+11     .454    2600.00
     LOW  /  2.200E+30   -4.800   5560.00/
     TROE/   .7580   94.00  1555.00  4200.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH2O<=>HCO+H2                           5.740E+07    1.900    2742.00
H+CH2OH(+M)<=>CH3OH(+M)                   1.055E+12     .500      86.00
     LOW  /  4.360E+31   -4.650   5080.00/
     TROE/   .600  100.00  90000.0  10000.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH2OH<=>H2+CH2O                         2.000E+13     .000        .00
H+CH2OH<=>OH+CH3                          1.650E+11     .650    -284.00
H+CH2OH<=>CH2(S)+H2O                      3.280E+13    -.090     610.00
H+CH3O(+M)<=>CH3OH(+M)                    2.430E+12     .515      50.00
     LOW  /  4.660E+41   -7.440   14080.0/
     TROE/   .700  100.00  90000.0 10000.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH3O<=>H+CH2OH                          4.150E+07    1.630    1924.00
H+CH3O<=>H2+CH2O                          2.000E+13     .000        .00
H+CH3O<=>OH+CH3                           1.500E+12     .500    -110.00
H+CH3O<=>CH2(S)+H2O                       2.620E+14    -.230    1070.00
H+CH3OH<=>CH2OH+H2                        1.700E+07    2.100    4870.00
H+CH3OH<=>CH3O+H2                         4.200E+06    2.100    4870.00
H+C2H(+M)<=>C2H2(+M)                      1.000E+17   -1.000        .00
     LOW  /  3.750E+33   -4.800   1900.00/
     TROE/   .6464  132.00  1315.00  5566.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C2H2(+M)<=>C2H3(+M)                     5.600E+12     .000    2400.00
     LOW  /  3.800E+40   -7.270   7220.00/
     TROE/   .7507   98.50  1302.00  4167.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C2H3(+M)<=>C2H4(+M)                     6.080E+12     .270     280.00
     LOW  /  1.400E+30   -3.860   3320.00/
     TROE/   .7820  207.50  2663.00  6095.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C2H3<=>H2+C2H2                          3.000E+13     .000        .00
H+C2H4(+M)<=>C2H5(+M)                     0.540E+12     .454    1820.00
     LOW  /  0.600E+42   -7.620   6970.00/
     TROE/   .9753  210.00   984.00  4374.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C2H4<=>C2H3+H2                          1.325E+06    2.530   12240.00
H+C2H5(+M)<=>C2H6(+M)                     5.210E+17    -.990    1580.00
     LOW  /  1.990E+41   -7.080   6685.00/
     TROE/   .8422  125.00  2219.00  6882.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C2H5<=>H2+C2H4                          2.000E+12     .000        .00
H+C2H6<=>C2H5+H2                          1.150E+08    1.900    7530.00
H+HCCO<=>CH2(S)+CO                        1.000E+14     .000        .00
H+CH2CO<=>HCCO+H2                         5.000E+13     .000    8000.00
H+CH2CO<=>CH3+CO                          1.130E+13     .000    3428.00
H+HCCOH<=>H+CH2CO                         1.000E+13     .000        .00
H2+CO(+M)<=>CH2O(+M)                      4.300E+07    1.500   79600.00
```

```
     LOW  /  5.070E+27   -3.420  84350.00/
     TROE/   .9320  197.00  1540.00 10300.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
OH+H2<=>H+H2O                             2.160E+08    1.510    3430.00
2OH(+M)<=>H2O2(+M)                        7.400E+13    -.370        .00
     LOW  /  2.300E+18    -.900  -1700.00/
     TROE/   .7346   94.00  1756.00  5182.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./
2OH<=>O+H2O                               3.570E+04    2.400   -2110.00
OH+HO2<=>O2+H2O                           1.450E+13     .000    -500.00
 DUPLICATE
OH+H2O2<=>HO2+H2O                         2.000E+12     .000     427.00
 DUPLICATE
OH+H2O2<=>HO2+H2O                         1.700E+18     .000   29410.00
 DUPLICATE
OH+C<=>H+CO                               5.000E+13     .000        .00
OH+CH<=>H+HCO                             3.000E+13     .000        .00
OH+CH2<=>H+CH2O                           2.000E+13     .000        .00
OH+CH2<=>CH+H2O                           1.130E+07    2.000    3000.00
OH+CH2(S)<=>H+CH2O                        3.000E+13     .000        .00
OH+CH3(+M)<=>CH3OH(+M)                    2.790E+18   -1.430    1330.00
     LOW  /  4.000E+36   -5.920   3140.00/
     TROE/   .4120  195.0  5900.00  6394.00/
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
OH+CH3<=>CH2+H2O                          5.600E+07    1.600    5420.00
OH+CH3<=>CH2(S)+H2O                       6.440E+17   -1.340    1417.00
OH+CH4<=>CH3+H2O                          1.000E+08    1.600    3120.00
OH+CO<=>H+CO2                             4.760E+07    1.228      70.00
OH+HCO<=>H2O+CO                           5.000E+13     .000        .00
OH+CH2O<=>HCO+H2O                         3.430E+09    1.180    -447.00
OH+CH2OH<=>H2O+CH2O                       5.000E+12     .000        .00
OH+CH3O<=>H2O+CH2O                        5.000E+12     .000        .00
OH+CH3OH<=>CH2OH+H2O                      1.440E+06    2.000    -840.00
OH+CH3OH<=>CH3O+H2O                       6.300E+06    2.000    1500.00
OH+C2H<=>H+HCCO                           2.000E+13     .000        .00
OH+C2H2<=>H+CH2CO                         2.180E-04    4.500   -1000.00
OH+C2H2<=>H+HCCOH                         5.040E+05    2.300   13500.00
OH+C2H2<=>C2H+H2O                         3.370E+07    2.000   14000.00
OH+C2H2<=>CH3+CO                          4.830E-04    4.000   -2000.00
OH+C2H3<=>H2O+C2H2                        5.000E+12     .000        .00
OH+C2H4<=>C2H3+H2O                        3.600E+06    2.000    2500.00
OH+C2H6<=>C2H5+H2O                        3.540E+06    2.120     870.00
OH+CH2CO<=>HCCO+H2O                       7.500E+12     .000    2000.00
2HO2<=>O2+H2O2                            1.300E+11     .000   -1630.00
 DUPLICATE
2HO2<=>O2+H2O2                            4.200E+14     .000   12000.00
 DUPLICATE
HO2+CH2<=>OH+CH2O                         2.000E+13     .000        .00
HO2+CH3<=>O2+CH4                          1.000E+12     .000        .00
HO2+CH3<=>OH+CH3O                         3.780E+13     .000        .00
HO2+CO<=>OH+CO2                           1.500E+14     .000   23600.00
HO2+CH2O<=>HCO+H2O2                       5.600E+06    2.000   12000.00
C+O2<=>O+CO                               5.800E+13     .000     576.00
C+CH2<=>H+C2H                             5.000E+13     .000        .00
```

```
C+CH3<=>H+C2H2                          5.000E+13     .000        .00
CH+O2<=>O+HCO                           6.710E+13     .000        .00
CH+H2<=>H+CH2                           1.080E+14     .000    3110.00
CH+H2O<=>H+CH2O                         5.710E+12     .000    -755.00
CH+CH2<=>H+C2H2                         4.000E+13     .000        .00
CH+CH3<=>H+C2H3                         3.000E+13     .000        .00
CH+CH4<=>H+C2H4                         6.000E+13     .000        .00
CH+CO(+M)<=>HCCO(+M)                    5.000E+13     .000        .00
     LOW  /  2.690E+28   -3.740   1936.00/
     TROE/   .5757  237.00  1652.00  5069.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
CH+CO2<=>HCO+CO                         1.900E+14     .000   15792.00
CH+CH2O<=>H+CH2CO                       9.460E+13     .000    -515.00
CH+HCCO<=>CO+C2H2                       5.000E+13     .000        .00
CH2+O2=>OH+H+CO                         5.000E+12     .000    1500.00
CH2+H2<=>H+CH3                          5.000E+05    2.000    7230.00
2CH2<=>H2+C2H2                          1.600E+15     .000   11944.00
CH2+CH3<=>H+C2H4                        4.000E+13     .000        .00
CH2+CH4<=>2CH3                          2.460E+06    2.000    8270.00
CH2+CO(+M)<=>CH2CO(+M)                  8.100E+11     .500    4510.00
     LOW  /  2.690E+33   -5.110   7095.00/
     TROE/   .5907  275.00  1226.00  5185.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
CH2+HCCO<=>C2H3+CO                      3.000E+13     .000        .00
CH2(S)+N2<=>CH2+N2                      1.500E+13     .000     600.00
CH2(S)+AR<=>CH2+AR                      9.000E+12     .000     600.00
CH2(S)+O2<=>H+OH+CO                     2.800E+13     .000        .00
CH2(S)+O2<=>CO+H2O                      1.200E+13     .000        .00
CH2(S)+H2<=>CH3+H                       7.000E+13     .000        .00
CH2(S)+H2O(+M)<=>CH3OH(+M)              4.820E+17   -1.160    1145.00
     LOW  /  1.880E+38   -6.360   5040.00/
     TROE/   .6027  208.00  3922.00  10180.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH2(S)+H2O<=>CH2+H2O                    3.000E+13     .000        .00
CH2(S)+CH3<=>H+C2H4                     1.200E+13     .000    -570.00
CH2(S)+CH4<=>2CH3                       1.600E+13     .000    -570.00
CH2(S)+CO<=>CH2+CO                      9.000E+12     .000        .00
CH2(S)+CO2<=>CH2+CO2                    7.000E+12     .000        .00
CH2(S)+CO2<=>CO+CH2O                    1.400E+13     .000        .00
CH2(S)+C2H6<=>CH3+C2H5                  4.000E+13     .000    -550.00
CH3+O2<=>O+CH3O                         3.560E+13     .000   30480.00
CH3+O2<=>OH+CH2O                        2.310E+12     .000   20315.00
CH3+H2O2<=>HO2+CH4                      2.450E+04    2.470    5180.00
2CH3(+M)<=>C2H6(+M)                     6.770E+16   -1.180     654.00
     LOW  /  3.400E+41   -7.030   2762.00/
     TROE/   .6190  73.20  1180.00  9999.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
2CH3<=>H+C2H5                           6.840E+12     .100   10600.00
CH3+HCO<=>CH4+CO                        2.648E+13     .000        .00
CH3+CH2O<=>HCO+CH4                      3.320E+03    2.810    5860.00
CH3+CH3OH<=>CH2OH+CH4                   3.000E+07    1.500    9940.00
CH3+CH3OH<=>CH3O+CH4                    1.000E+07    1.500    9940.00
CH3+C2H4<=>C2H3+CH4                     2.270E+05    2.000    9200.00
CH3+C2H6<=>C2H5+CH4                     6.140E+06    1.740   10450.00
HCO+H2O<=>H+CO+H2O                      1.500E+18   -1.000   17000.00
```

```
HCO+M<=>H+CO+M                            1.870E+17   -1.000   17000.00
H2/2.00/ H2O/ .00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./
HCO+O2<=>HO2+CO                           13.45E+12     .000     400.00
CH2OH+O2<=>HO2+CH2O                       1.800E+13     .000     900.00
CH3O+O2<=>HO2+CH2O                        4.280E-13    7.600   -3530.00
C2H+O2<=>HCO+CO                           1.000E+13     .000    -755.00
C2H+H2<=>H+C2H2                           5.680E+10    0.900    1993.00
C2H3+O2<=>HCO+CH2O                        4.580E+16   -1.390    1015.00
C2H4(+M)<=>H2+C2H2(+M)                    8.000E+12     .440   86770.00
     LOW  /  1.580E+51   -9.300  97800.00/
     TROE/   .7345  180.00  1035.00  5417.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
C2H5+O2<=>HO2+C2H4                        8.400E+11     .000    3875.00
HCCO+O2<=>H+CO+CO2                        1.600E+12     .000     854.00
2HCCO<=>2CO+C2H2                          1.000E+13     .000        .00
O+CH3=>H+H2+CO                            3.370E+13     .000        .00
O+C2H4<=>H+CH2CHO                         6.700E+06    1.830     220.00
O+C2H5<=>H+CH3CHO                         1.096E+14     .000        .00
OH+HO2<=>O2+H2O                           0.500E+16     .000   17330.00
  DUPLICATE
OH+CH3=>H2+CH2O                           8.000E+09     .500   -1755.00
CH+H2(+M)<=>CH3(+M)                       1.970E+12     .430    -370.00
   LOW/ 4.820E+25  -2.80  590.0 /
   TROE/ .578  122.0  2535.0  9365.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
CH2+O2=>2H+CO2                            5.800E+12     .000    1500.00
CH2+O2<=>O+CH2O                           2.400E+12     .000    1500.00
CH2+CH2=>2H+C2H2                          2.000E+14     .000   10989.00
CH2(S)+H2O=>H2+CH2O                       6.820E+10     .250    -935.00
C2H3+O2<=>O+CH2CHO                        3.030E+11     .290      11.00
C2H3+O2<=>HO2+C2H2                        1.337E+06    1.610    -384.00
O+CH3CHO<=>OH+CH2CHO                      2.920E+12     .000    1808.00
O+CH3CHO=>OH+CH3+CO                       2.920E+12     .000    1808.00
O2+CH3CHO=>HO2+CH3+CO                     3.010E+13     .000   39150.00
H+CH3CHO<=>CH2CHO+H2                      2.050E+09    1.160    2405.00
H+CH3CHO=>CH3+H2+CO                       2.050E+09    1.160    2405.00
OH+CH3CHO=>CH3+H2O+CO                     2.343E+10    0.730   -1113.00
HO2+CH3CHO=>CH3+H2O2+CO                   3.010E+12     .000   11923.00
CH3+CH3CHO=>CH3+CH4+CO                    2.720E+06    1.770    5920.00
H+CH2CO(+M)<=>CH2CHO(+M)                  4.865E+11    0.422   -1755.00
    LOW/ 1.012E+42  -7.63  3854.0/
    TROE/ 0.465  201.0  1773.0  5333.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
O+CH2CHO=>H+CH2+CO2                       1.500E+14     .000       .00
O2+CH2CHO=>OH+CO+CH2O                     1.810E+10     .000       .00
O2+CH2CHO=>OH+2HCO                        2.350E+10     .000       .00
H+CH2CHO<=>CH3+HCO                        2.200E+13     .000       .00
H+CH2CHO<=>CH2CO+H2                       1.100E+13     .000       .00
OH+CH2CHO<=>H2O+CH2CO                     1.200E+13     .000       .00
OH+CH2CHO<=>HCO+CH2OH                     3.010E+13     .000       .00
CH3+C2H5(+M)<=>C3H8(+M)                    .9430E+13     .000       .00
     LOW/ 2.710E+74  -16.82  13065.0 /
     TROE/ .1527  291.0  2742.0  7748.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
```

```
O+C3H8<=>OH+C3H7                          1.930E+05    2.680   3716.00
H+C3H8<=>C3H7+H2                          1.320E+06    2.540   6756.00
OH+C3H8<=>C3H7+H2O                        3.160E+07    1.800    934.00
C3H7+H2O2<=>HO2+C3H8                      3.780E+02    2.720   1500.00
CH3+C3H8<=>C3H7+CH4                       0.903E+00    3.650   7154.00
CH3+C2H4(+M)<=>C3H7(+M)                   2.550E+06    1.600   5700.00
      LOW/ 3.00E+63  -14.6  18170./
      TROE/ .1894  277.0  8748.0  7891.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
O+C3H7<=>C2H5+CH2O                        9.640E+13     .000       .00
H+C3H7(+M)<=>C3H8(+M)                     3.613E+13     .000       .00
      LOW/ 4.420E+61  -13.545  11357.0/
      TROE/ .315  369.0  3285.0  6667.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C3H7<=>CH3+C2H5                         4.060E+06    2.190    890.00
OH+C3H7<=>C2H5+CH2OH                      2.410E+13     .000       .00
HO2+C3H7<=>O2+C3H8                        2.550E+10    0.255   -943.00
HO2+C3H7=>OH+C2H5+CH2O                    2.410E+13     .000       .00
CH3+C3H7<=>2C2H5                          1.927E+13   -0.320       .00
!*********************************************
!********** HYDROGEN/OXYGEN/FLUORINE **********
!*********************************************
!*********************************************
!*** HF, F, F2: Combination, decomposition ***
!*********************************************
H + F + M = HF + M                        1.70e21  -2.0        0.
H2/2.00/ H2O/9.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./
!*******************************
!*** HF, F, F2: Atom transfer ***
!*******************************
H2      + F    = H       + HF       2.56E12   0.50     650.
OH      + F    = O       + HF       5.00E13   0.00        0.
HO2     + F    = O2      + HF       2.89E12   0.50       0.
H2O     + F    = OH      + HF       1.30E09   1.50       0.
H2O2    + F    = HO2     + HF       1.73E12   0.50       0.
!************************************
!********** C1 FLUOROCARBONS **********
!************************************
!*********************************************
!*** FLUOROMETHANES: THERMAL DECOMPOSITIONS ***
!*********************************************
CH3F (+M) = CH2(S) + HF (+M)        1.00E14   0.0    85000.
LOW /1.50E16   0.0          67499./
H2/2.00/ H2O/9.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/
CHF      + H2  = CH3F               2.25E17  -2.85   13000.
CH2F     + H   = CH3F               3.03E21  -3.38    3460.
!*********************************************
CH2F2(+M)           = CHF        + HF(+M)         1.5E+15   0.00    81800.
   LOW  /   0.65E+18   0.00    62600./
   TROE/ 0.08  1E-30  1E+30            /
   H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
   HF/2.0/  CH2F2/2.0/  CH3-CHF2/2.0/  CH2F-CF3/2.0/ CF2O /5./ CF4 /6./
```

```
CF2      + H2  = CH2F2              1.70E06  -0.71   40900.
CHF2     + H   = CH2F2              2.75E06  -0.32    7690.
!*********************************************

CHF3  (+M)  = CF2    + HF(+M)    5.0E+15   0.00    74000.
                           LOW/ 1.23E+16   0.00    51700./
     H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/
     CH2F2 /2.00/ CHF3 /2.00/ HF /2.00/ CF2O /5./  CH2F-CF3 /2.0/

!*********************************************

CF4 (+ M) = CF3 + F (+ M)              6.31E16   0.0    128940.
     LOW /9.0E34  -4.64     122400./
H2/2.00/ H2O/9.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./

!*********************************************
!*** FLUOROMETHANES: ABSTRACTION TO METHYLS ***
!*********************************************

!*************************************
!*** Fluoromethanes: Reactions with H ***
!*************************************
CH3F    + H    = CH2F    + H2       6.51E07   1.96   10710.
CH2F2   + H    = CHF2    + H2       5.72E03   2.69   12340.
CHF3    + H    = CF3    +  H2       7.83E06   2.06   12300.
!*************************************
CH3F    + H    = CH3     + HF       1.73E08   1.77   31000.
CH3F    + H    = CH4     + F        2.83E08   1.61   38350.
CH2F2   + H    = CH2F    + HF       4.90E08   1.73   35370.
CHF3    + H    = CHF2    + HF       2.11E08   1.77   39800.
CHF3    + H    = CH2F2    + F       4.32E08   1.60   62990.
CF4     + H    = CF3     + HF       3.07e09    1.58   41330.
CF4     + H    = CHF3     + F       9.15e08    1.45   63590.
CH2F2   + H    = CH3F    +  F       4.87E00    1.61   51070.
!*************************************************
!*** Fluoromethanes: Reactions with O, OH, HO2 ***
!*************************************************
CH3F    + O    = CH2F    + OH       3.01E03   3.13    4890.
CH2F2   + O    = CHF2    + OH       1.20E03   3.17    5410.
CHF3    + O    = CF3     + OH       3.07E14   0.00    18950.

!*************************************************
CH3F    + OH   = CH2F    + H2O      2.60E08   1.50    2940
CH2F2   + OH   = CHF2    + H2O      2.64E02   3.27     950.
CHF3    + OH   = CF3     + H2O      1.25E07   1.55    3670.
!*************************************************

!*********************************************
!*** Fluoromethanes: Reactions with CH3, C2H3 ***
!*********************************************
CH3F    + CH3  = CH2F    + CH4      1.50E11   0.00   11400.
CH2F2   + CH3  = CHF2    + CH4      8.70E10   0.00   10200.
CF3     + CH4  = CHF3    + CH3      8.34E11   0.00   10920.
CF4 + CH3 = CH3F + CF3              9.64e04   2.41   26130.
```

```
!************************************************
CH3F    + C2H3 = CH2F    + C2H4     1.50E11   0.00   10300.
CH2F2   + C2H3 = CHF2    + C2H4     9.00E10   0.00    9200.
CF3     + C2H4 = CHF3    + C2H3     8.00E11   0.00   12000.

!****************************************************************************
!*** FLUOROMETHYLS ***********************************************************
!****************************************************************************
CF3 (+ M) = CF2 + F (+ M)              1.0e15      0.0     82370.
   LOW / 5.0e15  0.0  59660. /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./

!*** Fluoromethyls: Reactions with Fluoromethanes ***
!************************************************
CH3F    + CF3  = CH2F    + CHF3     5.75E11   0.00   11210.
CH2F2   + CH2F = CHF2    + CH3F     9.00E10   0.00   14000
CH2F2   + CF3  = CHF2    + CHF3     4.27E11   0.00   11300.
!************************************************
!*** Fluoromethyls: Reactions with CH3O, CH2O, HCO ***
!************************************************
CH3OH   + CH2F = CH3O    + CH3F     1.44E01   3.10    9800.
CH3OH   + CHF2 = CH3O    + CH2F2    1.44E01   3.10    9000
CH3OH   + CF3  = CH3O    + CHF3     1.44E01   3.10    5500
!************************************************
CH3OH   + CH2F = CH2OH   + CH3F     3.20E01   3.20   10000.
CH3OH   + CHF2 = CH2OH   + CH2F2    3.20E01   3.20    9300.
CH3OH   + CF3  = CH2OH   + CHF3     3.20E01   3.20    5700.
!************************************************
CH2O    + CH2F = HCO     + CH3F     5.54E03   2.81    8300.
CH2O    + CHF2 = HCO     + CH2F2    5.54E03   2.81    7800.
CH2O    + CF3  = HCO     + CHF3     5.54E03   2.81    4600.
!************************************************
HCO     + CH2F = CO      + CH3F     9.00E13   0.00       0.
HCO     + CHF2 = CO      + CH2F2    9.00E13   0.00       0.
HCO     + CF3  = CO      + CHF3     9.00E13   0.00       0.
!************************************************
HCO     + CH2F = CH2CO   + HF       3.00E13   0.00       0.
HCO     + CHF2 = CHFCO   + HF       3.00E13   0.00       0.
HCO     + CF3  = CF2CO   + HF       2.70E13   0.00       0.

!************************************************
!*** Fluoromethyls: Reactions with H2O2 ***
!************************************************
CH2F    + H2O2 = CH3F    + HO2      1.20E10   0.00    -600.
CHF2    + H2O2 = CH2F2   + HO2      1.20E10   0.00    -600.
CF3     + H2O2 = CHF3    + HO2      1.20E10   0.00    -600.
!************************************************
!*** Fluoromethyls + H
!************************************************
CH2F     + H <=> CH2(S) + HF        11.000E+13     0.0      0.0
CH2F     + H <=> CHF + H2           5.000E+13     .000      0.0
CHF2     + H   = CHF     + HF       1.49E14     -0.11       101.
CHF2     + H   = CF2     + H2       5.50E03      2.42      -420.
```

```
CF3      + H   = CF2     + HF       5.33E13  0.00        0.
!*********************************************

!*** Fluoromethyls + F *************************
CH3      + F   = CH2(S)  + HF       1.62E16  -0.88    -981.
CH3      + F   = CH2F    + H        1.36E12  -0.39    -265.
CH2F     + F   = CHF     + HF       5.00E13   0.00       0.
CHF2     + F   = CF2     + HF       3.00E13   0.00       0.

!*************************************************
!*** Fluoromethyls: Reaction with O2, O, OH, HO2 ***
!*************************************************

CH2F     + O2  => CHFO   + O + H    1.32E14   0.00   25000.
CH2F     + O2  = CHFO   + OH        10.3E11   0.0   8940.
CHF2     + O2  = CF2O   + OH        4.9E10    0.0     3490.
CF3      + O2   = CF3O    + O        3.4E09   1.14   21000.

!*************************************************
CH2F     + O    = CHFO   + H        5.70E13   0.00       0.
CHF2     + O    = CF2O   + H        3.70E13   0.00       0.
CF3      + O    = CF2O   + F        1.54E13   0.00       0.

!*************************************************
CH2F     + OH   = CH2O    + HF      2.50E13   0.00       0.
CHF2     + OH   = CHFO   + HF       1.00E13   0.00       0.
CF3      + OH   = CF2O   + HF       1.46E13  -0.06    -266.

!*************************************************
CH2F     + HO2  => CHFO  + OH + H   1.50E13   0.00       0.
CHF2     + HO2  => CF2O  + OH + H   1.50E13   0.00       0.
CF3      + HO2  = CF3O    + OH      1.00E13   0.00       0.
!*************************************************
CH2F     + HO2  = CH3F    + O2       3.00E12   0.00       0.
CHF2     + HO2  = CH2F2   + O2       3.00E12   0.00       0.
CF3      + HO2  = CHF3    + O2       2.00E12   0.00       0.

!************
!*** CF3O ***
!************
CF3O     + M    = CF2O + F          9.03E26  -3.42   21700.
CF3O     + H    = CF2O + HF         1.00E14   0.00       0.
CF3O     + H2   => CF2O+HF + H      1.00E13   0.00    5000.
CF3O     + H2O  => CF2O+HF + OH     5.13E07    1.40    6220.
CF3O     + CH4  => CF2O+HF + CH3    2.70E12   0.00    3200.
CF3O     + C2H6 => CF2O+HF + C2H5   6.81E12   0.00    1280.
CF3O     + C2H4 => CF2O+HF + C2H3   1.00E13   0.00    5000.
CF3O     + C2H2 => CF2O    + CH2CF 1.00E13   0.00    5000.
CF3O     + CH2O => CF2O+HF + HCO    5.00E12   0.00    5000.
CF3O     + HCO  => CF2O+HF + CO     5.00E12   0.00    2000.
CF3O     + F    = F2  + CF2O        6.e13     0.00    7000.
!*****************************************************************************
!*** FLUOROCARBENES: (CH2SING,) CHF, CF2 *************************************
!*****************************************************************************
```

```
!************************************************
!*** Fluorocarbenes: Reaction with O2, O, OH, H2O ***
!************************************************
CHF     + O2   = CHFO  + O              2.0E14    0.00    2100.
CF2        + O2    = CF2O  + O          2.7E13    0.00   26500.    !

!*********************************************
CHF     + O    = CO      + HF        9.00E13   0.00       0.
CF2     + O    = CFO     + F        5.0E12   0.00       0.
!*********************************************
CHF     + OH   = CHFO   + H         2.00E13   0.00       0.
CF2     + OH   = CF2O   + H         3.00E12   0.00    3500.
CHF     + OH   = HCO     + HF        4.00E12   0.00       0.
CF2     + OH   = CFO    + HF        1.00E13   0.00       0.
!*********************************************
CHF     + HO2  = CHFO   + OH        1.00E13   0.00       0.
CF2     + HO2  = CF2O   + OH        1.00E13   0.00    3500.
CHF     + HO2  = CH2F    + O2        2.00E12   0.00       0.
CF2     + HO2  = CHF2    + O2        5.00E11   0.00    4500.
!*********************************************
CHF     + H2O  = CH2O    + HF        5.00E12   0.00   6500.
CF2     + H2O  = CHFO   + HF        5.00E12   0.00  25000.

!************************************
!*** Fluorocarbenes ***
!************************************

CF2 (+ M) = CF + F (+ M)             5.3E14    0.0  118300.
   LOW / 2.29e15  0.0  95470. /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./

!************************************
!*** Fluorocarbenes: Reaction wih H ***
!************************************
CHF     + H    = CH     + HF        0.65E14   0.00       0.
CHF     + H    = CF     + H2        2.30E14   0.00       0.
CF2     + H    = CF     + HF        3.98E13   0.00    4540.

!************************************
!*** Fluorocarbenes: Reaction with RH ***
!************************************
CH2O    + CHF  = HCO     + CH2F     1.00E13   0.00  15000.
CH2O    + CHF  = CH2CO   + HF       1.00E13   0.00  15000.
!************************************
CH2O    + CF2  = HCO     + CHF2     1.00E13   0.00  41000.
CH2O    + CF2  = CHFCO   + HF       1.00E13   0.00  41000.
!************************************
HCO     + CHF  = CO      + CH2F     2.00E13   0.00  15000.
HCO     + CF2  = CO      + CHF2     2.00E13   0.00  41000.

!************************************
!*** Fluorocarbene misc. reactions ***
!************************************
CH2(S)  + HF  = CHF     + H2       2.08E07   1.27    8330.
```

```
CHF + HF = CF2 + H2                9.0e11      0.0        0.
!**********
!*** CF ***
!**********
CF      + O2   = CFO    + O        6.62E12   0.00   1690.
CF      + H2O  = CHFO   + H        2.00E13   0.00  17000.
CF      + H    = C       + HF       8.00E13   0.00   1160.
CF      + O    = CO + F             8.00E13   0.00   1410.
CF      + OH   = CO      + HF       8.00E13   0.00   1410.
CF      + HO2  =>CFO    + OH       3.00E13   0.00      0.
CF      + CH3  =>CH2CF  + H        3.00E13   0.00      0.
CF      + C2H3 =>C2HF    + CH2      3.00E13   0.00      0.
CF      + CH2  =>C2HF    + H        3.00E13   0.00      0.
CF    + CH2(S) => C2HF  + H        3.00E13   0.00      0.
CF      + CH4  =>CH2CHF + H        5.00E12   0.00  10000.
CF      + C2H4 =>C2H2    + CH2F     1.00E13   0.00      0.
CF      + CH2O =>CHF     + HCO      1.00E13   0.00   8000.
CF      + HCO  =>CHF     + CO       1.00E13   0.00      0.
CH      + HF   = CF      + H2       2.00E13   0.00      0.

!*********************************
!*** Oxidized C1 Fluorocarbons ***
!*********************************
CF3O + CO = CO2 + CF3               3.13e10   0.0        0.

!************************************
!*** CHFO & CF2O Decompositions ***
!************************************
CHFO   + M    = CO      + HF       2.48E25  -3.00   43000.
CFO    + F    = CF2O              1.00E12   0.00       0.

!************************************
!*** CHFO & CF2O: Reactions with H ***
!************************************
!CHFO   + H    = CFO    + H2       1.10E08   1.77    3000.
!************************************
CF2O    + H   = CFO    + HF       2.40E07   1.88   35900.
DUP
CF2O    + H   = CFO    + HF       1.20E10   0.83   22300.
DUP
CF2O    + H   = CFO    + HF       5.50E08   1.42   18900.
DUP
!*****************************************************
!*** CHFO & CF2O: Reactions with H2O, O, OH, HO2 ***
!*****************************************************
CF2O   + H2O  => CO2 + HF + HF     7.40E-3   3.84   25100.
CHFO   + O    = CFO    + OH       9.00E12   0.00    3080.
CHFO   + OH   = CFO    + H2O      2.83E13   0.00    6620.
CF2O   + OH   => CO2 + F + HF      2.70E03   2.38   21000.
CFO    + H2O2 = CHFO   + HO2      1.00E11   0.00    3900.

!*******************************************
!*** CHFO & CF2O: Reactions with Methyls ***
!*******************************************
CHFO   + CH3  = CFO    + CH4      2.00E12   0.00    9000.
```

```
CHFO   + CH2F = CFO    + CH3F     2.00E12   0.00    9000
CHFO   + CHF2 = CFO    + CH2F2    2.00E12   0.00    9000.
CHFO   + CF3  = CFO    + CHF3     2.00E12   0.00    9000.
CHFO   + C2H3 = CFO    + C2H4     2.00E12   0.00    5000.
!*********************
!*** CFO Reactions ***
!*********************
CO  + F + M    = CFO    + M        3.09E19  -1.40    -487.
H2/2.00/ H2O/18.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./

CFO    + H    = CO      + HF       2.50E13   0.00       0.
CFO    + O    = CO2     + F        3.00E13   0.00       0.
CFO    + OH   = CO2     + HF       3.00E13   0.00       0.
CFO    + HO2  => CO2    + F + OH   3.00E13   0.00       0.
CFO    + CH3  = CH2CO   + HF       2.70E13   0.00       0.
CFO    + CH2F = CHFCO   + HF       2.70E13   0.00       0.
CFO    + CFO = CO      + CF2O      2.23E13   0.00     318.
CFO    + CHF2 = CF2CO   + HF       2.70E13   0.00   20000.
CFO + CF2 = CF3 + CO               5.4e11    0.0        0.

!************************
!*** C2 FLUOROCARBONS ***
!************************

!*****************************************************
!*** Fluoroethanes: (C2H6,) CH3F, CH2F2, CHF3, CF4 ***
!*****************************************************

!*****************************************************
!*** Fluoroethane <A name=c2h6d>decompositions (HF elimination)</A> ***
!*****************************************************
CH3-CH2F (+M)    = C2H4 + HF (+M)    1.83E13    0.00   59900.
 LOW  /  0.87E+69   -14.94  75710.00/
     TROE/   .652  10.00  1496.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/

CH3-CHF2         = CH2CHF  + HF    7.9E13   0.00    63800.
CH3-CF3          = CH2CF2  + HF    1.00E14   0.00   68700.
CH2F-CH2F        = CH2CHF  + HF    2.50E13   0.00   62900.
CH2F-CHF2        = CHFCHF[Z]+HF    1.26E14   0.00   69100.
CH2F-CHF2        = CH2CF2  + HF    1.00E13   0.00   65400.
CH2F-CF3         = CHFCF2  + HF    5.70E11   0.00   62690.
CHF2-CHF2        = CHFCF2  + HF    2.00E13   0.00   69400.
CHF2-CF3         = CF2CF2  + HF    4.00E13   0.00   71600.

!*****************************************
!*** Ethyl + Hydrogen with HF elimination ***
!*****************************************
CH2F-CH2 + H    = C2H4     + HF     1.44E20  -2.12    1730.
CH3-CHF  + H    = C2H4     + HF     2.27E20  -2.21    1950.
CH2F-CHF + H    = CH2CHF  + HF     2.06E23  -3.23    2280.
!*****************************************
CHF2-CH2 + H    = CH2CHF  + HF     5.24E16  -0.933    880.
CH3-CF2  + H    = CH2CHF  + HF     2.09E16  -0.854    848.
```

```
CHF2-CHF + H    = CHFCHF[Z]+HF     1.86E20  -2.29    1750.
CHF2-CHF + H    = CH2CF2  + HF     9.95E19  -2.34    1780.
CH2F-CF2 + H    = CHFCHF[Z]+HF     6.32E19  -2.21    1630.
CH2F-CF2 + H    = CH2CF2  + HF     3.36E19  -2.26    1660.
CF3-CH2  + H    = CH2CF2  + HF     1.12E21  -2.27    2240.
CF3-CHF + H   = CHFCF2 + HF        6.56E24  -3.57    4225
CHF2-CF2 + H    = CHFCF2  + HF     1.81E22  -2.92    3070.
CF3-CF2  + H    = CF2CF2  + HF     1.41E21  -2.40    3630.

!****************************************
!*** Ethyl + Hydrogen with C-C breakage ***
!****************************************
CH2F-CH2 + H    = CH3      + CH2F   3.80E11   0.635    633.
CH3-CHF  + H    = CH3      + CH2F   3.47E10   0.90    1370.
CH2F-CHF + H    = CH2F     + CH2F   1.79E14  -0.105   1320.
!****************************************
CHF2-CH2 + H    = CH3      + CHF2   2.02E06   2.16     451.
CH3-CF2  + H    = CH3      + CHF2   1.62E05   2.50    1370.
CHF2-CHF + H    = CH2F     + CHF2   6.36E12   0.318   1460.
CH2F-CF2 + H    = CH2F     + CHF2   3.64E12   0.329   1180.
CF3-CH2  + H    = CH3      + CF3    2.48E11   0.816   2870.
CF3-CHF + H = CF3 + CH2F           4.28E16   -0.74    4750.
CHF2-CF2 + H    = CHF2     + CHF2   3.25E15  -0.524   3000.
CF3-CF2  + H    = CHF2     + CF3    4.37E16  -0.746   4360.

!*********************************************
!*** Ethyl + Hydrogen with stablized product ***
!*********************************************
CH2F-CH2 + H    = CH3-CH2F          1.19E35  -8.51    8140.
CH3-CHF  + H    = CH3-CH2F          9.57E38  -9.24    7360.
CH2F-CHF + H    = CH2F-CH2F         1.56E45 -10.80    8070.
CHF2-CH2 + H    = CH3-CHF2          2.96E37  -9.05    7160.
CH3-CF2  + H    = CH3-CHF2          3.11E40  -9.59    7190.
CHF2-CHF + H    = CH2F-CHF2         1.20E44 -10.60    7520.
CH2F-CF2 + H    = CH2F-CHF2         2.74E43 -10.50    7670.
CF3-CH2  + H    = CH3-CF3           7.27E42  -9.86    7360.
CHF2-CF2 + H    = CHF2-CHF2         3.77E46 -10.80    8980.
CF3-CF2  + H    = CHF2-CF3          1.12E47 -10.80    4100.

!*****************************************************
!*** Methyl + Methyl combination with HF elimination ***
!*****************************************************
CH3      + CH2F = C2H4     + HF     1.85E19  -1.86    1870.
CH2F     + CH2F = CH2CHF   + HF     7.56E21  -2.79    2590.
CH3      + CHF2 = CH2CHF   + HF     1.30E15  -0.586    634.
CH2F     + CHF2 = CHFCHF[Z]+HF      3.88E20  -2.35    2888.
CH2F     + CHF2 = CH2CF2   + HF     2.23E20  -2.41    2910.
CH3      + CF3  = CH2CF2   + HF     5.53E19  -1.94    2440.
CHF2     + CHF2 = CHFCF2   + HF     2.20E19  -1.95    4100.
CHF2     + CF3  = CF2CF2   + HF     7.00E16  -1.17    4330.
CH4     + CF2  = CH3-CHF2           1.5e11    0.0    39000.
!************************************************
!*** Methyl + Methyl with product stabilization ***
!************************************************
CH3      + CH2F = CH3-CH2F          1.57E31  -6.27    4440.
```

```
CH2F     + CH2F = CH2F-CH2F         2.37E24  -3.79    2290.
CH3      + CHF2 = CH3-CHF2          1.93E35  -7.69    5760.
CH2F     + CHF2 = CH2F-CHF2         9.61E38  -8.36    6940.
CH3      + CF3  = CH3-CF3           1.78E33  -6.64    5020.
CHF2     + CHF2 = CHF2-CHF2         2.26E24  -3.50    3360.
CHF2     + CF3  = CHF2-CF3          2.61E26  -4.16    4100.
CF3  + CF3 (+M) = CF3-CF3 (+M)      9.69e10   0.77       0.0 !
     LOW / 2.12e60  -12.51   5910. /
     TROE / 0.069  260. 880. /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/

!*********************************************
!*** Ethyl + Hydrogen with H atom disprop. ***
!*********************************************
CH2F-CH2 + H    = CH3-CHF  + H      1.87E01   3.10     137.
CHF2-CH2 + H    = CH3-CF2  + H      1.59E-3   4.35     157.
CH2F-CF2 + H    = CHF2-CHF + H      0.64E00   3.53    1830.
!*****************************************************
CF3-CF3 + H    = CF3-CF2 + HF       1.00E15   0.00   30000.
!***********************************************************
!*** Methane + Methylene combination with HF elimination ***
!***********************************************************
!*****************************************************
!*** Fluorocarbenes: Reaction with Fluoromethanes ***
!*****************************************************
CH3F +CH2(S)  = C2H4    + HF      3.00E13   0.00      0.
CH2F2+CH2(S)  = CH2CHF + HF       2.00E13   0.00      0.
CHF3 +CH2(S)  = CH2CF2 + HF       1.00E13   0.00      0.
CF4  +CH2(S)  = CHFCF2 + HF       4.00E13   0.00  31000.
!*****************************************************
CH4     + CHF  = C2H4    + HF      4.00E13   0.00  15000.
CH3F    + CHF  = CH2CHF + HF       3.00E13   0.00  15000.
CH2F2   + CHF  = CH2CF2 + HF       1.00E13   0.00  15000.
CH2F2   + CHF  = CHFCHF[Z]+HF      1.00E13   0.00  15000.
CHF3    + CHF  = CHFCF2 + HF       1.00E13   0.00  15000.
CF4     + CHF  = CF2CF2 + HF       4.00E13   0.00  31000.
!*****************************************************
CH4     + CF2  = CH2CHF + HF       4.00E13   0.00  41000.
CH3F    + CF2  = CH2CF2 + HF       1.50E13   0.00  41000.
CH3F    + CF2  = CHFCHF[Z]+HF      1.50E13   0.00  41000.
CH2F2   + CF2  = CHFCF2 + HF       2.00E13   0.00  41000.
CHF3    + CF2  = CF2CF2 + HF       1.00E13   0.00  41000.
CF4     + CF2  => CF3-CF3          4.00E13   0.00  51000.
!*****************************************************
CH3     + CH2F = CH4     + CHF     3.00E13   0.00   3400.
CH2F    + CH2F = CH3F    + CHF     3.00E13   0.00   4800.
CHF2    + CH2F = CH2F2   + CHF     1.00E13   0.00   4400.
CF3     + CH2F = CHF3    + CHF     3.00E13   0.00   4600.
!*****************************************************


CH2F    + CHF2 = CH3F    + CF2     3.00E13   0.00   2200.
CHF2    + CHF2 = CH2F2   + CF2     1.00E13   0.00   1600.

!*************************************************
```

```
!****************************************
!*** FLUOROETHANES: ABSTRACTION REACTIONS</A> ***
!****************************************

!************************************
!*** CH3-CH2F: Reactions with H,O,OH ***
!************************************
CH3-CH2F  + H    = CH2F-CH2 + H2    5.50E08   1.60    9100.
CH3-CH2F  + O    = CH2F-CH2 + OH    2.90E08   1.60    6100.
CH3-CH2F  + OH   = CH2F-CH2 + H2O   2.23E02   3.58    1040.
!************************************
CH3-CH2F  + H    = CH3-CHF  + H2    3.30E08   1.60    9100.
CH3-CH2F  + O    = CH3-CHF  + OH    1.60E08   1.60    6100.
CH3-CH2F  + OH   = CH3-CHF  + H2O   1.94E04   2.85     250.
!************************************
!*** CH3-CHF2: Reactions with H,O,OH ***
!************************************

CH3-CHF2  + H    = CH3-CF2  + H2    2.0E+4     2.67   6280.
CH3-CHF2  + H    = CHF2-CH2 + H2    0.747e5     2.66   9720.
CH3-CHF2  + O    = CH3-CF2  + OH    3.31E+03   2.97   5624.
CH3-CHF2  + O    = CHF2-CH2 + OH    7.83E+02   3.32   6936.
CH3-CHF2  + OH   = CHF2-CH2 + H2O   3.73E+03   2.81   1696.
CH3-CHF2  + OH   = CH3-CF2  + H2O   3.37E+05   2.11   1012.
CH3-CHF2  + F    = CH3-CF2  + HF    3.0E13   0.00    1700.
CH3-CHF2  + F    = CHF2-CH2 + HF    7.7E13   0.00    2700.
!************************************
!*** CH3-CF3: Reactions with H,O,OH ***
!************************************
CH3-CF3   + H    = CF3-CH2  + H2    4.00E10   1.10   12700.
CH3-CF3   + O    = CF3-CH2  + OH    2.00E10   1.10    9700.
CH3-CF3   + OH   = CF3-CH2  + H2O   4.08E09   1.10    4670.

!****************************************
!*** CH2F-CH2F: Reactions with H,O,OH ***
!****************************************
CH2F-CH2F + H    = CH2F-CHF + H2    6.00E08   1.70    9600.
CH2F-CH2F + O    = CH2F-CHF + OH    3.00E08   1.70    6600.
CH2F-CH2F + OH   = CH2F-CHF + H2O   6.16E07   1.70    1610.

!****************************************
!*** CH2F-CHF2: Reactions with H,O,OH ***
!****************************************
CH2F-CHF2 + H    = CHF2-CHF + H2    2.00E08   1.70    9800.
CH2F-CHF2 + O    = CHF2-CHF + OH    1.00E08   1.70    6800.
CH2F-CHF2 + OH   = CHF2-CHF + H2O   2.05E07   1.70    1800.
!****************************************
CH2F-CHF2 + H    = CH2F-CF2 + H2    1.00E08   1.70   11000.
CH2F-CHF2 + O    = CH2F-CF2 + OH    5.00E07   1.70    8000.
CH2F-CHF2 + OH   = CH2F-CF2 + H2O   1.06E07   1.70    3000.
!************************************
!*** CH2F-CF3: Reactions with H,O,OH ***
!************************************
CH2F-CF3  + H    = CF3-CHF  + H2    2.00E08   1.70   10500.
```

```
CH2F-CF3  + O    = CF3-CHF  + OH    1.4300E07   1.70    7500.
CH2F-CF3  + OH   = CF3-CHF  + H2O   2.10E07   1.70    2524.

!*************************************
!*** CHF2-CHF2: Reactions with H,O,OH ***
!*************************************
CHF2-CHF2 + H    = CHF2-CF2 + H2    1.60E07   1.70   10600.
CHF2-CHF2 + O    = CHF2-CF2 + OH    8.00E07   1.70    7600.
CHF2-CHF2 + OH   = CHF2-CF2 + H2O   1.60E07   1.70    2643.

!*************************************
!*** CHF2-CF3: Reactions with H,O,OH ***
!*************************************
CHF2-CF3  + H    = CF3-CF2  + H2    1.40E07   1.60   10200.
CHF2-CF3  + O    = CF3-CF2  + OH    7.00E07   1.60    12700.
CHF2-CF3  + OH   = CF3-CF2  + H2O   1.40E07   1.60    2246.

!*********************************************
!*** Abstraction from fluoroethanes: By HO2 ***
!*********************************************
CH3-CHF   + H2O2 = CH3-CH2F + HO2   9.00E09   0.00    1000.
CH3-CF2   + H2O2 = CH3-CHF2 + HO2   9.00E09   0.00    1000.
CH2F-CH2  + H2O2 = CH3-CH2F + HO2   9.00E09   0.00    1000.
CH2F-CHF  + H2O2 = CH2F-CH2F+ HO2   9.00E09   0.00    1000.
CH2F-CF2  + H2O2 = CH2F-CHF2+ HO2   9.00E09   0.00    1000.
CHF2-CH2  + H2O2 = CH3-CHF2 + HO2   9.00E09   0.00    1000.
CHF2-CHF  + H2O2 = CH2F-CHF2+ HO2   9.00E09   0.00    1000.
CHF2-CF2  + H2O2 = CHF2-CHF2+ HO2   9.00E09   0.00    1000.
CF3-CH2   + H2O2 = CH3-CF3  + HO2   9.00E09   0.00    1000.
CF3-CHF   + H2O2 = CH2F-CF3 + HO2   9.00E09   0.00    1000.
CF3-CF2   + H2O2 = CHF2-CF3 + HO2   9.00E09   0.00    1000.

!*************************************
!*** CH3-CH2F: Abstraction by CH3,C2H3 ***
!*************************************
CH3-CH2F  + CH3  = CH2F-CH2 + CH4   2.00E11   0.00   13400.
CH3-CH2F  + C2H3 = CH2F-CH2 + C2H4  2.00E11   0.00   10000.
!*************************************
CH3-CH2F  + CH3  = CH3-CHF  + CH4   1.50E11   0.00   10000.
CH3-CH2F  + C2H3 = CH3-CHF  + C2H4  1.50E11   0.00    7000.

!*************************************
!*** CH3-CHF2: Abstraction by CH3,C2H3 ***
!*************************************
CH3-CHF2  + CH3  = CHF2-CH2 + CH4   2.00E11   0.00   12000.
CH3-CHF2  + C2H3 = CHF2-CH2 + C2H4  2.00E11   0.00    9000.
!*************************************
CH3-CHF2  + CH3  = CH3-CF2  + CH4   8.00E10   0.00   10000.
CH3-CHF2  + C2H3 = CH3-CF2  + C2H4  8.00E10   0.00    7000.

!*************************************
!*** CH3-CF3: Abstraction by CH3,C2H3 ***
!*************************************
CH3-CF3   + CH3  = CF3-CH2  + CH4   2.00E11   0.00   12000.
CH3-CF3   + C2H3 = CF3-CH2  + C2H4  2.00E11   0.00    9000.
```

```
!****************************************
!*** CH2F-CH2F: Abstraction by CH3,C2H3 ***
!****************************************
CH2F-CH2F + CH3  = CH2F-CHF + CH4   3.00E11   0.00   10400.
CH2F-CH2F + C2H3 = CH2F-CHF + C2H4  3.00E11   0.00    7000.

!****************************************
!*** CH2F-CHF2: Abstraction by CH3,C2H3 ***
!****************************************
CH2F-CHF2 + CH3  = CHF2-CHF + CH4   2.00E11   0.00   10000.
CH2F-CHF2 + C2H3 = CHF2-CHF + C2H4  2.00E11   0.00    7000.
!****************************************
CH2F-CHF2 + CH3  = CH2F-CF2 + CH4   1.00E11   0.00    9600.
CH2F-CHF2 + C2H3 = CH2F-CF2 + C2H4  1.00E11   0.00    7000.

!****************************************
!*** CH2F-CF3: Abstraction by CH3,C2H3 ***
!****************************************
CH2F-CF3  + CH3  = CF3-CHF  + CH4   2.00E11   0.00   10000.
CH2F-CF3  + C2H3 = CF3-CHF  + C2H4  2.00E11   0.00    7000.

!****************************************
!*** CHF2-CHF2: Abstraction by CH3,C2H3 ***
!****************************************
CHF2-CHF2 + CH3  = CHF2-CF2 + CH4   3.00E11   0.00   10000.
CHF2-CHF2 + C2H3 = CHF2-CF2 + C2H4  3.00E11   0.00    7000.

!****************************************
!*** CH2F-CF3: Abstraction by CH3,C2H3 ***
!****************************************
CHF2-CF3  + CH3  = CF3-CF2  + CH4   5.70E10   0.00    9500.
CHF2-CF3  + C2H3 = CF3-CF2  + C2H4  6.00E10   0.00    7000.

!****************************************
!*** CH2F-CF3: Abstraction by CH3CH2 etc.
!****************************************
CHF2-CF3  + C2H5       = CF3-CF2 + C2H6    5.7E10 0.0 11800.
CHF2-CF3  + C3H7      = CF3-CF2 + C3H8     5.7E10 0.0 10300.
DUPLICATE
CHF2-CF3  + C3H7      = CF3-CF2 + C3H8     5.7E10 0.0 13500.
DUPLICATE

!*****************************************************
!*** Fluoroethanes: CH2SING insertion & CH3 elimination ***
!*****************************************************
!*********************************************
!*** Abstraction from fluoroethanes: By CH2F ***
!*********************************************
CH3-CH2F  + CH2F = CH2F-CH2 + CH3F  2.00E11   0.00   13000.
CH3-CH2F  + CH2F = CH3-CHF  + CH3F  1.50E11   0.00   10000.
CH3-CHF2  + CH2F = CHF2-CH2 + CH3F  2.00E11   0.00   12000.
CH3-CHF2  + CH2F = CH3-CF2  + CH3F  8.00E10   0.00   10000.
CH3-CF3   + CH2F = CF3-CH2  + CH3F  2.00E11   0.00   12000.
CH2F-CH2F + CH2F = CH2F-CHF + CH3F  3.00E11   0.00   10000.
```

```
CH2F-CHF2 + CH2F = CHF2-CHF + CH3F  2.00E11   0.00   10000.
CH2F-CHF2 + CH2F = CH2F-CF2 + CH3F  1.00E11   0.00   10000.
CH2F-CF3  + CH2F = CF3-CHF  + CH3F  2.00E11   0.00   10000.
CHF2-CHF2 + CH2F = CHF2-CF2 + CH3F  3.00E11   0.00   11000.
CHF2-CF3  + CH2F = CF3-CF2  + CH3F  2.00E11   0.00   10000.

!*********************************************
!*** Abstraction from fluoroethanes: By CHF2 ***
!*********************************************
CH3-CH2F  + CHF2 = CH2F-CH2 + CH2F2 2.00E11   0.00   13000.
CH3-CH2F  + CHF2 = CH3-CHF  + CH2F2 1.50E11   0.00   10000.
CH3-CHF2  + CHF2 = CHF2-CH2 + CH2F2 2.00E11   0.00   12000.
CH3-CHF2  + CHF2 = CH3-CF2  + CH2F2 8.00E10   0.00   10000.
CH3-CF3   + CHF2 = CF3-CH2  + CH2F2 2.00E11   0.00   12000.
CH2F-CH2F + CHF2 = CH2F-CHF + CH2F2 3.00E11   0.00   10000.
CH2F-CHF2 + CHF2 = CHF2-CHF + CH2F2 2.00E11   0.00   10000.
CH2F-CHF2 + CHF2 = CH2F-CF2 + CH2F2 1.00E11   0.00   10000.
CH2F-CF3  + CHF2 = CF3-CHF  + CH2F2 2.00E11   0.00   10000.
CHF2-CHF2 + CHF2 = CHF2-CF2 + CH2F2 3.00E11   0.00   10000.
CHF2-CF3  + CHF2 = CF3-CF2  + CH2F2 2.00E11   0.00   10000.

!*********************************************
!*** Abstraction from fluoroethanes: By CF3 ***
!*********************************************
CH3-CH2F  + CF3  = CH2F-CH2 + CHF3  9.50E11   0.00    8200.
CH3-CH2F  + CF3  = CH3-CHF  + CHF3  9.50E11   0.00    8200.
CH3-CHF2  + CF3  = CHF2-CH2 + CHF3  3.10E10   0.00    7100.
CH3-CHF2  + CF3  = CH3-CF2  + CHF3  3.10E10   0.00    7100.
CH3-CF3   + CF3  = CF3-CH2  + CHF3  1.45E12   0.00   13500.
CH2F-CH2F + CF3  = CH2F-CHF + CHF3  5.00E11   0.00    7600.
CH2F-CHF2 + CF3  = CHF2-CHF + CHF3  3.00E11   0.00    7200.
CH2F-CHF2 + CF3  = CH2F-CF2 + CHF3  2.00E11   0.00    8000.
CH2F-CF3  + CF3  = CF3-CHF  + CHF3  6.00E10   0.00    6400.
CHF2-CHF2 + CF3  = CHF2-CF2 + CHF3  5.70E11   0.00   11900.
CHF2-CF3  + CF3  = CF3-CF2  + CHF3  1.40E11   0.00   10100.
CF3-CF3   + CF3  = CF4 + CF3-CF2    7.1e11     0.0    12300.

!*********************************************************
!*** Fluoroethyl decompositions (see H + fluoroethene) ***
!*********************************************************

CF3-CHF (+M)=CHFCF2 + F (+M)                        4.5E13   0.0    70000.0
LOW /5.5E19   0.0  70000.0/
H2O/9.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./
CF3-CF2 = CF2 + CF3                                 4.27e14  0.0     56240.

!************************************
!*** Fluoroethyl associations: + O2 ***
!************************************
CH3-CHF   + O2   = CH2CHF  + HO2   2.56E18  -2.77    1977.
CH3-CF2   + O2   = CH2CF2  + HO2   1.23E17  -1.87    1400.
!************************************

CH2F-CH2  + O2   = CH2CHF  + HO2   2.56E18  -2.77    1977.
```

```
CH2F-CHF  + O2   = CHFCHF[Z]+HO2   2.56E19  -2.77    1977.
CH2F-CF2  + O2   = CHFCF2  + HO2   2.56E19  -2.77    1977.
!************************************

CHF2-CH2  + O2   = CH2CF2  + HO2       1.23E17  -1.87    1400.
CHF2-CHF  + O2   = CHFCF2  + HO2       2.56E19  -2.77    1977.
CHF2-CF2  + O2   = CF2CF2  + HO2       2.56E19  -2.77    1977.
!************************************
CF3-CH2   + O2   => CF3 + CH2O + O   1.30E13    0.00    44000.
CF3-CHF   + O2   => CHFO + CF3+O     1.55E11    0.00    23000.
CF3-CF2   + O2   => CF3 + CF2O+ O    1.30E13    0.00    23000.
CF3-CHF  + O2  = CF2CF2 + HO2         5.5E8     0.00    -7800.

!************************************
!*** Fluoroethyl associations: + O ***
!************************************
!************************************
CH2F-CH2  + O    = CH2CO+HF + H     6.60E13   0.         0.
CHF2-CH2  + O    = CHFCO+HF + H     6.60E13   0.         0.
CF3-CH2   + O    = CF2CO+HF + H     6.60E13   0.         0.

!************************************
CH3-CHF   + O    = CH2CO+HF + H     4.40E13   0.         0.
CH2F-CHF  + O    = CHFCO+HF + H     4.40E13   0.         0.
!CHF2-CHF  + O    = CF2CO+HF + H     4.40E13   0.         0.
CF3-CHF   + O    = CF3 + CHFO       4.40E13   0.         0.

!************************************
CH3-CF2   + O    = CH2CO+HF + F     2.20E13   0.         0.
CH2F-CF2  + O    = CHFCO+HF + F     2.20E13   0.         0.
CHF2-CF2  + O    = CF2CO+HF + F     2.20E13   0.         0.
CF3-CF2   + O    =>CF3+CFO + F     2.20E13   0.         0.
!************************************
CH2F-CH2  + O    = CH2O     + CH2F  3.30E13   0.         0.
CHF2-CH2  + O    = CH2O     + CHF2  3.30E13   0.         0.
CF3-CH2   + O    = CH2O     + CF3   3.30E13   0.         0.
!************************************
CH3-CHF   + O    = CHFO    + CH3   2.20E13   0.         0.
CH2F-CHF  + O    = CHFO    + CH2F  2.20E13   0.         0.
CHF2-CHF  + O    = CHFO    + CHF2  2.20E13   0.         0.

!************************************
CH3-CF2   + O    = CF2O    + CH3   1.10E13   0.         0.
CH2F-CF2  + O    = CF2O    + CH2F  1.10E13   0.         0.
CHF2-CF2  + O    = CF2O    + CHF2  1.10E13   0.         0.
CF3-CF2   + O    = CF2O    + CF3   1.10E13   0.         0.

!************************************
!*** Fluoroethyl associations: + OH ***
!************************************
CH2F-CH2  + OH   =>CH2CO+HF + H2    6.60E13   0.         0.
CHF2-CH2  + OH   =>CHFCO+HF + H2    6.60E13   0.         0.
CF3-CH2   + OH   =>CF2CO+HF + H2    6.60E13   0.         0.
!************************************
CH3-CHF   + OH   =>CH2CO+H2 + HF    4.40E13   0.         0.
```

```
CH2F-CHF  + OH   =>CH2CO+HF + HF    4.40E13   0.         0.
CHF2-CHF  + OH   =>CHFCO+HF + HF    4.40E13   0.         0.
CF3-CHF   + OH   = CF3CHO + HF      4.40E13   0.         0.

!************************************

CH3-CF2   + OH   =>CH2CO+HF + HF    1.0E12   0.         10000.
CH3-CF2   + OH   =>CH3 + CFO +HF    1.0E12   0.         10000.
CH2F-CF2  + OH   =>CHFCO+HF + HF    2.20E13   0.         0.
CHF2-CF2  + OH   =>CF2CO+HF + HF    2.20E13   0.         0.
CF3-CF2   + OH   =>CF3+CFO + HF     2.20E13   0.         0.
!************************************
CH2F-CH2  + OH   = CH2CHF  + H2O   6.60E13   0.      3000.
CHF2-CH2  + OH   = CH2CF2  + H2O   4.40E13   0.      3000.
!************************************
CH3-CHF   + OH   = CH2CHF  + H2O   6.60E13   0.      3000.
CH2F-CHF  + OH   = CHFCHF[Z]+H2O   4.40E13   0.      3000.
CHF2-CHF  + OH   = CHFCF2  + H2O   2.20E13   0.      3000.
!************************************
CH3-CF2   + OH   = CH2CF2  + H2O   6.60E13   0.      3000.
CH2F-CF2  + OH   = CHFCF2  + H2O   4.40E13   0.      3000.
CHF2-CF2  + OH   = CF2CF2  + H2O   2.20E13   0.      3000.

!************************************
!*** Disproportionation with CH3 *****
!************************************
CH2F-CH2  + CH3  = CH2CHF  + CH4   1.30E13  -0.5        0.
CHF2-CH2  + CH3  = CH2CF2  + CH4   6.50E12  -0.5        0.
!************************************
CH3-CHF   + CH3  = CH2CHF  + CH4   1.95E13  -0.5        0.
CH2F-CHF  + CH3  = CHFCHF[Z]+CH4   1.30E13  -0.5        0.
CHF2-CHF  + CH3  = CHFCF2  + CH4   6.50E12  -0.5        0.
!************************************
CH3-CF2   + CH3  = CH2CF2  + CH4   1.95E13  -0.5        0.
CH2F-CF2  + CH3  = CHFCF2  + CH4   1.30E13  -0.5        0.
CHF2-CF2  + CH3  = CF2CF2  + CH4   6.50E12  -0.5        0.

!************************************
!*** Fluoroethyls reaction with HO2 ***
!************************************
CH3-CHF   + HO2  =>CH3+CHFO+ OH   3.00E13    0.         0.
CH3-CF2   + HO2  =>CH3+CF2O+ OH   3.00E13    0.         0.
CH2F-CH2  + HO2  =>CH2F+CH2O+ OH   3.00E13    0.         0.
CH2F-CHF  + HO2  =>CH2F+CHFO+OH   3.00E13    0.         0.
CH2F-CF2  + HO2  =>CH2F+CF2O+OH   3.00E13    0.         0.
CHF2-CH2  + HO2  =>CHF2+CH2O+ OH   3.00E13    0.         0.
CHF2-CHF  + HO2  =>CHF2+CHFO+OH   3.00E13    0.         0.
CHF2-CF2  + HO2  =>CHF2+CF2O+OH   3.00E13    0.         0.
CF3-CH2   + HO2  =>CF3 +CH2O+ OH   3.00E13    0.         0.
CF3-CHF   + HO2  =>CF3 +CHFO+OH   3.00E13    0.         0.
CF3-CF2   + HO2  =>CF3 +CF2O+OH   3.00E13    0.         0.
!************************************************************
CH3-CHF   + HO2  = CH2CHF  + H2O2 3.00E11    0.         0.
CH3-CF2   + HO2  = CH2CF2  + H2O2 3.00E11    0.         0.
CH2F-CH2  + HO2  = CH2CHF  + H2O2 2.00E11    0.         0.
```

```
CH2F-CHF  + HO2  = CHFCHF[Z]+H2O2 4.00E11    0.         0.
CH2F-CF2  + HO2  = CHFCF2  + H2O2 2.00E11    0.         0.
CHF2-CH2  + HO2  = CH2CF2  + H2O2 1.00E11    0.         0.
CHF2-CHF  + HO2  = CHFCF2  + H2O2 1.00E11    0.         0.
CHF2-CF2  + HO2  = CF2CF2  + H2O2 1.00E11    0.         0.
!*********************************************************
CH3-CHF   + HO2  = CH3-CH2F + O2   3.00E11    0.         0.
CH3-CF2   + HO2  = CH3-CHF2 + O2   3.00E11    0.         0.
CH2F-CH2  + HO2  = CH3-CH2F + O2   3.00E11    0.         0.
CH2F-CHF  + HO2  = CH2F-CH2F+ O2   3.00E11    0.         0.
CH2F-CF2  + HO2  = CH2F-CHF2+ O2   3.00E11    0.         0.
CHF2-CH2  + HO2  = CH3-CHF2 + O2   3.00E11    0.         0.
CHF2-CHF  + HO2  = CH2F-CHF2+ O2   3.00E11    0.         0.
CHF2-CF2  + HO2  = CHF2-CHF2+ O2   3.00E11    0.         0.
CF3-CH2   + HO2  = CH3-CF3  + O2   3.00E11    0.         0.
CF3-CHF   + HO2  = CH2F-CF3 + O2   3.00E11    0.         0.
CF3-CF2   + HO2  = CHF2-CF3 + O2   3.00E11    0.         0.
!************
CH3-CHF   + CH2O = CH3-CH2F + HCO  5.50E03    2.80    5900.
CH3-CF2   + CH2O = CH3-CHF2 + HCO  5.50E03    2.80    5900.
CH2F-CH2  + CH2O = CH3-CH2F + HCO  5.50E03    2.80    5900.
CH2F-CHF  + CH2O = CH2F-CH2F+ HCO  5.50E03    2.80    5900.
CH2F-CF2  + CH2O = CH2F-CHF2+ HCO  5.50E03    2.80    5900.
CHF2-CH2  + CH2O = CH3-CHF2 + HCO  5.50E03    2.80    5900.
CHF2-CHF  + CH2O = CH2F-CHF2+ HCO  5.50E03    2.80    5900.
CHF2-CF2  + CH2O = CHF2-CHF2+ HCO  5.50E03    2.80    5900.
CF3-CH2   + CH2O = CH3-CF3  + HCO  5.50E03    2.80    5900
CF3-CHF   + CH2O = CH2F-CF3 + HCO  5.50E03    2.80    5900.
CF3-CF2   + CH2O = CHF2-CF3 + HCO  5.50E03    2.80    5900.

!***********************
!*** FLUOROETHYLENES ***
!***********************

!************************************
!*** Fluoroethylenes: Isomerization ***
!************************************

!*******************************************
!*** Fluoroethylenes: HF elimination (kINF) ***
!*******************************************
CH2CHF        = C2H2    + HF     2.31e14   0.00    71300.          !
CH2CF2(+M)           = C2HF        + HF(+M)         5.19E14   0.00    86400.
   LOW  /   1.48E39   -12.85    87150./
   TROE/ 0.917  1192.  39.  6181. /
H2/2.00/ H2O/6.00/
CO/1.50/ CO2/2.00/
HF/2.0/  CH2F2/2.0/  CH3-CHF2/2.0/  CH2F-CF3/2.0/

CHFCHF[Z] (+M)  = C2HF    + HF  (+M)  2.50E14   0.00 78000.
LOW   /   9.00E15   1.00   78000./
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./

CHFCF2  (+M)   = C2F2    + HF   (+M)  2.0E14   0.00   80000.
```

```
LOW  /  1.50E15  1.00  80000./
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./

CF2CF2  ( + M)    = CF2 + CF2 (+ M)    5.01e14   0.0    68070.
     LOW/3.96E50  -9.06   85300./
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./

!************************************
!*** Fluoroethylenes: Decomposition ***
!************************************
CH2(S)   + CHF  = C2H2      + HF  17.02E19  -2.12    2380.
CH2(S)   + CF2  = C2HF      + HF  17.02E19  -2.12    2380.
CHF      + CHF  = C2HF      + HF   2.70E+13   .00   -5000.
CHF       + CF2  = C2F2      + HF   8.51E19 -2.12    2380.
!************************************
CH2(S)   + CHF  = CH2CHF          3.10E24  -3.80    2830.
CH2(S)   + CF2  = CH2CF2          3.10E24  -3.80    2830.
CHF       + CHF  = CHFCHF[Z]       3.10E24  -3.80    2830
CHF       + CF2  = CHFCF2          3.10E24  -3.80    2830.
!************************************
CH2(S)   + CHF  = CH2CF    + H    1.64E07   1.56    5740.
CH2(S)   + CHF  = CHFCH[Z] + H    1.64E07   1.56    5740.
CH2(S)   + CF2  = CF2CH    + H    3.28E07   1.56    5740.
CHF       + CHF  = CHFCF[Z] + H    1.64E07   1.56    5740.
CHF       + CF2  = CF2CF    + H    1.64E07   1.56    5740.
!************************************
CH2CF    + H    = C2H2      + HF   5.98E20  -2.31    1940.
CHFCH[Z] + H    = C2H2      + HF   5.98E20  -2.31    1940.
CF2CH    + H    = C2HF      + HF   2.0E20  -2.31    1940.
CHFCF[Z] + H    = C2HF      + HF   5.98E20  -2.31    1940.
CF2CF    + H    = C2F2      + HF   5.98E20  -2.31    1940.
!************************************
CH2CF    + H    = CH2CHF          2.40E34  -7.11    5040.
CHFCH[Z] + H    = CH2CHF          2.40E34  -7.11    5040.
CF2CH    + H    = CH2CF2          2.40E34  -7.11    5040.
CHFCF[Z] + H    = CHFCHF[Z]       2.40E34  -7.11    5040.
CF2CF    + H    = CHFCF2          2.40E34  -7.11    5040.
!************************************

!*************************************************
!*** Fluoroethylene + H: Association/Stabilization ***
!*************************************************
CH2CHF   + H(+M)= CH2F-CH2  (+M)   4.20E08   1.5      990.
     LOW/3.19E27   -2.8     -54./
     H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/
CH2CHF   + H(+M)= CH3-CHF   (+M)   4.20E08   1.5      990.
     LOW/3.19E27   -2.8     -54./
     H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/
CH2CF2   + H(+M)= CHF2-CH2  (+M)   4.20E08   1.5      990.
     LOW/3.19E27   -2.8     -54./
     H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/
CH2CF2   + H(+M)= CH3-CF2   (+M)   4.20E08   1.5      990.
     LOW/3.19E27   -2.8     -54./
```

```
     H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/

CHFCHF[Z]+ H(+M)= CH2F-CHF  (+M)   8.40E08   1.5      990.
     LOW/6.37E27   -2.8     -54./
     H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/
CHFCF2   + H(+M)= CHF2-CHF  (+M)   4.20E08   1.5      990.
     LOW/3.19E27   -2.8     -54./
     H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/
CHFCF2   + H(+M)= CH2F-CF2  (+M)   4.20E08   1.5      990.
     LOW/3.19E27   -2.8     -54./
     H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/
CF2CF2   + H(+M)= CHF2-CF2  (+M)   8.40E08   1.5      990.
     LOW/6.37E27   -2.8     -54./
     H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/

!************************************************************
!*** Fluoroethylene + H: Association with HF-Elimination ***
!************************************************************

!****************************************
!*** Fluoroethylenes + H: H-Abstraction ***
!****************************************
CH2CHF   + H    = CHFCH[Z]+ H2    0.33E06  2.53    14300.
CH2CHF   + H    = CH2CF   + H2    0.33E06  2.53    14300.
CH2CF2   + H    = CF2CH   + H2    0.67E06  2.53    14300.
CHFCHF[Z]+ H    = CHFCF[Z]+ H2    0.33E06  2.53    14300.
CHFCF2   + H    = CF2CF   + H2    0.33E06  2.53    12241.

!****************************************
!*** Fluoroethylenes + F: H-Elimination ***
!****************************************
C2H4      + F    = CH2CHF  + H     2.00E13  0.00        0.
CH2CHF    + F    = CH2CF2  + H     2.00E12  0.00        0.
CH2CHF    + F    = CHFCHF[Z]+H     5.00E12  0.00        0.
CHFCHF[Z] + F    = CHFCF2  + H     4.00E12  0.00        0.
CH2CF2 + F = CHFCF2 + H            1.0E13   0.0         0.

!CHFCF2    + F    = CF2CF2  + H     2.00E12  0.00        0
!CHFCF2    + F    = CF2CF2  + H     3.00E12  0.00        0.
!CHFCF2    + F    = CF2CF2  + H     5.00E12  0.00        0
!CHFCF2    + F    = CF2CF2  + H     8.1500E12  0.00        0.
!CHFCF2    + F    = CF2CF2  + H     1.200E13  0.00        0.
!CHFCF2    + F    = CF2CF2  + H     1.200E13  0.00        0.
CHFCF2    + F    = CF2CF2  + H     5.00E12   0.00        0.
CH2CHF    + F    = CH2CF  + HF     5.700E13  0.00     3000.
CH2CHF    + F    = CHFCH[Z]  + HF  7.00E13   0.00     4000.
CH2CF2    + F    = CF2CH  + HF     7.00E13   0.00     5000
!****************************************
CF2CF2 + F = CF3-CF2                3.15e13  0.0      7770.

!*****************************************************
!*** Fluoroethylene + O: Isomerization/decomposition ***
!*****************************************************
CH2CHF   + O    = CH2F     + HCO   1.750E09  1.00     1310.  !
CHFCHF[Z]+ O    = CH2F     + CFO  7.00E09  1.00     1590.
```

```
CH2CF2   + O    = CHF2     + HCO  0.550E09  1.00     3700.
CH2CF2   + O    = CF2O + CH2      1.10E12  0.00     7400.
CHFCF2   + O    = CHF2     + CFO  6.00E09  1.00     1150.
CHFCF2  +  O    = CF2 + CHFO      0.48E07 2.00        0.
CHFCF2  + O     = CHF + CF2O      0.48E07 2.00      2000.
CF2CF2   + O    = CF2      + CF2O 1.01E08  1.48        0.
!****************************************************
CH2CHF   + O    = CH3      + CFO  1.33E09  1.00     2300.
CH2CHF     + O  = CH2CO    + HF   3.7e12   0.00     2100.

!*****************************************
!*** Fluoroethylene + OH: Abstraction of H ***
!*****************************************
CH2CHF   + OH   = CHFCH[Z]+ H2O   4.00E06  2.00     2850.
CH2CHF   + OH   = CH2CF   + H2O   4.00E06  2.00     2850.
CH2CHF   + OH   = CHFO   + CH3   1.50E06  2.00     5550.
CHFCHF[Z]+ OH   = CHFCF[Z]+ H2O   2.00E06  2.00     2850.
CH2CF2   + OH   = CF2CH   + H2O   2.00E06  2.00     6100.
CHFCF2   + OH   = CF2CF   + H2O   1.00E06  2.00     2850.
CHFCF2 +OH  = CF2O + CH2F         2.0E06   2.00     2850.
CHFCF2 + OH = CHFO + CHF2         4.0E06   2.00     2850.

!*************************************************************************
!*** FLUOROVINYLS ********************************************************
!*************************************************************************

!*********************************************
!*** Fluorovinyl + O2: Addition/decomposition ***
!*********************************************
CH2CF    + O2   = CH2O     + CFO  1.12E25   -4.55   5480.
DUP
CH2CF    + O2   = C2HF    + HO2   1.0e11   0.0   10000.
CHFCH[Z] + O2   = CHFO    + HCO   1.12E25   -4.55   5480
DUP
CHFCF[Z] + O2   = CHFO    + CFO  4.48E26   -4.55   5480.
DUP
CF2CH    + O2   = CF2O    + HCO   5.0e11   0.0   8000.
CF2CF    + O2   = CF2O    + CFO  4.48E26   -4.55   5480
DUP
!*********************************************
CH2CF    + O2   = CH2O     + CFO  1.05E38   -8.22   7030.
DUP
CHFCH[Z] + O2   = CHFO    + HCO   1.05E38   -8.22   7030.
DUP
CHFCF[Z] + O2   = CHFO    + CFO  1.05E38   -8.22   7030.
DUP
CF2CF    + O2   = CF2O    + CFO  1.05E38   -8.22   7030.
DUP
!*********************************************

!*********************************************
!*** Fluorovinyl + O Addition/decomposition ***
!*********************************************
CH2CF    + O    = CH2CO    + F     9.00E13  0.00        0.
```

```
CHFCH[Z] + O    = CHFCO    + H     9.00E13  0.00        0.
CHFCF[Z] + O    = CHFCO    + F     3.00E13  0.00        0.
CF2CH    + O    = CF2CO    + H     3.00E13  0.00        0.
CF2CF    + O    = CF2CO    + F     3.00E13  0.00        0.

!*********************************************
!*** Fluorovinyl + OH: Addition/decomposition ***
!*********************************************
CH2CF    + OH   = CH2CO    + HF    3.00E13  0.00        0.
CHFCH[Z] + OH   = CH2CO    + HF    3.00E13  0.00        0.
CHFCF[Z] + OH   = CHFCO    + HF    2.00E13  0.00        0.
CF2CF    + OH   = CF2CO    + HF    1.00E13  0.00        0.
!*********************************************
CH2CF    + OH   = CH3      + CFO  3.00E13  0.00        0.
CHFCH[Z] + OH   = CH2F     + HCO   3.00E13  0.00        0.
CHFCF[Z] + OH   = CH2F     + CFO  4.00E13  0.00        0.
CF2CF    + OH   = CHF2     + CFO  5.00E13  0.00        0.

!*****************************************************************************
!*** FLUOROETHYNES ***********************************************************
!*****************************************************************************
CF + CF = C2F2                       5.0e13   0.0         0.
!*************************************************
!*** Fluoroethynes + H Addition/stabilization ***
!*************************************************
C2HF      +H (+M)= CH2CF   (+M)    2.80E12  0.00     2410.
     LOW/1.33E27   -3.5     2410./
     H2/2./ CO/2./ CO2/3./ H2O/5./
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./
C2HF      +H (+M)= CHFCH[Z](+M)    1.40E12  0.00     2410.
     LOW/0.67E27   -3.5     2410./
     H2/2./ CO/2./ CO2/3./ H2O/5./
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./
C2F2      +H (+M)= CHFCF[Z](+M)    2.80E12  0.00     2410.
     LOW/1.33E27   -3.5     2410./
     H2/2./ CO/2./ CO2/3./ H2O/5./
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./
C2HF      +F (+M)= CF2CH   (+M)    8.40E12  0.00     2410.
     LOW/4.00E27   -3.5     2410./
H2/2./ CO/2./ CO2/3./ H2O/5./
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./
C2HF      +F (+M)= CHFCF[Z]   (+M)    8.40E12  0.00     2410.
     LOW/4.0E27   -3.5     2410./
H2/2./ CO/2./ CO2/3./ H2O/5./
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./


!*****************************************
!*** FLUORO-ACETYLENE DESTRUCTION PATHWAYS ***
!*****************************************
!*****************************************
C2HF  + O      = CFCO    + H                    2.25E12    0.00     4530.
C2HF       + O      = CO         + CHF           9.00E+13   0.00     2000.
C2F2  + O      = CFCO    + F        1.00E07    2.00   1900.
!*****************************************
```

```
C2HF  + OH     = CHFCO   + H        2.18E-4    4.50  -1000.
C2HF  + OH     = CH2F    + CO       2.50E-4    4.00  -2000.
C2HF  + OH     = HCCO    + HF       2.50E-4    4.00  -2000.
C2F2  + OH     = CF2CO   + H        2.18E-4    4.50  -1000.
C2F2  + OH     = CFCO    + HF       2.50E-4    4.00  -2000.

!***********************************
!*** Fluoromethylenes (CHF, CF2): ***
!***********************************

!*************************
!*** Radical combination ***
!*************************
CH2F      + CH2  = CH2CHF   + H    4.00E13   0.00       0.
CH2F      + CH2  = C2H4      + F    4.00E13   0.00      0.
CHF2      + CH2  = CH2CF2   + H    4.00E13   0.00       0.
CHF2      + CH2  = CH2CHF   + F    4.00E13   0.00       0.
CF3       + CH2  = CH2CF2   + F    4.00E13   0.00       0.

!************************************
!*** Insertion into bonds of methyls ***
!************************************
CH2F   + CH2(S) = CH2CHF   + H    4.00E12   0.00       0.
CH2F   + CH2(S) = C2H4      + F    2.00E12   0.00       0.
CHF2   + CH2(S) = CH2CF2   + H    2.00E12   0.00       0.
CHF2   + CH2(S) = CH2CHF   + F    4.00E12   0.00       0.
CF3    + CH2(S) = CH2CF2   + F    6.00E12   0.00       0.
!************************************
CH3    + CHF    = CH2CHF   + H     6.00E12   0.00       0.
CH2F   + CHF    = CHFCHF[Z]+ H     4.00E12   0.00       0.
CH2F   + CHF    = CH2CHF   + F     2.00E12   0.00       0.
CHF2   + CHF    = CHFCF2   + H     2.00E12   0.00       0.
CHF2   + CHF    = CHFCHF[Z]+ F     4.00E12   0.00       0.
CF3    + CHF    = CHFCF2   + F     6.00E12   0.00       0.
!************************************
CH3    + CF2    = CH2CF2   + H     6.00E12   0.00    3500.
CH2F   + CF2    = CH2CF2   + F     2.00E12   0.00    3500.
CH2F   + CF2    = CHFCF2   + H     2.00E12   0.00    3500.
CHF2   + CF2    = CF2CF2   + H     2.00E12   0.00    20000.
CHF2   + CF2    = CHFCF2   + F     1.00E11   0.00    8500.

!*****************************
!*** FLUOROKETENE CHEMISTRY ***
!*****************************
CHFCO + H      = CH2F    + CO       1.13E13    0.00   3428.
CHFCO + H      = CFCO    + H2       5.00E13    0.00   8000.
CF2CO + H      = CHF2    + CO       1.13E13    0.00   3428.
!*****************************
CHFCO + O      = CHFO   + CO       1.00E13    0.00   8000.
CF2CO + O      = CF2O   + CO       1.00E13    0.00   8000.
CHFCO + OH     = CFCO    + H2O      7.50E12    0.00   2000.
!*****************************
CFCO    + H    = CHF     + CO       1.00E14    0.00      0.
CFCO    + O    = CFO    + CO        1.00E14    0.00      0.
HCCO    + F    = CHF     + CO       9.00E13    0.00      0.
```

```
CFCO    + F    = CF2     + CO       3.00E13    0.00      0.

!**************************************
!*** Fluoromethanes Reactions with F ***
!**************************************
CH4     + F    = CH3     + HF       5.90E12   0.50     450.
CH3F    + F    = CH2F    + HF       1.35E14   0.00    1200.
CH2F2   + F    = CHF2    + HF       3.1E07   2.10       30.
CHF3    + F    = CF3     + HF       9.00E03   2.69     990.

!**************************************
!*** CHFO & CF2:O: Reactions with F ***
!**************************************
CH3OH   + F    = CH3O    + HF       2.62E09   1.44    -205.
CH3OH   + F    = CH2OH   + HF       4.62E07   1.97    -300.
!**************************************
CH2O    + F    = HCO     + HF       6.00E13   0.00    2000.
CHFO   + F    = CFO    + HF       2.65E13   0.00    1800.
!**************************************
CH3O    + F    = CH2O    + HF       3.00E13   0.00       0.
HCO     + F    = CO      + HF       1.00E13   0.00       0.

!***********************************************
!*** Abstraction from fluoroethanes: By F-atom ***
!***********************************************
C2H6      + F  = C2H5     + HF       8.00E12   0.00     300.
CH3-CH2F  + F  = CH2F-CH2 + HF       9.00E13   0.00     800.
!CH3-CHF2  + F  = CHF2-CH2 + HF       1.00E14   0.00     800.
CH3-CF3   + F  = CF3-CH2  + HF       1.00E14   0.00    4000.
!***********************************************
CH3-CH2F  + F  = CH3-CHF  + HF       6.00E13   0.00     200.
CH2F-CH2F + F  = CH2F-CHF + HF       1.30E14   0.00     800.
CH2F-CHF2 + F  = CHF2-CHF + HF       1.30E14   0.00     800.
CH2F-CF3  + F    = CF3-CHF  + HF     1.6E13    0.00    4500.

!***********************************************
!CH3-CHF2  + F  = CH3-CF2  + HF       3.00E13   0.00     800.
CH2F-CHF2 + F  = CH2F-CF2 + HF       3.00E13   0.00    1200.
CHF2-CHF2 + F  = CHF2-CF2 + HF       1.25E5    2.49     790.
CHF2-CF3  + F  = CF3-CF2  + HF       7.11E3    2.72    -910.
!***********************************************
CF3-CF2 + F = CF3 + CF3              3.16e13   0.0        0.

!***********************************************
C2H4     + F    = C2H3      + HF     1.00E14   0.00    2000.
CF2CF2  + F    = CF3       + CF2    3.00E13   0.00       0.

!*********************************************
!*** Fluorovinyl + F: Addition/decomposition ***
!*********************************************
C2H3      + F   = C2H2     + HF     2.00E13   0.00       0.
CHFCF[Z]  + F   = CHF      + CF2    1.00E13   0.00       0.
CF2CF     + F   = CF2      + CF2    2.00E13   0.00       0.

!
```

```
! **** CF3CHO,CF3OF, CF3CO reactions ****
CF3CO (+M) = CF3 + CO (+M)                              2.65e14    0.00  12000.00
 LOW /2.05E16 0.0 9200.0 /
 TROE/ 1.0  100.0  520.0 /
CF3CO + F = CF3 + CFO                                   3.e12       0.0       0.0
CF3CO + F = CF4 + CO                                    5.e12       0.0       0.0

!*****
CF3CHO + H  = CF3CO + H2                                4.00e13   0.00    4200.00
CF3CHO + OH = CF3CO + H2O                               7.0e12    0.00    1410.0
CF3CHO + O  = CF3CO + OH                                1e12      0.0        0.0
CF3CHO + CH3 = CF3CO + CH4                              1e11      0.00    7400.0
CF3CHO + CF3 = CHF3 + CF3CO                             1e12      0.00    8400.0
CF3CHO (+M) = CF2CO + HF (+M)                           1e13      0.00    85000.0
  LOW /8.75E17 0.0 85000.0 /
H2O/9.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./
CF3CHO + F = CF3CO + HF                                 4e13      0.00    1000.0
CF3CHO (+M) = CF3 + HCO (+M)                            4e16      0.00   80000.00
  LOW /3.50E21 0.0 80000.0 /
H2O/9.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./
CF3COF+ H = CF3CO + HF                                  2e13     0.00    3000.00
CF3COF(+M) =CF3+CFO(+M)                                4.3E+16    0.00   90000.00
LOW /3.76E21   0.0  90000.0/
H2O/9.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./
CF3COF + CF3 = CF3CO + CF4                              2.e12       0.0     9000.
CF3COF + CF3-CF2 = CF3CO + CF3-CF3                      3.e11       0.0     14000.
CF3COF + F = CF3 + CF2O                                 2.e12       0.0      4500.
CF3COF + O = CF3O + CFO                                 2.e12       0.0      9500.

! *** F2 reactions ***
F + F + M = F2 + M                                      1.0e14      0.0         0.
F2 + H = F + HF                                         2.9e9       1.4      1330.
F2 + CF3 = CF4 + F                                      2.65e12     0.0      2500.
CH3 + F2 = CH3F + F                                     4.e12       0.0      1100.
CF2 + F2 = CF3 + F                                      1.2e12      0.0      3000.
CFO + F2 = CF2O + F                                     1.e12       0.0         0.
H2 + F2 = HF + F + H                                    3.44e12     0.0     19790.
F2 + CO = CFO + F                                      4.7e11      0.0     13500.
C + F2 = CF + F                                         1.7e12      0.0      1500.
CF + F2 = CF2 + F                                       2.4e12      0.0         0.
C2H4 + F2 = CH2F-CH2 + F                                4.8e10      0.0      4590.
CH4 + F2 = CH3 + HF + F                                 2.e12       0.0     11230.
OH + F2 = HF + F + O                                    7.e13       0.0      9000.

!************************************************
! *** 2-BTP reactions ***
  CF3CHCH2 + OH    = CF3COCH3     + H                    1.0E+12   0.00     4780.

! TRIFLUOROPROPENE
CF3CHCH2+H=C2H4+CF3                                      0.7E13   0.0     9100.
  CF3CHCH2 + H     = CF3CCH2 + H2                       3.0E+13   0.00    14000.
  CF3CHCH2 + H     = CF3CHCH + H2                       4.3E+13   0.00    14000.
```

```
CF3CHCH2 + O     = CH3CO   + CF3                    1.5E+13   0.00     4000.
CF3CHCH2 + OH    = CH3CHO  + CF3                    5.0E+12   0.00      1500.0
CF3CHCH2 + CH3   = C3H6    + CF3                    5.0E+12   0.00    11850.
CF3CHCH2 + F = HF + CF3CCH2                          2.e13     0.0      5000.
CF3CHCH2 + F = HF + CF3CHCH                          2.7e13    0.0      5000.
CF3CHCH2 + F = CF4 + C2H3                            4.e12     0.0      6000.
CF3CHCH2 + F = CF3 + CH2CHF                          3.e13    0.0       8000.

CF3CHCH2 + CF3 = CHF3 + CF3CCH2                      1.2e13     0.0     12500.
CF3CHCH2 + CF3 = CHF3 + CF3CHCH                      1.7e13     0.0     15000.
CF3CHCH2 + CF3 = CF3-CF3 + C2H3                      2.e13    0.0      15500.

CF3CHCH2 = CF3 + C2H3                               8.e16    0.0      109000.
CF3CHCH2 = CF3CCH + H2                              9.7e13    0.0      67500.
CF3CHCH2 = CHF3 + C2H2                              9.21e13    0.0    71000.0
CF3CHCH2 = CF2 + CH2CHF                             5.e12     0.0     77000.

!! TRIFLUOROPROPENYL REACTIONS
  CF3CCH   + H     = CF3CCH2                        6.0E+14   0.00     4780.
  CF3CCH   + H     = CF3CHCH                        4.0E+14   0.00     4780.
  CF3CCH2          = C2H2    + CF3                 2.E+13    0.00    37000.
  CF3CHCH          = C2H2    + CF3                 2.E+13    0.00    37000.

  CF3CCH2  + O2    = CF3CCH  + HO2                  2.0E+13   0.00    23900.
  CF3CCH2  + H     = C2H3    + CF3                  4.0E+13   0.00     4780.
  CF3CCH2  + H     = CF3CCH  + H2                   2.0E+13   0.00        0.
CF3CHCH  + O2    = CF3CCH  + HO2                    1.0E+13   0.00    23900.
  CF3CHCH  + H     = C2H3    + CF3                  2.0E+13   0.00     4780.
  CF3CHCH  + H     = CF3CCH  + H2                   2.0E+13   0.00        0.

  CF3CCH2  + O     = CH2CO   + CF3                  5.0E+13   0.00        0.0
  CF3CCH2  + O     = CF3CCH  + OH                   5.0E+13   0.00     2390.
  CF3CCH2  + OH    = CH2CO   + CF3   +  H           5.0E+13   0.00     9560.
  CF3CCH2  + OH    = CF3CCH  + H2O                  5.0E+13   0.00     4780.
  CF3CCH2  + CH3   = CH3CCH2 + CF3                  4.0E+13   0.00     4780.
  CF3CCH2  + CH3   = CF3CCH + CH4                   1.0E+13   0.00        0.

  CF3CHCH  + O     = CH2CO   + CF3                  5.0E+13   0.00        0.0
  CF3CHCH  + O     = CF3CCH  + OH                   5.0E+13   0.00     2390.
  CF3CHCH  + OH    = CF3CCH  + H2O                  5.0E+13   0.00     4780.

  CF3CHCH  + CH3   = CH3CCH2 + CF3                  4.0E+13   0.00     4780.
  CF3CHCH  + CH3   = CF3CCH + CH4                   1.0E+13   0.00        0.

CF3CCH2 + F = CF3CCH + HF                           5.e13     0.0        0.
CF3CCH2 + CF2 = CHF2 + CF3CCH                       3.e13     0.0      3500.
CF3CCH2 + CF3 = CHF3 + CF3CCH                       2.e13     0.0        0.

CF3CHCH + F = CF3CCH + HF                           5.e13     0.0        0.
CF3CHCH + CF2 = CHF2 + CF3CCH                       3.e13     0.0      3500.
CF3CHCH + CF3 = CHF3 + CF3CCH                       2.e13     0.0        0.

! TRIFLUOROPROPYNE REACTIONS
CF3CCH   + H     = C2H2   + CF3                    2.0E+14   0.00     9560.
```

```
  CF3CCH   + O     = HCCO   + CF3                    4.0E+13   0.00     1500.
  CF3CCH   + OH    = CH2CO  + CF3                    2.0E+14   0.00     3300.

!! TRIFLUOROPROPANONE  REACTIONS
  CH3CO    + CF3   = CF3COCH3                        4.0E+13   0.00       0.0
  CH3CO    + CF3   = CH2CO + CHF3                    1.0E+13   0.00       0.0
  CH3CO    + F   = CH2CO + HF                        1.0E+13   0.00       0.0
  CH3CO + CF3   = CO + CH3 +CF3                      2.0E+13   0.00    9560.0
  CF3COCH3 + CF3   = CH2CO +CHF3+CF3                 2.0E+13   0.00   21500.0
  CF3COCH3 + H     = CH2CO + H2  + CF3               6.0E+14   0.00   23900.
  CF3COCH3 + OH    = CH2CO + H2O + CF3               5.0E+13   0.00    3585.

CF3COCH3 + F = HF + CH2CO + CF3                      1.e13     0.0     10000.
CF3CCH + F = CF3 +C2HF                               7.e12     0.0     12500.
CF3CCH + CF2 = CF2CF2 + C2HF                        5.e11     0.      50000.
CF3CCH + CF3 = CF2CF2 + CF2CH                       1.e12     0.      60000.
CF3CCH   + O     = CO  + CHFCF2                     3.0E+12   0.00     1500.
CHFCCF3 = CF3 + C2HF                               2.e13     0.0     54000.

C3H8 + F = C3H7 + HF                                 3.5e13    0.0        0.
DUPLICATE
C3H8 + F = C3H7 + HF                                 4.1e13    0.0        0.
DUPLICATE
C3H8 + CF3 = C3H7 + CHF3                             5.4e11    0.0     8540.
DUPLICATE
C3H8 + CF3 = C3H7 + CHF3                             1.8e11    0.0     6520.
DUPLICATE
C3H8 + CF3-CF2 = C3H7 + CHF2-CF3                     3.9e11    0.0     7800.
DUPLICATE
C3H8 + CF3-CF2 = C3H7 + CHF2-CF3                     3.3e11    0.0     6100.
DUPLICATE

! ************************************************************************
!***HFO1234zee**********************************************************
!************************************************************************
CHFCHCF3 = HF + CF3CCH                               4.72e52 -10.897  102870.
CHFCHCF3 = CF3 + CHFCH[Z]                           0.5e16     0.0    116000.
CHFCHCF3 + O2 = CFCHCF3 + HO2                        4.02e12   0.0     57640.
CHFCHCF3 + O2 = CHFCCF3 + HO2                        3.02e12   0.0     57640.

CHFCCF3 + H = CHFCHCF3                               0.1e14     0.0     0.0
CFCHCF3 + H = CHFCHCF3                               0.1e14     0.0     0.0

!*** Abstraction, association/decomposition

CHFCHCF3 + H = CFCHCF3 + H2                          3.5e13    0.0      16000.
CHFCHCF3 + H = CHFCCF3 + H2                          2.5e13    0.0      18000.
CHFCHCF3 + H = CF3 + CH2CHF                          0.9e13    0.0       5000.

CHFCHCF3 + O = CFCHCF3 + OH                          1.2e12   0.7      15000.
CHFCHCF3 + O = CHFCCF3 + OH                          1.e12    0.7      17000.

CHFCHCF3 + O = CF3 + CH2F + CO                      3.25e6   1.83        0.
CHFCHCF3 + O = CFO + CF3-CH2                        1.3e7    1.83        0.
```

```
CHFCHCF3 + OH = CFCHCF3 + H2O                          1.5e13   0.0       7500.
CHFCHCF3 + OH = CHFCCF3 + H2O                          1.5e13   0.0       9000.
CHFCHCF3 + OH = CHFO + CF3-CH2                        3.75e11   0.0        240.

CHFCHCF3 + F = HF + CFCHCF3                           9.3e13    0.        4500.
CHFCHCF3 + F = HF + CHFCCF3                           1.1e13    0.        7500.
CHFCHCF3 + F = CF3 + CH2CF2                           0.2e13    0.        8200.
CHFCHCF3 + F = CF3 + CHFCHF[Z]                        0.5e13    0.        9000.

CHFCHCF3 + CF3 = CHF3 + CFCHCF3                        5.e12    0.        17000.
CHFCHCF3 + CF3 = CHF3 + CHFCCF3                        5.e12    0.        15000.

!*** consumption of CFCHCF3, CHFCCF3, radical reactions ***
!CHFCCF3 = CF3 + C2HF                                  2.e13    0.       56000.
CFCHCF3 = CF3 + C2HF                                  1.e13    0.       55000.
CHFCCF3 + O2 = HO2 + CFCCF3                           3.e11    0.       17000.
CFCHCF3 + O2 = HO2 + CFCCF3                           3.e11    0.       18500.
CHFCCF3 + H = CF3 + CHFCH[Z]                          2.e13    0.        8000.
CFCHCF3 + H = CF3 + CH2CF                             2.e13    0.        8000.
CHFCCF3 + H = H2 + CFCCF3                             2.e13    0.        3000.
CHFCCF3 + H = HF + CF3CCH                             3.e13    0.        2000.
CFCHCF3 + H = H2 + CFCCF3                             2.e13    0.        3000.
CFCHCF3 + H = HF + CF3CCH                             3.e13    0.        2000.
CHFCCF3 + OH = H2O + CFCCF3                           2.e13    0.           0.
CFCHCF3 + OH = H2O + CFCCF3                           2.e13    0.           0.
CHFCCF3 + OH = CF3 + CH2CFO                           5.e12    0.        3000.
CFCHCF3 + OH = CF3 + CH2CFO                           5.e12    0.        4000.
CHFCCF3 + CH3 = CH4 + CFCCF3                          5.e12    0.0       2000.
CFCHCF3 + CH3 = CH4 + CFCCF3                          3.e12    0.0       3000.
CHFCCF3 + CF3 = CHF3 + CFCCF3                         3.e12    0.0       1000.
CFCHCF3 + CF3 = CHF3 + CFCCF3                         2.e12    0.0       2000.
CHFCCF3 + CF2 = CHF2 + CFCCF3                         8.e12    0.0       7000.
CFCHCF3 + CF2 = CHF2 + CFCCF3                         7.e12    0.0       7000.
CHFCCF3 + F = HF + CFCCF3                             1.e13    0.0       1000.
CFCHCF3 + F = HF + CFCCF3                             1.e13    0.0       1000.
 CHFCCF3 + F = CF3 + CHFCF[Z]                         3.5e12   0.0       9000.
CFCHCF3 + F = CF3 + CHFCF[Z]                          3.5e12   0.0      10000.
CH2CFO (+M) = CH2F + CO (+M)                          2.e13    0.00     30000.
 LOW /2.0E16 0.0 30000.0 /
 TROE/ 1.0  100.0  520.0 /
CH2CFO + H = CH3 + CFO                               8.e12    0.0   11000.0
CH2CFO + F = CH2F + CFO                              5.e12    0.0    9000.0
CH2CFO + CF3 = CF3-CH2 + CFO                         3.e12    0.0    8000.0

!*****************
!*** 1234yf ******
!*****************
CH2CFCF3 (+M) => CF3 +CH2CF (+M) 5.0E+16   0.00       107000.00
LOW /5.40E18   0.0  108700.0/
H2O/9.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/ CF2O /5./ CF4 /6./ CH2CFCF3/10./

CH2CFCF3 = CF3CCH + HF         1.1E+44  -8.492        99304.00          !100kPa
CF3CCH2 + F = CH2CFCF3         5.0e13         0.               0.
CF3CHCH + F = CHFCHCF3         5.0e13         0.               0.
```

```
CH-CFCF3 + H = CH2CFCF3        5.0e13         0.              0.
CH2CFCF3 + O2 = CH-CFCF3 + HO2 6.02e12        0.0          57640.
CH2CFCF3 + H = CH-CFCF3 + H2   2.5e13         0.           16000.
CH2CFCF3 + H = CH2CHF + CF3    2.5e13         0.            5000.
CH2CFCF3 + OH = CH-CFCF3 + H2O  2.e13         0.            6800.
CH2CFCF3 + OH = CH3 + CF3COF    7.5e11        0.             240.
CH2CFCF3 + O = CH-CFCF3 + OH    0.6e12         0.7          15000.
CH2CFCF3 + O = CF3-CHF + HCO    3.25e6         1.83             0.
CH2CFCF3 + O = CH2F + CO + CF3  1.7e6          1.83             0.
CH2CFCF3 + CF3 = CH-CFCF3 + CHF3 1.5e13        0.           22000.
CH2CFCF3 + CH3 = CH-CFCF3 + CH4  1.e13         0.           20000.
CH2CFCF3 + F = CH-CFCF3 + HF    6.7e13         0.            5400.
CH2CFCF3 + F = CH2CF2 + CF3     1.2e12         0.            8300.
CH2CFCF3 + F = CHFCHF[Z]+ CF3   2.0e12         0.            8000.

CH-CFCF3 = CF3CCH + F           1.e13          0.           57000.
CH-CFCF3 = CF3 + C2HF           2.e13          0.           45000.

CH-CFCF3 + O2 = HO2 + CFCCF3    3.e11          0.           25000.
CH-CFCF3 + H = CF3 + CH2CF      2.e13          0.            5000.
CH-CFCF3 + H = H2 + CFCCF3      2.e13          0.            3000.
CH-CFCF3 + H = HF + CF3CCH      3.e13          0.            2000.

CH-CFCF3 + OH = CF3 + CH2CFO        5.e12       0.            4000.
CH-CFCF3 + OH = H2O + CFCCF3    2.e13          0.              0.
CH-CFCF3 + CH3 = CH4 + CFCCF3   5.e12          0.            3000.
CH-CFCF3 + CF3 = CHF3 + CFCCF3  5.e12          0.            1500.
CH-CFCF3 + CF2 = CHF2 + CFCCF3  7.e12          0.            8000.
CH-CFCF3 + F = HF + CFCCF3      1.e13          0.            1000.
CH-CFCF3 + F = CF3 + CHFCF[Z]   3.5e12         0.            9000.
CFCCF3 + H = CF3 + C2HF         5.e13          0.            7500.
CFCCF3 + O = CF3 + CFCO         1.e13          0.              0.
CFCCF3 + OH = CF3 + CHFCO       3.e13          0.            5000.
CFCCF3 + F = CF3 + C2F2         1.e13          0.            7000.
CFCCF3 = CF2 + C2F2              3.e15          0.           89000.
! *******
CH2CF + CF3 <=> CF3CCH + HF                          1.180E+13     0.000   5880.
F + CH2CO <=> HF + HCCO                             1.5000E+13     0.000   3000.
CF3-CF3 + F = CF3 + CF4                              7.e11          0.0    7500.

!************************************************
C3F7H+O =  C3F7+OH                                   7.000E+07   1.60    7200.00
C3F7H+CF3 =  C3F7+CHF3                               1.400E+11   0.00   10100.00
C3F7H (+M)  =  CF3+CF3-CHF (+M)                      7.900E+15   0.00   85000.00
LOW /3.46E21 0.0 85000.0/
H2O/9.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ C3F7H /12.00/ HF /2.00/

C3F7H (+M) =  C3F6+HF (+M)                           7.900E+12   0.00   69600.00
LOW /3.46E18 0.0 69600.0 /
H2O/9.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ C3F7H /12.00/ HF /2.00/

C3F7H+F =  C3F7+HF                                   4.000E+13   0.00    2400.00
C3F7H+CH3 =  C3F7+CH4                                5.700E+10   0.00    9500.00
```

```
C3F7H+C2H3 =  C3F7+C2H4                                  6.000E+10   0.00    7000.00
C3F7H+CH2F =  C3F7+CH3F                                  2.000E+11   0.00   10000.00
C3F7H+CHF2 =  C3F7+CH2F2                                 2.000E+11   0.00   10000.00
C3F7H+OH =  C3F7+H2O                                     9.92e5      1.7     1400.0
C3F7H+H = C3F7+H2                                        1.400E+07   1.60   10200.00
C3F7+H =  C3F6+HF                                        2.415E+63  -13.87  44675.00
C3F7+H =  CF3-CHF+CF3                                    5.284E+70  -15.71  57151.00
C3F7+H =  C3F7H                                          8.551E+64  -14.85  32739.00
C3F7+F = CF3-CF2 + CF3                                   2.5e11      0.      6000.0
!
C3F7O = C3F6O + F                                         2e14       0.00  55000.00
C3F7O = CF3COF + CF3                                      1e15       0.00  10000.00
C3F6O = CF3CO + CF3                                       8.5e16     0.00  76000.00
C3F6O + H = CF3CHO + CF3                                  1.3e11     0.00  3000.00
CF3CO = CF3 + CO                                          2.2e13     0.00  10000.00
C3F7(+M) = CF2CF2 + CF3(+M)                               1.0e14     0.00  76000.00
LOW /4.38E19   0.0  76000.0/
H2O/9.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ C3F7H/12.00/ HF /2.00/
C3F7 (+M)= C3F6 + F (+M)                                  2.0e14     0.00  69000.00
LOW /8.75E19   0.0  69000.0/
H2O/9.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ C3F7H/12.00/ HF /2.00/
!*******
CF3-CHF+CF3 =  C3F6+HF                                   7.000E+16  -1.17    4330.00
C3F7+H2O2 =  C3F7H+HO2                                   9.000E+09   0.00    1000.00
C3F7+HO2 =  O2+C3F7H                                     3.000E+11   0.00       0.00
C3F7+CH2O =  C3F7H+HCO                                   5.500E+03   2.80    5900.00
C3F7+O2 =  C3F7O2                                        3.954E+66 -16.34   24194.00
C3F7+O2 =  C3F7O+O                                       1.033E+20  -1.86   20065.00
!****
C3F7OH => C3F6O + HF                                    2.000E+14    0.00   57000.00
C3F7 + OH = CF3 + HF + CF3CO                             2.2E13       0.0        0.0
C3F7OH+H => C3F7 + H2O                                  1.0E+13      0.00    5000.00
C3F7+O =  CF3COF+CF3                                    2.400E+13    0.00       0.00
C3F6+OH = CF3-CHF + CF2O                                5.0e+12      0.00       0.00
C3F6+F = CF3-CF2 + CF2                                  3.000E+13    0.00       0.00
C3F6+O =  CF3COF+CF2                                    5.800E+12    0.00    2500.00
C3F6+O =  CF2CF2+CF2O                                   3.500E+12    0.00    6300.00
C3F6(+M)=CF3+CF2CF (+M)                                 3.200E+13    0.00  105600.00
LOW /1.40E19   0.0  105600.0/
H2O/9.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ C3F7H/12.00/ HF /2.00/
C3F6(+M)=CF2CF2+CF2(+M)                                 3.200E+13   0.00   94000.00
LOW /1.40E19   0.0  94000.0/
H2O/9.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ C3F7H/12.00/ HF /2.00/
C3F6+H =  CF3+CHFCF2                                     1.170E+21  -2.213   9912.00

end
```

Appendix C: Transport properties of fluorine-containing species (Chemkin format).

1. Species name
2. Molecule index: 0 = atom, 1= linear molecule, 2 = nonlinear molecule
3. L-J potential well depth, ε/k_b (K)
4. L-J collision diameter, A^o
5. Dipole moment in Debye
6. Polarizability in cubic Angstroms
7. Rotational relaxation number, Z_{rot} at 298K
8. Reference, comment

```
1                 2   3          4        5        6        7     8
F                 0    80.000    2.750    0.000    0.000    0.000 ! [60]
F2                1   125.700    3.301    0.000    1.600    3.800 ! [60]
HF                1   330.000    3.148    1.920    2.460    1.000 !
[60](sv/mec)
HOF               2   107.400    3.458    0.000    0.000    0.000 !
[60](ois)
F2O               2   107.400    3.458    0.000    0.000    0.000 !prwH2O2?
FO                1   109.600    3.412    0.000    0.000    0.000 !
[60](ois)
HOOF              2   107.400    3.458    0.000    0.000    0.000 !prwH2O2?
F2O2              2   107.400    3.458    0.000    0.000    0.000 !prwH2O2?
FO2               2   107.400    3.458    0.000    0.000    0.000 !prwH2O2?
CH3F              2   262.       4.123    1.8      0.000    0.000 ! [61]
CH2F2             2   318.       4.08     1.8      0.0      0.0   ! [60]sve
CHF3              2   240.       4.33     0.0      0.0      1     ! [60]sve
CF4               2   265.57     4.35     0.0      0.0      0.0   ! [62]
CH2F              2   276.7      4.15     1.8      0.0      0.0   !wtc*
CHF2              2   288.2      4.29     1.8      0.0      0.0   !wtc*
CF3               2   297.2      4.45     0.0      0.0      1     !wtc*
CHF               2   276.0      4.14     1.8      0.0      0.0   !wtc*
CF2               2   287.6      4.28     0.0      0.0      1     !wtc*
CF                1   94.2       3.635    0.0      0.0      1     !
[60](Svehla)
CF3OH             2   305.0      4.61     0.0      0.0      0.0   !wtc*
CF3OF             2   314.0      4.8      0.0      0.0      0.0   !wtc*
CH2FO             2   287.0      4.27     0.0      0.0      0.0   !wtc*
CHF2O             2   296.2      4.43     0.0      0.0      0.0   !wtc*
CF3O              2   304.5      4.6      0.0      0.0      0.0   !wtc*
CHFO              2   286.5      4.27     0.0      0.0      0.0   !wtc*
CF2O              2   350.5      4.906    0.0      0.0      0.0   !(ois)
CFO               2   285.9      4.26     0.0      0.0      0.0   !wtc*
CH3-CH2F          2   312.2      4.583    2.       0.0      0.0   ! [61]
CH3-CHF2          2   323.4      4.798    2.3      0.0      0.0   ! [61]
CH2F-CH2F         2   312.2       4.583   2.       0.0      0.0   ! [61]
CH3-CF3           2   289.1       4.911   2.3      0.0      0.0   ! [61]
CH2F-CHF2         2   323.4       4.798   2.3      0.0      0.0   ! [61]
CH2F-CF3          2   323.4       4.85    2.3      0.0      0.0   ! [61]
CHF2-CHF2         2   323.4       4.85    2.       0.0      0.0   ! [61]
CHF2-CF3          2   265.77      4.6831  1.5      0.0      0.0   ! [63]
CF3-CF3           2   231.8       4.969   0.0      0.0      0.0   ! [61]
CH3-CHF           2   285.9       4.26    2.0      0.0      0.0   !wtc*
```

CH2F-CH2	2	285.9	4.26	2.0	0.0	0.0	!wtc*
CH3-CF2	2	295.3	4.41	2.3	0.0	0.0	!wtc*
CH2F-CHF	2	295.3	4.41	2.	0.0	0.0	!wtc*
CHF2-CH2	2	295.3	4.21	2.3	0.0	0.0	!wtc*
CH2F-CF2	2	303.6	4.58	2.3	0.0	0.0	!wtc*
CHF2-CHF	2	303.6	4.58	2.3	0.0	0.0	!wtc*
CHF2-CF2	2	312.3	4.76	2.	0.0	0.0	!wtc*
CF3-CH2	2	303.6	4.58	2.3	0.0	0.0	!wtc*
CF3-CHF	2	312.3	4.76	2.3	0.0	0.0	!wtc*
CF3-CF2	2	323.3	4.96	1.5	0.0	0.0	!wtc*
CH2CHF	2	272.2	4.322	1.4	0.0	0.0	! [61]
CH2CF2	2	251.5	4.442	1.4	0.0	0.0	! [61]
CHFCHF-E	2	251.5	4.442	1.4	0.0	0.0	! [61]
CHFCHF-Z	2	251.5	4.442	1.4	0.0	0.0	! [61]
CHFCHF[Z]	2	251.5	4.442	1.4	0.0	0.0	! [61]
CHFCHF(Z)	2	251.5	4.442	1.4	0.0	0.0	! [61]
CHFCF2	2	303.1	4.57	1.4	0.0	0.0	!wtc*
CF2CF2	2	254.2	4.647	0.0	0.0	0.0	! [61]
CH2CF	2	284.7	4.24	1.4	0.0	0.0	!wtc*
CHFCH-E	2	284.7	4.24	1.4	0.0	0.0	!wtc*
CHFCH-Z	2	284.7	4.24	1.4	0.0	0.0	!wtc*
CHFCH[Z]	2	284.7	4.24	1.4	0.0	0.0	!wtc*
CHFCF-E	2	294.3	4.39	1.4	0.0	0.0	!wtc*
CHFCF-Z	2	294.3	4.39	1.4	0.0	0.0	!wtc*
CHFCF[Z]	2	294.3	4.39	1.4	0.0	0.0	!wtc*
CF2CH	2	294.3	4.39	1.4	0.0	0.0	!wtc*
CF2CF	2	302.7	4.56	1.4	0.0	0.0	!wtc*
C2HF	1	225.	4.25	1.	0.0	0.0	! [61]
C2F2	1	240.	4.4	0.0	0.0	0.0	! [61]
C2F	1	283.5	4.23	0.0	0.0	0.0	!wtc*
CHFCO	2	292.9	4.37	0.0	0.0	0.0	!wtc*
CF2CO	2	301.3	4.53	0.0	0.0	0.0	!wtc*
FCCO-E	2	292.4	4.36	0.0	0.0	0.0	!wtc*
CFCO	2	292.4	4.36	0.0	0.0	0.0	!wtc*
C3F7H	2	380.2	5.62	0.0	0.0	0.0	!wtc*
C3F7	2	378.5	5.6	0.0	0.0	0.0	!wtc*
C3F6	2	351.9	5.35	0.0	0.0	0.0	!wtc*
CF3CO	2	354.4	4.87	0.0	0.0	0.0	! [64]
CF3CHO	2	310.8	4.73	0.0	0.0	0.0	!wtc*
CF3COF	2	321.2	4.93	0.0	0.0	0.0	!wtc*
C3F6O	2	373.7	5.56	0.0	0.0	0.0	!wtc*
C3F7OH	2	410.2	5.85	0.0	0.0	0.0	!wtc*
C3F7O	2	408.1	5.84	0.0	0.0	0.0	!wtc*
C3F7O2	2	445.4	6.08	0.0	0.0	0.0	!wtc*
C2F5COC3F7	2	1045.0	8.2	0.0	0.0	0.0	!mw-cor.[65]
C3F7CO	2	398.4	6.16	0.0	0.0	0.0	! [64]
C2F5CO	2	376.4	5.59	0.0	0.0	0.0	! [64]
C3F7CHO	2	437.8	6.03	0.0	0.0	0.0	!wtc*
C2F5CHO	2	349.5	5.32	0.0	0.0	0.0	!wtc*
CF3CHCH2	2	335.	4.7	0.0	0.0	0.0	!btp-spec,wtc*
CF3CCH2	2	333.	4.7	2.444	6.006	0.0	!wtc*
CF3CHCH	2	333.	4.7	2.444	6.006	0.0	!wtc*
CF3CCH	2	331.	4.7	0.0	0.0	0.0	!wtc*

```
CF3COCH3          2   367.        5.0       0.0       0.0       0.0    !wtc*
CH2CFCF3          2   371.        4.9       0.0       0.0       0.0
!est,anal/cor
CFCCF3            2   361.        4.8       0.0       0.0       0.0
!est,anal/cor
CH-CFCF3          2   367.        4.9       0.0       0.0       0.0
!est,anal/cor
CHFCHCF3          2   371.        4.9       0.0       0.0       0.0    !R1234yf
CFCHCF3           2   335.000     4.700     2.722     4.631     1.000
!eCHCFCF3, [29]
CHFCCF3           2   335.000     4.700     2.722     4.631     1.000
!eCHCFCF3, [29]
CH2CFO            2   312.200     4.583     3.302     3.442     1.000  ! [29]

! * - estimation, mw correlations
```

Appendix D: Tables of burning velocity data in figures.

Key: CVM: Constant volume method; CPM: constant pressure method; Tube: Vertical tube metod.

Table A- 1: Burning velocity as a function of ϕ for R-32/air mixtures. [5, 10, 16], CVM, $X_{\text{R-32, stoic}} = 0.1736$; initial conditions: $T_i = 298$ K, $P_i = 1$ bar.

Takizawa et al. [10] CVM		Burrell et al. [5] CVM			Kim et al. [16] CVM		
ϕ	S_u [cm/s]	ϕ	S_u [cm/s] (OTL)	S_u [cm/s] (ADI)	ϕ	S_u [cm/s] (UV)	S_u [cm/s] (HP)
0.9	5.97	0.9	6.1	7.04	0.9	5.161	4.996
0.95	6.38	0.95	6.58	7.59	1	6.718	6.452
1	6.56	1	6.81	7.8	1.05	7.02	6.758
1.05	6.71	1.05	7.06	8.03	1.1	6.973	6.77
1.1	6.71	1.1	7.06	8.13	1.2	6.599	6.513
1.2	6.35	1.2	6.66	7.75	1.3	5.881	5.846
1.3	5.7	1.3	5.95	6.96	1.4	4.675	4.66
1.4	4.68	1.4	4.99	5.97			

Table A- 2: Burning velocity as a function of ϕ for R-134a/O_2 mixtures from Burrell et al. [18], CVM, $X_{\text{R-134a,stoic}} = 0.400$ when $X_{O_2,\text{ox}} = 1.0$; initial conditions: $T_i = 298$ K, $P_i = 1$ bar.

ϕ	S_u [cm/s]
0.6	10.26

0.7	10.74
0.8	10.45
0.9	10.16
1	9.58
1.1	9.06
1.2	8.22

Table A- 3: Burning velocity as a function of the volume fraction of refrigerant in the air X_i for R-143/air mixtures [10] and R-143a/air mixtures [6, 10]; initial conditions: T_i = 298 K, P_i = 1 bar.

Takizawa et al. [10] CVM		Takizawa et al. [10] CVM		Clodic and Jabbour [6] Tube	
$X_{R\text{-}143}$	S_u [cm/s]	$X_{R\text{-}143a}$	S_u [cm/s]	$X_{R\text{-}143a}$	S_u [cm/s]
0.0734	8.37	0.0897	6.75	0.0901	5.94
0.0732	9.43	0.0954	6.44	0.0952	6.31
0.0787	10.77	0.0952	7.01	0.0951	6.57
0.0894	12.6	0.101	6.97	0.1051	6.59
0.0948	12	0.1066	6.86	0.1052	6.67
0.0947	13.2	0.1118	6.43	0.1151	6.01
0.1005	13.2	0.118	5.55	0.1251	4.36
0.112	12.4	0.12368	5.18		

Table A- 4: Burning velocity as a function of ϕ for R-152a/air mixtures [6, 10, 16, 18]; $X_{R\text{-}152a,stoic}$ = 0.0775; initial conditions: T_i = 298 K, P_i = 1 bar.

Takizawa et al. [10] CVM		Takizawa et al. [10] CPM		Burrell et al. [18] CVM		Clodic & Jabbour [6] CVM		Kim et al. [16] CVM	
ϕ	S_u [cm/s]	ϕ	S_u [cm/s]	ϕ	S_u [cm/s]	ϕ	S_u [cm/s]	ϕ	S_u [cm/s]
0.76	15.07	0.757	13.47	0.8	15.55	0.638	7.92	0.8	16.37
0.826	18.14	1	21.39	0.85	17.54	0.719	11.75	0.9	20.01
0.897	20.62			0.9	18.79	0.719	11.9	1	23.6
0.962	22.34			0.95	21.09	0.909	19.74	1.1	24.43
1.034	23.76			1	21.89	0.908	20.66	1.2	22.96
1.104	23.47			1.05	22.54	0.964	22.3	1.3	19.31
1.176	22.74			1.1	23.22	1	23.03	1.4	15.15
1.251	21.2			1.15	23.01	1	23.21		
1.317	17.48			1.2	22.23	1.03	23.07		
				1.3	19.61	1.11	22.96		
						1.1	24.05		

1.18	20.77
1.18	21.42
1.32	16.17
1.34	17.15

Table A- 5: Burning velocity as a function of ϕ for R-1234yf/O_2/N_2 mixtures from Takizawa et al. [11]; CVM; $X_{\text{R-1234yf,stoic}}$ = 0.167, 0.153, 0.116, and 0.0775 when $X_{O_2,ox}$ = 0.5, 0.45, 0.33, and 0.21, respectively; initial conditions: T_i = 298 K, P_i = 1 bar;

$X_{O_2,ox}$ = 0.5		$X_{O_2,ox}$ = 0.45		$X_{O_2,ox}$ = 0.33		$X_{O_2,ox}$ = 0.21	
ϕ	S_u [cm/s]	ϕ	S_u [cm/s]	ϕ	S_u [cm/s]	ϕ	S_u [cm/s]
0.8	15.5	0.904	13.64	1	6.721	0.828	0.882
0.9	16.3	1.003	14.29	1.041	7.037	0.83	0.945
1	16.75	1.058	14.52	1.141	7.352	0.894	1.22
1.1	17.2	1.136	14.63	1.242	7.73	0.964	1.306
1.27	17	1.221	14.77	1.35	7.538	0.966	1.188
1.4	15.45	1.307	14.33	1.457	7.197	0.996	1.259
		1.394	13.78			0.996	1.436
						1	1.527
						1.035	1.416
						1.037	1.365
						1.104	1.325
						1.109	1.42
						1.175	1.459
						1.178	1.53
						1.25	1.427
						1.25	1.494
						1.321	1.454
						1.328	1.399
						1.396	1.454
						1.471	1.501
						1.473	1.571
						1.546	1.504

Table A- 6: Burning velocity as a function of ϕ for R-1243zf/O_2/N_2 mixtures from Takizawa et al. [11]; CVM; $X_{R\text{-}1243yf,stoic}$ = 0.0567, 0.0654, and 0.0769 when $X_{O_2,ox}$ = 0.21, 0.25, and 0.30, respectively; initial conditions: T_i = 298 K, P_i = 1 bar.

$X_{O_2,ox}$ = 0.21		$X_{O_2,ox}$ = 0.25		$X_{O_2,ox}$ = 0.30	
ϕ	S_u [cm/s]	ϕ	S_u [cm/s]	ϕ	S_u [cm/s]
0.752	11.05	0.766	18.6	0.754	28.2
0.833	12.82	0.834	20.34	0.81	25.56
0.91	13.92	0.903	21.06	0.87	30.35
0.958	14.14	1.0	20.98	0.928	30.65
0.994	14.11	1.044	20.76	1.0	30.28
1.025	13.99	1.116	19.87	1.0497	29.6
1.075	13.61			1.113	28.69
1.158	12.48				
1.242	11.01				
1.328	9.31				

Table A-7: Burning velocity as a function of the mole fraction $X_{i,f}$ of R-1234yf the mixture of (R-32/R-1234yf); CPM, 0g [22]; CVM, 1g [22]; Tube, 1g [7]; ϕ = 1; initial conditions: T_i = 298 K, P_i = 1 bar.

Takizawa et al. [22], CPM, 0g		Takizawa et al. [22], CVM, 1g		Papas et al. [7], Tube, 1g	
$X_{i,f}$	S_u [cm/s]	$X_{i,f}$	S_u [cm/s]	$X_{i,f}$	S_u [cm/s]
0.3	2.27	0.488	1.74	0	6.61
0.502	1.71	0.7	1.4	0.102	4.81
		1	1.55	0.201	3.79
		1	1.22	0.3	2.86

Table A- 7: Burning velocity as a function of ϕ for R-152a/R-134a mixtures with air; CVM; data are shown for two values (0.2, 0.5) of the mole fraction $X_{i,f}$ of R-134a in the R-152a/R-134a fuel; $X_{i,stoic}$ = 0.0837 and 0.0951 at $X_{i,f}$ = 0.2 and 0.5; initial conditions: T_i = 298 K, P_i = 1 bar.

Takizawa et al. [19], CVM		Takizawa et al. [19], CVM		Kim et al. [16], CVM		Kim et al. [16], CVM	
$X_{R\text{-}134a,f}$ = 0.2		$X_{R\text{-}134a,blend}$ = 0.5		$X_{R\text{-}134a,blend}$ = 0.2		$X_{R\text{-}134a,blend}$ = 0.5	
ϕ	S_u [cm/s]	ϕ	S_u [cm/s]	ϕ	S_u [cm/s]	ϕ	S_u [cm/s]
0.755	14.3	0.77	9.37	0.8	12.11	0.85	8.26
0.887	17.72	0.826	10.96	0.9	15.96	0.9	9.41
1	19.5	0.939	11.47	1	18.2	1	10.13
1.15	17.85	0.995	11.43	1.1	18.51	1.1	10.2
1.28	13.46	1.12	10.31	1.2	17.31	1.2	9.22
		1.23	8.09	1.3	14.2	1.3	8
				1.4	11.05	1.4	6.47

Table A- 8: Burning velocity as a function of ϕ for R-152a/R-125 mixtures with air from Takizawa et al. [19]; CVM; data are shown for two values (0.2, 0.4) of the mole fraction $X_{i,f}$ of R-125 in the R-152a/R-125 blend; $X_{i,stoic}$ = 0.0871 and 0.0995 at $X_{i,fuel}$ = 0.2 and 0.4; initial conditions: T_i = 298 K, P_i = 1 bar.

$X_{i,fuel}$ = 0.2		$X_{R\text{-}125,fuel}$ = 0.4	
ϕ	S_u [cm/s]	ϕ	S_u [cm/s]
0.73	12.67	0.838	7.72
0.847	15.34	0.947	7.84
0.998	17.64	1	7.44
1.17	15.95	1.06	7.16
1.29	12.05	1.12	6.92
		1.24	5.35

Table A- 9: Burning velocity as a function of ϕ for R-152a/R-116 mixtures with air from Takizawa et al. [19]; CVM; data are shown for two values (0.2, 0.4) of the mole fraction $X_{i,f}$ of R-116 in the R-152a/R-116 blend; $X_{i,stoic}$ = 0.0909 and 0.110 at $X_{i,f}$ = 0.2 and 0.4; initial conditions: T_i = 298 K, P_i = 1 bar.

$X_{R\text{-}116,fuel}$ = 0.2		$X_{R\text{-}116,fuel}$ = 0.4	
ϕ	S_u [cm/s]	ϕ	S_u [cm/s]
0.752	13.76	0.8	5.25
0.869	15.01	0.847	5.86
0.998	15.18	0.898	5.46
1.11	14.42	1	4.78
1.24	11.56		

Table A- 10: Burning velocity as a function of ϕ for R-152a/R-1234yf mixtures with air from Kim et al. [16]; CVM; data are shown for two values (0.5, 0.6) of the mole fraction $X_{i,f}$ of R-1234yf in the R-152a/R-1234yf blend; $X_{i,stoic}$ = 0.0775 at $X_{i,f}$ = 0.5 and 0.6; initial conditions: T_i = 298 K, P_i = 1 bar.

$X_{R\text{-}1234yf,\ fuel}$ = 0.5		$X_{R\text{-}1234yf,\ fuel}$ = 0.6	
ϕ	S_u [cm/s]	ϕ	S_u [cm/s]
0.8	10.88	0.9	9.23
0.9	12.68	1	9.81
1	13.47	1.1	9.14
1.1	13.55	1.2	8.02
1.2	12.41	1.3	6.7
1.3	10.2	1.4	5.52
1.4	8.14		
1.5	6.61		

Table A- 11: Burning velocity as a function of $X_{i,f}$ of R-1234yf in R-1234yf/C_3H_8 mixtures in air from Papas et al. [7]; tube method; $\phi = 1$; initial conditions: $T_i = 298$ K, $P_i = 1$ bar.

$X_{R\text{-}1234yf,fuel}$	S_u [cm/s]
0.721	22.4
0.777	18.25
0.838	13.81
0.902	7.1
1	1.29

Table A- 12: Burning velocity as a function of the volume fraction $X_{i,f}$ of R-134a in R-134a/CH_4 mixtures in air with $X_{O_2,ox} = 0.185$ from Choi et al. [24]; CPM; $\phi = 1$; initial conditions: $T_i = 298$ K, $P_i = 1$ bar;

$X_{134a,fuel}$	S_u [cm/s]
0	26.67
0.1	20.53
0.2	17.03
0.3	13.36
0.4	10.07
0.5	7.36
0.6	5.55
0.7	3.52
0.75	1.27

Table A- 13: Burning velocity as a function of the volume fraction $X_{i,f}$ of R-134a in R-134a/CH_4 mixtures in air with $X_{O_2,ox} = 0.30$ from Choi et al. [24]; $\phi = 1$; CPM; initial conditions: $T_i = 298$ K, $P_i = 1$ bar;

$X_{134a,fuel}$	S_u [cm/s]
0	78.45
0.1	63.82
0.2	49.55
0.3	38
0.4	31.23
0.5	23.23
0.6	15.97
0.7	9.02
0.8	3.36
0.85	1.54

Table A- 14: Burning velocity as a function of the volume fraction $X_{i,f}$ of R-134a in R-134a/CH_4 mixtures in air with $X_{O_2,ox} = 0.40$ from Choi et al. [24]; CPM; $\phi = 1$; initial conditions: $T_i = 298$ K, $P_i = 1$ bar;

$X_{134a,fuel}$	S_u [cm/s]
0	129.7
0.1	102.1
0.2	82.56
0.3	64.18
0.4	51.25
0.5	40.37
0.6	28.62
0.7	18.08
0.8	5.908
0.9	2.2
0.95	1.44

Table A- 15: Burning velocity as a function of ϕ for R-161/air and R-152/air mixtures from Takizawa et al. [17]; CVM; $X_{R\text{-}152,stoic} = 0.0775$, $X_{R\text{-}161,stoic} = 0.0654$; initial conditions: $T_i = 298$ K, $P_i = 1$ bar.

R-152		**R-161**	
ϕ	S_u [cm/s]	ϕ	S_u [cm/s]
0.756	20.7	0.593	13.2
0.823	24.2	0.668	19.5
0.893	27	0.75	26.1
0.962	29.1	0.834	31.3
1.031	30.4	1.156	36.7
1.103	30.3	1.24	33.1
1.172	28.7	1.324	27.7
1.249	26.9	1.407	21.2
1.319	23.2		

Table A- 16: Burning velocity as a function of ϕ for R-41/air mixtures from Takizawa et al. [17]; CVM; $X_{\text{R-41,stoic}}$ =0.1228; initial conditions: T_i = 298 K, P_i = 1 bar.

ϕ	S_u [cm/s]
0.706	15.5
0.749	18.4
0.794	21.3
0.838	23.9
0.883	26
0.926	27.4
0.972	28.6
0.998	28.4
1.019	28.4
1.067	27.7
1.113	26.1
1.162	23.9
1.217	20.3