UNCLASSIFIED

LEGAL NOTICE

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, express or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission to the extent that such employee or contractor prepares, handles or distributes, or provides access to, any information pursuant to his employment or contract with the Commission.

UNCLASSIFIED

7

K-220(II(Del.))

UNITED STATES ATOMIC ENERGY COMMISSION

FLUOROCARBONS AND FLUOROORGANIC COMPOUNDS. SECTION II

By

J. L. Gabbard

J. D. Gibson

A. V. Faloon

K. E. Rapp

S. E. Frey

D. V. Walker

August 2, 1948

Photostat Price \$ 66.60

Microfilm Price \$ 11.10

Available from the
Office of Technical Services
Department of Commerce
Washington 25, D. C.

Carbide and Carbon Chemicals Corporation
K-25 Plant, Oak Ridge, Tennessee

Technical Information Service Extension, Oak Ridge, Tenn.

220 1A

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

FOREWORD

The following references have been declassified and are presented below with their corresponding MDDC number.

A-199	MDDC-523
A-311	MDDC-514
A-312	MDDC-347
A-1575	MDDC-955
A-3468	MDDC-898
M-3113	MDDC-1177

~~CONFIDENTIAL~~

DECLASSIFIED

INTRODUCTION

This section covers information on fluoroorganic compounds prepared for research purposes. It is a supplement of Section I which consists of information on fluoroorganic compounds which were produced commercially and used on or for the Manhattan Project. The material in both sections was taken from reports of the Manhattan Project and the Atomic Energy Commission and from unpublished data obtained by the Fluorocarbon Section of the K-25 Laboratories.

Since no proposed system for naming fluoroorganic compounds has been adopted by the American Chemical Society, the general system employed by Chemical Abstracts has been followed.

In some instances, the values considered to be the best available are set apart and underlined.

Where physical property data are plotted the figures will be found in numerical sequence at the end of the report.

CONFIDENTIAL

220

2

TABLE OF CONTENTS

	Page
Properties of Fluorocarbons	xxxii
CF ₄ , Tetrafluoromethane	127
Preparation	127
Heat of Formation	127
Melting Point	128
Boiling Point	128
Density	128
Refractive Index	129
Molecular Refraction	129
Vapor Pressure	129
Heat of Vaporization	129
Heat of Fusion	129
Heat of Transition	130
Entropy	130
Heat Capacity	130
Dielectric Constant	131
Polarization	131
Bond Distance	132
Infrared Absorption	132
Reaction	132
CF ₃ Cl, Chlorotrifluoromethane	133
Boiling Point	133
Bond Measurements	133
CF ₃ H, Trifluoromethane	134
Boiling Point	134
Bond Measurements	134
CF ₂ Cl ₂ , Dichlorodifluoromethane	135
Melting Point	135
Boiling Point	135
Density	135
Vapor Pressure	135
Viscosity	136
Critical Temperature	136
Critical Pressure	136
Critical Density	136
Heat of Vaporization	136
Entropy of Vaporization	136
Enthalpy of Vaporization	136
Compressibility Factor	137
Bond Distance	137
Toxicity	137
CF ₂ H ₂ , Difluoromethane	138
Bond Distance	138
CFO ₂ , Carbonyl fluoride	139
Preparation	139
Melting Point	139
Toxicity	139

	Page
CFCl ₃ , Trichlorofluoromethane	140
Melting Point	140
Boiling Point	140
Density	140
Vapor Pressure	140
Viscosity	141
Critical Temperature	141
Critical Pressure	141
Critical Density	141
Heat of Vaporization	141
Entropy of Vaporization	141
Enthalpy of Vaporization	141
Mass Spectrometer Data	142
Compressibility Factor	142
Bond Distance	142
Toxicity	142
CFH ₃ , Fluoromethane	143
Bond Distance	143
CF ₂ AsH ₃ , Methyl difluoroarsine	144
Preparation	144
Boiling Point	144
Toxicity	144
CF ₂ ClH, Chlorodifluoromethane	145
Melting Point	145
Boiling Point	145
Density	145
Vapor Pressure	145
Viscosity	145
Critical Temperature	146
Critical Pressure	146
Critical Density	146
Heat of Vaporization	146
Entropy of Vaporization	146
Enthalpy of Vaporization	146
Compressibility Factor	146
Bond Distance	146
CFCl ₂ H, Dichlorofluoromethane	147
Melting Point	147
Boiling Point	147
Density	147
Vapor Pressure	147
Viscosity	148
Critical Temperature	148
Critical Pressure	148
Critical Density	148
Heat of Vaporization	148
Entropy of Vaporization	148
Enthalpy of Vaporization	148
Compressibility Factor	148
Bond Distance	149
Mass Spectrometer Data	149
Toxicity	149

	Page
CFClH_2 , Chlorofluoromethane	150
Bond Distance	150
CFClO , Carbonyl chlorofluoride	151
Boiling Point	151
Toxicity	151
C_2F_6 , Hexafluoroethane	152
Preparation	152
Melting Point	152
Boiling Point	152
Density	152
Vapor Pressure	152
Heat of Vaporization	153
Dielectric Constant	153
Polarization	153
Bond Measurements	153
C_2F_4 , Tetrafluoroethylene <i>reflon</i>	154
Preparation	154
Freezing Point	154
Boiling Point	154
Bond Measurements	154
Reactions	154
$(\text{CF})_{2.4x}$, Tetrafluoroethylene polymer	155
Reactions	155
$\text{C}_2\text{F}_4\text{Cl}_2$, 1,1-Dichloro-1,2,2,2-tetrafluoroethane	156
Preparation	156
Boiling Point	156
$\text{C}_2\text{F}_4\text{Cl}_2$, 1,2-Dichloro-1,1,2,2-tetrafluoroethane	157
Preparation	157
Freezing Point	157
Boiling Point	157
Density	157
Vapor Pressure	158
Viscosity	158
Critical Temperature	158
Critical Pressure	158
Critical Density	158
Heat of Vaporization	158
Entropy of Vaporization	158
Enthalpy of Vaporization	158
Mass Spectrometer Data	159
$\text{C}_2\text{F}_4\text{H}_2$, 1,1,2,2-Tetrafluoroethane	160
Boiling Point	160
Bond Measurements	160
$\text{C}_2\text{F}_3\text{Br}$, Bromotrifluoroethylene	161
Reactions	161

	Page
$C_2F_3Cl_3$, 1,1,1,-Trichloro-2,2,2-trifluoroethane	162
Preparation	162
Freezing Point	162
Boiling Point	162
Refractive Index	162
Molecular Refraction	163
Bond Distance	163
$C_2F_3Cl_3$, 1,1,2-Trichloro-1,2,2-trifluoroethane	164
Preparation	164
Freezing Point	164
Boiling Point	164
Density	165
Refractive Index	165
Molecular Refraction	165
Vapor Pressure	165
Viscosity	166
Critical Temperature	166
Critical Pressure	166
Critical Density	166
Heat of Vaporization	166
Entropy of Vaporization	166
Enthalpy of Vaporization	166
Compressibility Factor	166
Mass Spectrometer Data	167
Uses	167
C_2F_3Cl , Chlorotrifluoroethylene <i>fluoroethene</i>	167a
$C_2F_3H_3$, 1,1,1-Trifluoroethane	168
Boiling Point	168
Bond Measurements	168
C_2F_3H , Trifluoroethylene	169
Boiling Point	169
Bond Measurements	169
$C_2F_2Cl_4$, 1,1,2,2-Tetrachloro-1,2-difluoroethane	170
Preparation	170
Boiling Point	170
Density	170
Refractive Index	170
$C_2F_2Cl_2$, 1,1-Dichloro-2,2-difluoroethylene	171
Preparation	171
Freezing Point	171
Boiling Point	171
Bond Measurements	171
Reactions	171
$C_2F_2Cl_2$, 1,2-Dichloro-1,2-difluoroethylene	172
Preparation	172
Freezing Point	172
Boiling Point	172
Density	172
Refractive Index	173

	Molecular Refraction	173
	Reaction	173
$C_2F_2Cl_2$	1,1-Difluoroethylene	174
	Boiling Point	174
	Bond Measurements	174
C_2FCl_3	Trichlorofluoroethylene	175
	Reactions	175
C_2F_3BrCl	1,2-Dibromo-1-chloro-1,2,2-trifluoroethane	176
	Preparation	176
	Freezing Point	176
	Boiling Point	176
	Density	176
	Refractive Index	176
	Molecular Refraction	176
$C_2F_3BrH_2$	2-Bromo-1,1,1-trifluoroethane	177
	Preparation	177
	Boiling Point	177
$C_2F_3ClH_2$	2-Chloro-1,1,1-trifluoroethane	178
	Boiling Point	178
	Bond Measurements	178
$C_2F_3H_3O$	2,2,2-Trifluoroethanol	179
	Preparation	179
	Boiling Point	179
$C_2F_3H_3O$	Trifluoromethyl methyl ether	180
	Density	180
	Molecular Volume	180
$C_2F_3HO_2$	Trifluoroacetic acid	181
	Preparation	181
$C_2F_3NaO_2$	Sodium trifluoroacetate	182
	Preparation	182
$C_2F_2AsH_5$	Ethyldifluoroarsine	183
	Preparation	183
	Boiling Point	183
	Toxicity	183
C_2FCl_4H	1,1,2,2-Tetrachloro-1-fluoroethane	184
	Preparation	184
	Melting Point	184
	Boiling Point	184
	Density	184
	Refractive Index	184
C_2FClH_2	1-Chloro-1-fluoroethylene	185
	Boiling Point	185
	Bond Distance	185

	Page
C_2F_5O , 2-Fluoroethanol	186
Preparation	186
Boiling Point	186
Vapor Pressure	186
Toxicity	186
$C_2F_6O_3P$, Dimethylfluorophosphate	187
Boiling Point	187
Volatility	187
Toxicity	187-188
C_3F_8 , Octafluoropropane	189
Preparation	189
Melting Point	189
Boiling Point	189
Density	189
Vapor Pressure	189
Heat of Vaporization	190
Bond Measurements	190
C_3F_6 , Hexafluoropropene	191
Preparation	191
C_3F_7Cl , 2-Chloro-1,1,1,2,3,3,3, heptafluoropropane	192
Preparation	192
Boiling Point	192
Reactions	192
$C_3F_6Br_2$, 1,2-Dibromo-1,1,2,3,3,3-hexafluoropropane	193
Preparation	193
Freezing Point	193
Boiling Point	193
Density	193
Refractive Index	193
Molecular Refraction	194
Reactions	194
$C_3F_6Cl_2$, 1,2-Dichloro-1,1,2,3,3,3-hexafluoropropane	195
Preparation	195
Freezing Point	195
Boiling Point	195
Density	196
Refractive Index	196
Molecular Refraction	196
Reactions	196
C_3F_6H , 1,1,1,3,3,3-Hexafluoropropane	197
Boiling Point	197
C_3F_6O , 1,1,1,3,3,3-Hexafluoro-2-propanone	198
Preparation	198
Boiling Point	198

	Page
C F Cl ₃ , 1,1,2-Trichloro-1,2,3,3,3-pentafluoropropane	199
Preparation	199
Boiling Point	199
Density	199
Refractive Index	199
Molecular Refraction	199
C F Cl ₃ , 1,2,2-Trichloro-1,1,3,3,3-pentafluoropropane	200
Preparation	200
Freezing Point	200
Boiling Point	200
Density	200
Refractive Index	200
Molecular Refraction	200
C F Cl ₃ , 1,2,3-Trichloro-1,1,2,3,3-pentafluoropropane	201
Preparation	201
Boiling Point	201
Density	201
Refractive Index	201
Molecular Refraction	201
Reactions	201
C F Cl ₃ , 1-Chloro-1,2,3,3,3-pentafluoropropene	202
Preparation	202
Boiling Point	202
C F Cl ₃ , 2-Chloro-1,1,3,3,3-pentafluoropropene	203
Preparation	203
Freezing Point	203
Boiling Point	203
Density	203
Refractive Index	204
Molecular Refraction	204
Reactions	204
Pyrolysis	204
C F Cl ₃ , 3-Chloro-1,1,2,3,3-pentafluoropropene	205
Preparation	205
Boiling Point	205
Density	205
Refractive Index	205
Molecular Refraction	205
Reactions	206
Pyrolysis	206
C F Cl ₄ , Tetrachlorotetrafluoropropane	207
Preparation	207
Boiling Point	207
Density	207
Refractive Index	207
Reactions	207

	Page
C F Cl ₁ , 2,3-Dichloro-1,1,3,3-tetrafluoropropene	208
3 4 2 Preparation	208
Freezing Point	208
Boiling Point	208
Density	208
Refractive Index	208
Molecular Refraction	208
C F Cl ₁ , Dichlorotetrafluoropropene	209
3 4 2 Preparation	209
Boiling Point	209
Density	209
Refractive Index	209
Reactions	209
C F Cl ₁ , 1,1,1,2,2-Pentachloro-3,3,3-trifluoropropane	210
3 3 5 Preparation	210
Freezing Point	210
Boiling Point	210
Density	210
Refractive Index	210
C F Cl ₁ , 1,1,2-Trichloro-3,3,3-trifluoropropene	211
3 3 3 Preparation	211
Freezing Point	211
Boiling Point	211
Density	211
Refractive Index	211
Molecular Refraction	211
Reactions	211
C F H ₅ , 1,1,1-Trifluoropropane	212
3 3 5 Boiling Point	212
Bond Measurements	212
C F H ₅ , 2,2-Difluoropropane	213
3 2 6 Boiling Point	213
Bond Measurements	213
C F H ₅ , 1,1-Difluoropropane	214
3 2 4 Boiling Point	214
C F Br Cl ₁ , 1,2-Dibromo-2-chloro-1,1,3,3,3-pentafluoropropane	215
3 5 2 Preparation	215
Boiling Point	215
C F Br Cl ₁ , 1,2-Dibromo-3-chloro-1,1,2,3,3-pentafluoropropane	216
3 5 2 Preparation	216
Freezing Point	216
Boiling Point	216
Density	216
Refractive Index	216
Molecular Refraction	216

	Page
$C_3F_3B_2Cl_2$, Dibromodichlorotetrafluoropropane	217
Preparation	217
Boiling Point	217
Density	217
Refractive Index	217
Reactions	217
$C_4F_4H_2O$, 1,1,2,2-Tetrafluor-1-methoxyethane	218
Preparation	218
Freezing Point	218
Boiling Point	218
Density	218
$C_3F_3Cl_4H$, 1,1,2,2-Tetrachloro-3,3,3-trifluoropropane	219
Boiling Point	219
Density	219
Refractive Index	219
$C_3F_5H_2O$, Methyl fluoroacetate	220
Preparation	220
Freezing Point	220
Boiling Point	220
Vapor Pressure	220
Toxicity	220
Absorption	221
$C_3F_4ClH_2O$, 2-Chloro-1,1,2-trifluoro-1-methoxyethane	222
Preparation	222
Freezing Point	222
Boiling Point	222
Density	222
Refractive Index	222
Molecular Refraction	223
Solubility	223
$C_3F_2Cl_2H_2O$, 2,2-Dichloro-1,1-difluoro-1-methoxyethane	224
Preparation	224
Freezing Point	224
Boiling Point	224
Density	224
Refractive Index	224
Molecular Refraction	225
Reactions	225
C_4F_{10} , Decafluorobutane	226
Preparation	226
Melting Point	226
Boiling Point	226
Density	227
Vapor Pressure	228
Critical Temperature	228
Critical Pressure	228
Critical Density	228
Heat of Vaporization	229
Entropy of Vaporization	229

220 11
note pg 11A
follows

	Page
C ₄ F ₈ , Octafluoro-1-butene	230
Preparation	230
Boiling Point	230
Density	230
Reactions	230
C ₄ F ₈ , Octafluoro-2-butene	231
Preparation	231
Melting Point	231
Boiling Point	231
Density	231
Reactions	231
C ₄ F ₈ , Octafluorocyclobutane	232
Preparation	232
Boiling Point	232
Density	232
C ₄ F ₆ , Hexafluoro-1,3-butadiene	233
Preparation	233
Freezing Point	233
Boiling Point	233
Density	233
Refractive Index	233
Molecular Refraction	234
Reactions	234
C ₄ F ₆ , Hexafluorocyclobutene	235
Preparation	235
Freezing Point	235
Boiling Point	235
Density	235
Refractive Index	236
Molecular Refraction	236
Reactions	236
C ₄ F ₈ Br ₂ , 2,3-Dibromo-1,1,1,2,3,4,4,4-octafluorobutane	237
Preparation	237
Boiling Point	237
Refractive Index	237
C ₄ F ₆ Br ₂ , Dibromohexafluorobutene	238
Preparation	238
Boiling Point	238
Density	238
Refractive Index	238
Reactions	238
C ₄ F ₈ Cl ₂ , 1,2-Dichloro-1,1,2,3,3,4,4,4-octafluorobutane	239
Preparation	239
Freezing Point	239
Boiling Point	239
Reaction	239

	Page
C F Cl ₄ 8 2, 1,4-Dichloro-1,1,2,2,3,4,4,4-octafluorobutane	240
Preparation	240
Boiling Point	240
C F Cl ₄ 8 2, 2,3-Dichloro-1,1,1,2,3,4,4,4-octafluorobutane	241
Preparation	241
Boiling Point	241
C F Cl ₄ 7 3, Trichloroheptafluorobutane	242
Preparation	242
Boiling Point	242
Density	242
Refractive Index	242
Molecular Refraction	242
C F Cl ₄ 7 3, Trichloroheptafluorobutane	243
Preparation	243
Boiling Point	243
Density	243
Refractive Index	243
Molecular Refraction	243
C F Cl ₄ 7, Chloroheptafluorobutene	244
Preparation	244
Boiling Point	244
Reaction	244
C F Cl ₄ 7, 2-Chloro-1,1,1,3,4,4,4-heptafluoro-2-butene	245
Preparation	245
Boiling Point	245
Density	245
Refractive Index	245
C F Br ₄ 6 4, 1,2,3,4-Tetrabromo-1,1,2,3,4,4,4-hexafluorobutane	246
Preparation	246
Boiling Point	246
Density	246
Refractive Index	246
C F Cl ₄ 6 4, 1,2,3,4-Tetrachloro-1,1,2,3,4,4,4-hexafluorobutane	247
Preparation	247
Boiling Point	247
Density	247
Refractive Index	247
Molecular Refraction	248
Reactions	248
C F Cl ₄ 6 2, 1,2-Dichloro-1,2,3,3,4,4-hexafluorocyclobutane	249
Preparation	249
Freezing Point	249
Boiling Point	249
Density	249
Refractive Index	249
Molecular Refraction	250
Reactions	250

	Page
$C_4F_6Cl_2$, 1,4-Dichloro-1,1,2,3,4,4-hexafluoro-2-butene	251
Preparation	251
Boiling Point	251
Reactions	251
$C_4F_6Cl_2$, 2,3-Dichloro-1,1,1,4,4,4-hexafluoro-2-butene	252
Preparation	252
Boiling Point	252
Density	252
Refractive Index	252
$C_4F_6Cl_2$, 3,4-Dichloro-1,1,2,3,4,4-hexafluoro-1-butene	253
Preparation	253
Boiling Point	253
Density	253
Refractive Index	253
Molecular Refraction	254
Reactions	254
$C_4F_5Cl_5$, Pentachloropentafluorobutane	255
Preparation	255
Boiling Point	255
Density	255
Refractive Index	255
Molecular Refraction	255
$C_4F_5Cl_3$, 3,3,4-Trichloro-1,1,2,4,4-pentafluoro-1-butene	256
Preparation	256
Boiling Point	256
$C_4F_4Cl_6$, 1,1,2,3,4,4-Hexachloro-1,2,3,4-tetrafluorobutane	257
Preparation	257
Boiling Point	257
Density	257
Refractive Index	257
Molecular Refraction	257
Reactions	257
$C_4F_4Cl_6$, 1,2,2,3,3,4-Hexachloro-1,1,4,4-tetrafluorobutane	258
Preparation	258
Boiling Point	258
Density	258
Refractive Index	258
Molecular Refraction	258
Reactions	258
$C_4F_4Cl_2$, 1,4-Dichloro-1,2,3,4-tetrafluoro-1,3-butadiene	259
Preparation	259
Boiling Point	259
Density	259
Refractive Index	259
Molecular Refraction	259
Reactions	260

	Page
$C_4F_4Cl_2$, 2,3-Dichloro-1,1,4,4-tetrafluoro-1,3-butadiene	261
Preparation	261
Boiling Point	261
Density	261
Refractive Index	261
Molecular Refraction	261
Reactions	262
$C_4F_3Cl_7$, Heptachlorotrifluorobutane	263
Preparation	263
Boiling Point	263
Density	263
Refractive Index	263
Molecular Refraction	263
C_4F_3H , 1,1,1-Trifluorobutane	264
Melting Point	264
$C_4F_2Cl_8$, 1,1,2,2,3,3,4,4-Octafluoro-1,4-difluorobutane	265
Preparation	265
Boiling Point	265
Density	265
Refractive Index	265
Molecular Refraction	265
Reactions	266
$C_4F_2Cl_4$, 1,2,3,4-Tetrachloro-1,4-difluoro-1,3-butadiene	267
Preparation	267
Melting Point	267
Boiling Point	267
Density	267
Refractive Index	267
Molecular Refraction	268
Reactions	268
$C_4F_2H_8$, 2,2-Difluorobutane	269
Preparation	269
Density	269
Molecular Volume	269
$C_4F_2H_6$, 1,1-Difluoro-1-butene	270
Boiling Point	270
$C_4F_6Br_2Cl_2$, 1,2-Dibromo-3,4-dichloro-1,1,2,3,4,4-hexafluorobutane	271
Preparation	271
Boiling Point	271
Density	271
Refractive Index	271
Molecular Refraction	271
Reaction	271
$C_4F_6Cl_2H_2$, Dichlorohexafluorobutane	272
Boiling Range	272
Density	272
Refractive Index	272

	Page
C_4F_5ClH , Chlorohexafluorobutene	273
Boiling Point	273
Density	273
Refractive Index	273
$C_4F_4Cl_3H$, Trichlorotetrachlorobutene	274
Boiling Point	274
Density	274
Refractive Index	274
$C_4F_3H_5O_2$, Ethyl trifluoroacetate	275
Preparation	275
Boiling Point	275
Refractive Index	275
$C_4F_2H_6O_2$, 2-Fluoroethyl fluoroacetate	276
Boiling Point	276
Toxicity	276
$C_4FCl_2H_5O_2$, Ethyl dichlorofluoroacetate	277
Preparation	277
$C_4FClH_6O_2$, 2-Chloroethyl fluoroacetate	278
Preparation	278
Boiling Point	278
Toxicity	278
$C_4FH_{10}O_3P$, Diethylfluorophosphate	279
Boiling Point	279
Volatility	279
Toxicity	279
C_5F_{12} , Dodecafluoropentane	280
Preparation	280
Boiling Point	280
C_5F_{12} , 1,1,1,2,3,3,4,4,4-Nonafluoro-2-trifluoroethylbutane	281
Preparation	281
Boiling Range	281
C_5F_{10} , Decafluorocyclopentane	282
Preparation	282
Melting Point	282
Boiling Point	282
Density	282
Refractive Index	283
Vapor Pressure	283
Heat of Vaporization	283
$C_5F_{11}Cl$, Chloroundecafluoropentane	284
Boiling Point	284
Density	284
Refractive Index	284

	Page
C ₅ F ₁₀ Cl ₂ , Dichlorodecafluoropentane	285
Boiling Point	285
Density	285
Refractive Index	285
C ₅ F ₉ Cl ₃ , Trichlorononafluoropentane	286
Boiling Point	286
Density	286
Refractive	286
C ₅ F ₆ Cl ₂ , 1,2 Dichloro-3,3,4,4,5,5-hexafluorocyclopentene	287
Preparation	287
Reactions	287
C ₅ F ₆ Cl ₂ , Dichlorohexafluoropentadiene	288
Boiling Point	288
Refractive Index	288
C ₅ F ₂ H ₁₀ , 2,2-Difluoropentane	289
Density	289
Molecular Volume	289
C ₅ F ₂ H ₁₀ , 3,3-Difluoropentane	290
Density	290
Molecular Volume	290
C ₅ F ₁₁ H, 1-Fluoropentane	291
Density	291
Molecular Volume	291
C ₅ F ₉ ClH, Dichlorononafluoropentane	292
Boiling Point	292
Refractive Index	292
C ₅ F ₈ ClH, Chlorooctafluoropentene	293
Preparation	293
Boiling Point	293
Refractive Index	293
C ₅ F ₆ Cl ₃ H, Trichlorohexafluoropentene	294
Preparation	294
Boiling Point	294
Refractive Index	294
C ₅ F ₆ H ₂ O, 1,1,1,5,5,5-Hexafluoro-2,4-pentanedione	295
Preparation	295
C ₅ F ₆ H ₂ O ₄ , Hexafluoroglutaric acid	296
Preparation	296
C ₅ F ₃ H ₅ O ₂ , 1,1,1-Trifluoro-2,4-pentanedione	297
Preparation	297

	Page
C_6F_{14} , Tetradecafluorohexane	298
Preparation	298
Boiling Point	298
C_6F_{12} , 2,3-Bis(trifluoromethyl)-1,1,1,4,4,4-hexafluoro-2-butene	299
Preparation	299
Boiling Point	299
Reactions	299
C_6F_{12} , Dodecafluorocyclohexane	300
Preparation	300
Melting Point	300
Boiling Point	300
Density	300
Refractive Index	301
Specific Refraction	301
Vapor Pressure	301
Heat of Vaporization	301
Solubility	301
Ultraviolet Absorption	302
Bond Distance	302
C_6F_6 , Hexafluorobenzene	303
Melting Point	303
Boiling Point	303
Density	303
Refractive Index	303
$C_6F_{14}O$, Bis(heptafluoroisopropyl)ether	304
$C_6F_{13}Cl$, Chlorotridecafluorohexane	305
Boiling Point	305
Density	305
Refractive Index	305
$C_6F_{12}Cl_2$, 2,3-Dichloro-2,3-bis(trifluoromethyl)-1,1,1,4,4,4-hexafluorobutane	306
Preparation	306
Melting Point	306
Boiling Point	306
Reactions	306
$C_6F_{12}Cl_2$, Dichlorododecafluorohexane	307
Boiling Point	307
Density	307
Refractive Index	307
$C_6F_{10}Cl_2$, Dichlorodecafluorocyclohexane	308
Boiling Point	308
Refractive Index	308

	Page
$C_6F_8Cl_6$, Hexachlorooctafluorohexane	309
Preparation	309
Boiling Point	309
Density	309
Refractive Index	309
Molecular Refraction	309
$C_6F_3H_3$, 1,2,4-Trifluorobenzene	310
Bond Distance	310
$C_6F_2H_2$, 2,2-Difluoro-4-methyl pentane	311
Density	311
Molecular Volume	311
$C_6F_2H_4$, p-Difluorobenzene	312
Preparation	312
Boiling Point	312
Bond Distance	312
C_6F_5H , Fluorobenzene	313
Boiling Point	313
Density	313
Molecular Volume	313
Bond Distance	313
Toxicity	313
$C_6F_2H_5N$, 2,5-Difluoroaniline	314
Preparation	314
Boiling Point	314
C_6FClH_4 , 1-Chloro-2-fluorobenzene	315
Boiling Point	315
Bond Distance	315
C_6FClH_4 , 1-Chloro-3-fluorobenzene	316
Boiling Point	316
Bond Distance	316
C_6FH_4N , 4-Fluoroaniline	317
Preparation	317
Boiling Point	317
$C_6F_2H_3NO_2$, 1,4-Difluoro-3-nitrobenzene	318
Preparation	318
Boiling Point	318
$C_6FH_4NO_2$, 1-Fluoro-4-nitrobenzene	319
Preparation	319
Boiling Point	319
$C_6F_3H_{12}OP$, Tris(2-fluoroethyl)phosphite	320
Preparation	320
Boiling Point	320
Toxicity	320

	Page
C ₆ FH ₁₄ O ₃ P, Di-isopropylfluorophosphate	321
Boiling Point	321
Volatility	321
Toxicity	321
C ₇ F ₁₆ , 1,1,1,3,4,4,4-Heptafluoro-2,2,3-tris(trifluoromethyl)butane	322
Preparation	322
Boiling Point	322
Density	322
Refractive Index	322
Specific Refraction	322
C ₇ F ₁₆ , Hexadecane <i>fluoro</i>	322a
C ₇ F ₁₆ , 1,1,1,2,3,4,4,5,5,5-Decafluoro-2,3-bis(trifluoromethyl)pentane	323
Preparation	323
Boiling Point	323
Density	323
Refractive Index	324
Specific Refraction	324
Purification	324
C ₇ F ₁₄ , Nonafluoro(pentafluoroethyl)cyclopentane	325
Preparation	325
Boiling Point	325
Density	325
Refractive Index	326
Specific Inductance Capacity	326
Infrared Absorption	326
C ₇ F ₁₄ , Undecafluoro(trifluoromethyl)cyclohexane	326a
C ₇ F ₁₄ , Octafluorobis(trifluoromethyl)cyclopentane	327
Preparation	327
Boiling Point	327
Density	327
Refractive Index	327
C ₇ F ₁₅ Cl, Chloropentadecafluoroheptane	328
Preparation	328
Boiling Point	328
Density	328
Refractive Index	328
Specific Inductance Capacity	329
Analysis	329
C ₇ F ₁₅ H, Pentadecafluoroheptane	330
Preparation	330
Boiling Point	330
Density	330
Refractive Index	330
Specific Inductance Capacity	331

	Page
$C_7F_{14}Cl_2$, Dichlorotetradecaheptane	332
Preparation	332
Boiling Point	332
Density	332
Refractive Index	332
Specific Inductance Capacity	332
$C_7F_{14}H_2$, Tetradecafluoroheptane	333
Preparation	333
Freezing Point	333
Boiling Point	333
Specific Inductance Capacity	333
$C_7F_{13}Cl$, Chlorodecafluoro(trifluoromethyl)cyclohexane	334
Preparation	334
Boiling Point	334
Density	334
Refractive Index	334
Mass Spectrometer Data	335
$C_7F_{13}Cl$, (Chlorodifluoromethyl)undecafluorocyclohexane	336
Boiling Point	336
Density	336
Refractive Index	336
$C_7F_{13}Cl$, Chlorotridecafluoroheptene	337
Boiling Point	337
Density	337
Refractive Index	337
$C_7F_{13}H_3$, Tridecafluoroheptane	338
Preparation	338
Boiling Point	338
$C_7F_{13}H$, Tridecafluoroheptene	339
Preparation	339
Boiling Point	339
Density	339
Refractive Index	339
Specific Refraction	339
$C_7F_{12}Cl_2$, Dichlorododecafluoroheptene	340
Boiling Point	340
Density	340
Refractive Index	340
$C_7F_{12}H_4$, Dodecafluoroheptane	341
Boiling Point	341
Density	341
Refractive Index	341
Specific Inductance Capacity	341
$C_7F_{12}H_2$, Dodecafluoroheptene	342
Preparation	342
Boiling Point	342

	Page
Refractive Index	342
$C_7F_5H_3$, 1,4-Difluoro-2-(trifluoromethyl)benzene	343
Boiling Point	343
$C_7F_4H_4$, 1-Fluoro-3-(trifluoromethyl)benzene	344
Density	344
Molecular Volume	344
Ultraviolet Absorption	344
$C_7F_4H_4$, 1-Fluoro-4-(trifluoromethyl)benzene	345
Ultraviolet Absorption	345
$C_7F_3H_5$, (Trifluoromethyl)benzene	346
Preparation	346
Freezing Point	346
Boiling Point	346
Density	347
Refractive Index	347
Vapor Pressure	348
Viscosity	348
Surface Tension	349
Parachor	349
Molecular Volume	349
Infrared Absorption	349
Ultraviolet Absorption	349
Bond Measurements	350
Reactions	350
$C_7F_2H_{14}$, 1,1-Difluoroheptane	351
Boiling Point	351
Density	351
Molecular Volume	351
$C_7F_2H_{14}$, 2,2-Difluoroheptane	352
Boiling Point	352
$C_7F_2H_6$, (Difluoromethyl)benzene	353
Density	353
Molecular Volume	353
$C_7F_2H_6$, 2,4-Difluorotoluene	354
Preparation	354
Ultraviolet Absorption	354
C_7FH_{15} , 1-Fluoroheptane	355
Boiling Point	355
C_7FH_7 , (Fluoromethyl)benzene	356
Density	356
Molecular Volume	356
C_7FH_7 , m-Fluorotoluene	357
Preparation	357
Density	357

	Molecular Volume	357
	Ultraviolet Absorption	358
C_7F_7H , p-Fluorotoluene		359
	Ultraviolet Absorption	359
$C_7F_{12}Cl_2H_2$, Dichlorododecafluoroheptane		360
	Preparation	360
	Boiling Point	360
$C_7F_{11}Cl_3H_2$, Trichloroundecafluoroheptane		361
	Preparation	361
	Boiling Point	361
$C_7F_{11}ClH_4$, Chloroundecafluoroheptane		362
	Boiling Point	362
	Density	362
	Refractive Index	362
	Specific Inductance Capacity	362
$C_7F_{11}ClH_2$, Chloroundecafluoroheptene		363
	Preparation	363
	Boiling Point	363
	Refractive Index	363
$C_7F_{10}Cl_4H_2$, Tetrachlorodecafluoroheptane		364
	Preparation	364
	Boiling Point	364
$C_7F_{10}Cl_2H_4$, Dichlorodecafluoroheptane		365
	Boiling Point	365
	Density	365
	Refractive Index	365
	Specific Inductance Capacity	365
$C_7F_{10}Cl_2H_2$, Dichlorodecafluoroheptene		366
	Preparation	366
	Boiling Point	366
	Refractive Index	366
$C_7F_9Cl_3H_4$, Trichlorononafluoroheptane		367
	Boiling Point	367
	Density	367
	Refractive Index	367
	Specific Inductance Capacity	367
$C_7F_9Cl_3H_2$, Trichlorononafluoroheptene		368
	Preparation	368
	Boiling Point	368
	Refractive Index	368
$C_7F_8Cl_2H_2$, Dichlorooctafluoroheptadiene		369
	Preparation	369
	Boiling Point	369
	Refractive Index	369

Reactions	Page
	369
$C_7F_3Cl_2H_3$, Dichloro(trifluoromethyl)benzene	370
Boiling Point	370
$C_7F_3ClH_4$, 1-Chloro-4-(trifluoromethyl)benzene	371
Boiling Point	371
C_8F_{18} , Octadecafluorooctane	372
Boiling Point	372
Density	372
Refractive Index	372
Specific Refraction	372
Molecular Refraction	373
Vapor Pressure	373
Viscosity	373
Surface Tension	373
Parachor	373
C_8F_{18} , 2,2,4-Tris(trifluoromethyl)-1,1,1,3,3,4,4,5,5,5-nonafluoropentane	374
Boiling Point	374
Density	374
Refractive Index	374
Specific Refraction	375
Molecular Refraction	375
Molecular Volume	375
C_8F_{16} , Decafluorobis(trifluoromethyl)cyclohexane	375a
C_8F_{12} , Hexafluoro-1,3-butadiene dimer	376
Preparation	376
Boiling Point	376
Density	376
Refractive Index	376
Reactions	376
C_8F_{12} , Hexafluoro-1,3-butadiene dimer	377
Preparation	377
Freezing Point	377
Boiling Point	377
Reactions	377
$C_8F_{17}N$, Bis(trifluoromethyl)undecafluorocyclohexylamine	378
Density	378
Molecular Volume	378
$C_8F_{15}Cl$, Chlorononafluorobis(trifluoromethyl)cyclohexane	379
Preparation	379
Boiling Point	379
Density	379
Refractive Index	379
Vapor Pressure	380
Viscosity	381
Surface Tension	381

	Page
Parachor	381
Heat of Vaporization	381
Entropy of Vaporization	382
Ultrasonic Velocity	382
Infrared Absorption	382
$C_8F_{14}Cl_4$, 1,6-Dichloro-1,1,2,2,3,4,5,5,6,6-decafluoro-3,4-bis(chlorodifluoromethyl)hexane	383
Preparation	383
Boiling Point	383
$C_8F_{14}Cl_2$, Dichlorooctabis(trifluoromethyl)cyclohexane	383a
$C_8F_{12}Cl_6$, Hexafluoro-1,3-butadiene dimer hexachloride	384
Preparation	384
Boiling Point	384
Refractive Index	384
Reactions	384
$C_8F_{12}Cl_4$, Hexafluoro-1,3-butadiene dimer tetrachloride	385
Preparation	385
Boiling Point	385
Refractive Index	385
Reaction	385
$C_8F_6Cl_4$, Tetrachlorobis(trifluoromethyl)benzene	386
Preparation	386
$C_8F_6H_4$, Bis(trifluoromethyl)benzene	386a
$C_8F_3Cl_7$, 1-(Dichlorotrifluoroethyl)-2,3,4,5,6-pentachlorobenzene	387
Preparation	387
Melting Point	387
$C_8F_2Cl_8$, 1-(Trichlorodifluoroethyl)-2,3,4,5,6-pentachlorobenzene	388
Preparation	388
Melting Point	388
$C_8F_2H_{16}$, 2,2-Difluorooctane	389
Density	389
Molecular Volume	389
$C_8F_7Cl_2H$, Dichlorofluorobis(trifluoromethyl)benzene	390
Preparation	390
Melting Point	390
Boiling Point	390
Reactions	390
$C_8F_6Cl_2H_2$, 1,2-Dichloro-3,5-bis(trifluoromethyl)benzene	391
Boiling Point	391
$C_8F_6Cl_2H_2$, Dichlorobis(trifluoromethyl)benzene	391a
$C_8F_6ClH_3$, 1-Chloro-2,4-bis(trifluoromethyl)benzene	392
Boiling Point	392

	Page
$C_8F_6ClH_3$, 1-Chloro-3,5-bis(trifluoromethyl)benzene	393
Boiling Point	393
Bond Distance	393
$C_8F_6ClH_3$, Chlorobis(trifluoromethyl)benzene	393a
$C_8F_4Cl_5H$, (Chlorotetrafluoroethyl)tetrachlorobenzene	394
Preparation	394
Boiling Point	394
$C_8F_3Cl_6H$, (Dichlorotrifluoroethyl)tetrachlorobenzene	395
Preparation	395
Boiling Point	395
$C_8F_3Cl_4H$, (Dichlorotrifluoroethyl)chlorobenzene	396
Preparation	396
Boiling Point	396
Density	396
Refractive Index	396
$C_8F_2Cl_4H_4$, (Trichlorodifluoroethyl)chlorobenzene	397
Preparation	397
Boiling Point	397
Density	397
Refractive Index	397
$C_8F_5H_2O_3S$, 1,1,1-Trifluoro-3-thenoylpropanone	398
Preparation	398
$C_{20}F_{19}$, Eicosafuorononane	399
Boiling Point	399
Density	399
Refractive Index	399
Specific Refraction	399
Viscosity	399
Surface Tension	400
Parachor	400
C_9F_{18} , Nonafluoro-1,2,4-tris(trifluoromethyl)cyclohexane	401
Boiling Point	401
Density	401
Refractive Index	401
C_9F_{18} , Nonafluoro-1,3,5-tris(trifluoromethyl)cyclohexane	402
Preparation	402
Melting Point	402
Boiling Point	403
Density	403
Refractive Index	403
Specific Refraction	403
Viscosity	404
Molecular Volume	404
Analysis	404

	Page
C_9F_{16} , Hexadecafluorooctahydroindene	405
Preparation	405
Freezing Point	405
Boiling Point	405
Density	405
Refractive Index	405
$C_9F_9H_3$, 1,3,5-Tris(trifluoromethyl)benzene	406
Preparation	406
Melting Point	406
Boiling Point	406
Density	406
Refractive Index	407
Bond Measurements	407
$C_9F_9H_2$, 2,4,6-Trifluoromesitylene	408
Freezing Point	408
Boiling Point	408
Bond Distance	408
$C_9F_9Cl_2H$, 2,4-Dichloro-1,3,5-tris(trifluoromethyl)benzene	409
Preparation	409
Melting Point	409
Boiling Point	409
$C_9F_9ClH_2$, 2-Chloro-1,3,5-tris(trifluoromethyl)benzene	410
Preparation	410
Melting Point	410
Boiling Point	410
Density	410
Refractive Index	411
Molecular Refraction	411
$C_{10}F_{20}$, 1-Trifluoromethyl-4-(heptafluoroisopropyl)decafluoro cyclohexane	412
Boiling Point	412
$C_{10}F_{18}$, Octadecafluorodecahydronaphthalene	413
Melting Point	413
Boiling Point	413
Density	413
Refractive Index	414
Specific Refraction	414
Molecular Refraction	414
Viscosity	414
Surface Tension	414
Parachor	414
Molecular Volume	415
$C_{10}F_{10}H_4$, Bis(pentafluoroethyl)benzene	416
Preparation	416
$C_{10}FH_7$, 1-Fluoronaphthalene	417
Density	417
Molecular Volume	417

	Page
$C_{11}F_{20}$, Heptadecafluoro-1-(trifluoromethyl)decahydronaphthalene	418
Melting Point	418
Boiling Point	418
Density	418
Refractive Index	418
$C_{11}F_{20}$, Heptadecafluoro-2-(trifluoromethyl)decahydronaphthalene	419
Melting Point	419
Boiling Point	419
Density	419
Refractive Index	419
$C_{12}F_{22}$, Docosafluorodicycloheyl	420
Melting Point	420
Boiling Point	420
$C_{12}F_{20}$, Eicosafluorododecahydroacenaphthylene	421
Freezing Point	421
Boiling Point	421
Density	421
Refractive Index	421
$C_{12}F_{18}$, Hexafluorobutadiene trimers	422
Preparation	422
Boiling Point	422
Density	422
Refractive Index	422
$C_{12}F_{22}O$, Docosafluorodicyclohexylether	423
Preparation	423
Boiling Point	423
$C_{12}F_8H_8$, 4,4'-Difluorodiphenyl	424
Melting Point	424
$C_{13}F_{22}$, Docosafluorododecahydrofluorene	425
Melting Point	425
Boiling Point	425
Density	425
Refractive Index	425
$C_{13}F_{11}$, Diphenylfluoromethane	426
Density	426
Molecular Volume	426
$C_{14}F_{24}$, Tetracosafuorotetradecahydroanthracene	427
Melting Point	427
Boiling Point	427
$C_{14}F_{24}$, Tetracosafuorotetradecahydrophenanthrene	428
Melting Point	428
Boiling Point	428
Density	428
Refractive Index	428

	Page
$C_{16}F_{34}$, Tetratriacontafluorohexadecane	429
Preparation	429
Melting Point	429
Boiling Point	429
Analysis	429
$C_{16}F_{26}$, Hexacosafuorohexadecahydrofluoranthene	430
Melting Point	430
Boiling Point	430
Density	430
Refractive Index	430
$C_{18}F_{38}$, Octatriacontafluorooctadecane	431
Specific Refraction	431
Molecular Refraction	431
$C_{18}F_{32}$, Docosafluoro-7-(heptafluoroisopropyl)-1-(trifluoromethyl) tetradecahydrophenanthrene	432
Boiling Point	432
Density	432
Refractive Index	432
Viscosity	432
$C_{18}F_{30}$, Triacontafluorooctahydrochrysene	433
Boiling Point	433
Density	433
Refractive Index	433
Viscosity	433

PROPERTIES OF FLUOROCARBONS

I. Physical Properties

Fluorocarbons are heavy, colorless, nearly odorless compounds. They have higher volatility and viscosity and lower surface tension than the corresponding hydrocarbons. As molecular weight is increased the liquids become viscous and rather tacky, finally becoming brittle solids having a waxy texture. Perhaps the most interesting properties of fluorocarbons arise from their stability and low internal energy.

Melting Point The melting point of fluorocarbons vary greatly depending on molecular symmetry. Comparison of the melting points of fluorocarbons with those of the corresponding hydrocarbons leads to the tentative conclusion that the fluorocarbons melt substantially higher, with the possible exception of CF_4 .

Boiling Point The boiling points of various fluorocarbons like those of other types of organic compounds are primarily dependent on molecular weight. The number of carbon atoms predicts the boiling point quite well and the number of fluorine atoms is of secondary importance provided the compounds are saturated.

Density The densities of both the perfluoroparaffin and naphthene series increase regularly with the number of carbon atoms. The increase per C-atom is, however, much larger than in the hydrocarbon series. The temperature coefficient of density is also very high. The density appears to approach a maximum of about 2.15 as the molecular size is increased. Density has been found to be a fair index of purity since unreplaced hydrogen in the molecule lowers the density appreciably.

Refractive Index The refractive indices of fluorocarbons are lower than those of any other known type of compounds, due to the very low atomic refraction of fluorine. For this reason those compounds of molecular weight below 500 or 600 cannot be measured on usual laboratory instruments. They can be measured by using a sugar refractometer or by employing the method of minimum deviation and using a hollow prism. As is to be expected, the temperature coefficient of the index is large. The atomic refraction of fluorine is not a constant but varies from about 0.95 in monofluoro compounds to about 1.24 in compounds such as C_7F_{16} . The indices of perfluoronaphthenes increase regularly with the number of carbon atoms. As expected, the refractive indices of the corresponding paraffins are lowered.

Vapor Pressure The volatility of fluorocarbons is quite striking, particularly if considered on the basis of molecular weight. Above C_4 , the fluorocarbons are much more volatile than the corresponding hydrocarbons. Structural isomerism is of much less importance than in the case of hydrocarbons; in fact, it is quite difficult to separate isomers by fractionation. At constant temperature, the rate of decrease of the vapor pressure with increasing number of carbon atoms is smaller than with hydrocarbons.

Viscosity The viscosities of fluorocarbons are somewhat higher than for those of the corresponding hydrocarbons and the temperature coefficients are considerably greater.

Surface Tension The surface tensions of fluorocarbons are lower than those of the analogous hydrocarbons.

Heat of Vaporization Fluorocarbons are normal liquids insofar as their heats of vaporization are concerned.

Solubility Liquid perfluorocarbons are remarkable in that they are very poor solvents for most organic as well as inorganic substances. Similarly, they are only slightly soluble in the common solvents. They are miscible with one another and are solvents for some volatile metallic fluorides.

Specifically, liquid perfluorocarbons are substantially insoluble in water, alcohols and hydrocarbons. They show appreciable solubility and at higher temperature, miscibility with chlorocarbons. They are completely miscible in ether and in some partly fluorinated hydrocarbons such as $C_6H_5CF_3$.

II. Chemical Properties

The saturated fluorocarbons are characterized by great stability and inertness toward even the most reactive chemicals. This is to be expected in view of the strength of the C-F bond and the large heat of formation of fluorocarbons.

The saturated fluorocarbons are inert to elemental fluorine at ordinary conditions. When ignited, fluorocarbons will explosively react with fluorine to yield CF_4 as the final stable fluorination product.

The fluorocarbons are thermally very stable. They can be heated to 400-500°C even in the presence of possible catalytic material, such as CaF_2 , without cracking. At red heat, however, decomposition to carbon and CF_4 takes place. Probably other compounds are also formed, in amounts depending on temperature, pressure, and time conditions.

With finely divided silica at temperatures above 400°C fluorocarbons will react to form CO_2 and SiF_4 .

Saturated fluorocarbons are not attacked by nitric acid, concentrated (96%) and fuming sulfuric acid, nitrating mixture, acid chromate and permanganate solutions.

They are stable toward air and do not burn by themselves. They crack, however, in the flame of Bunsen burner.

They do not decolorize bromine water and are stable against bromine and iodine.

Fluorocarbons react in the presence of catalyst with hydrogen under pressure at higher temperatures.

The fluorocarbons are stable toward dilute and concentrated alkali, at both room temperature and about 100°C.

1

Chemical Name	Tetrafluoromethane
Empirical Formula	CF ₄
Structural Formula	$\begin{array}{c} \text{F} \\ \\ \text{F} - \text{C} - \text{F} \\ \\ \text{F} \end{array}$
Molecular Weight	88.0
Formula Composition	13.6% C, 86.4 % F

Preparation

Difficult to control reaction when large amounts of carbon are used. A-3468 (22)

Some higher fluorocarbons obtained. MDDC-575 (1)

Heat of Formation

Bond	Bond energy, k cal/mol
C-F	107.0
F-F	63.5

For elements in standard states from monoatomic gases

Element	k cal/mol
C	124.3
F	31.8

Pauling, L, "Nature of Bond", 2nd ed., 1945.

ΔH calculated = -176.7 k cal/mol at 18°C Pauling, L, "Nature of Bond", 2nd ed., 1945.

Melting Point, °C

-186.8	A-1404 (10)
-184	A-312 (3)
	BR-319 (5)
-183.6 (triple point)	A-1404 (10)
	A-3649-2 (428)
-183.53	
-183.5	BR-319 (5)

Boiling Point, °C

-128.00	BR-319 (5)
-128	A-312 (3)
-127.8	BR-319 (5)

Density, g/cc

1. Solid

Temperature, °C

-273.1	2.1	
-195.1	1.98	
-195.1	1.96	BR-319 (5)
-184.1	1.96	A-312 (3)
Equation: $d_T = d_0 - 270 \times 10^{-5} T$		BR-319 (5)

2. Liquid

at m p	1.91	
at b p	1.62	A-312 (3)

Refractive Index

Wave Length, Å	At 25°C
6440	1.00045098
5462	1.00045281
5087	1.00045374
4801	1.00045456
4359	1.00045621
5462 ^a	1.0004943 ^b
5876 ^c	1.0004875 ^b

^agreen mercury line^bat 0°C^creported as 587.6×10^{-6} , assumed to be nm

See Figure 137

BR-319 (5)

Molecular Refraction (MR_D)

Temperature, °C

0

7.23

ibid

Vapor Pressure, mm Hg

$$\text{Equation: } \log p = \frac{-701.73}{T} + 1.75 \log T - 0.0076715 T + 5.04420$$

BR-319 (7)

Heat of Vaporization, cal/mol

Temperature, °C

-273.1

3209

-151.1

3120

-128.0

2947

BR-319 (6)

A-3649 (428)

BR-319 (6)

Trouton's constant

20.3

BR-319 (6)

20.2

A-1404 (10)

Heat of Fusion, cal/mol

Temperature, °C

-183.7

353

BR-319 (6)

220 33

Heat of Transition, cal/mol

Temperature, °C

-196.93

167.3

BR-319 (6)

Entropy, cal/mol/°C

Range

0 - 12°K	0.69
12 - 76.23°K	15.26
Transition	4.64
76.23 - 89.47°K	2.59
Melting	1.87
89.47 - 122°K	5.81
Vaporization at 0.1365 atm	25.55
122 - 298.2°K (gas)	<u>9.96</u>
	66.37
Compression from 0.1365 atm to 1 atm	<u>-3.94</u>
	62.43

From statistics $S_{298} = 62.81$

BR-319 (6)

Heat Capacity, cal/mol/°C

Temperature, °C

Cp for solid

-261.1	1.82
-258.1	2.98
-253.1	4.85
-248.1	6.50
-243.1	7.95
-238.1	9.16
-233.1	10.23
-228.1	11.21
-223.1	12.07
-218.1	12.95
-213.1	13.88
-208.1	15.02
-203.1	16.57
-198.1	20.79
-196.87	transition point
-193.1	16.10
-188.1	16.52
-186.1	16.48
-184.1	16.03
-183.63	melting point

See Figure 138

ibid

220 34

5

Temperature, °C	Cp for liquid
-183	18.75
-173	18.64
-163	18.64
-153	18.64
-143	18.73
-133	19.03
-128	19.11

See Figure 139

ibid

Temperature, °C	Cv for gas
-160	6.341
-100	7.912
-74	8.775
0	11.23
50	12.74
100	14.09
150	15.27
200	16.30
250	17.18
300	17.94

See Figure 140

ibid

Dielectric Constant (ε)

Pressure, mm

723	1.00113
629	1.00098
515	1.00081
429	1.00067
332	1.00052
223	1.00036
131	1.00021

See Figure 141

BR-319 (7)

Polarization, cc

10.15 < 2.86 (atomic)
 7.29 (electronic)

BR-319 (7)

220 35

6

Bond Distance, Å

Bond

C-F

1.36 ± 0.02

A-3786 (8)

Infrared AbsorptionNormal frequency, cm⁻¹W₁

904

W₂

437

W₃

1200*

W₄

635*

*Active fundamental frequencies W₃ and W₄ corrected to 1252 and 630.

BR-319 (7)

See Figure 142 Infrared spectra of CF₄.

This Laboratory

Reaction

Attempts to polymerize CF₄ in a carbon arc were unsuccessful both with and without pressure.

A-3468 (25)

Chemical Name Chlorotrifluoromethane

Empirical Formula CF₃Cl

Structural Formual
$$\begin{array}{c} \text{Cl} \\ | \\ \text{F} - \text{C} - \text{F} \\ | \\ \text{F} \end{array}$$

Molecular Weight 104.5

Formula Composition 11.5% C, 54.4% F, 34.0% Cl

Boiling Point, °C

-81.1

A-3786 (90)

Bond Measurements

Bond	Bond distance, Å	Bond angle, °	
C-F	1.34 ± 0.02	—	
C-Cl	1.72 ± 0.03	—	A-3786 (79)
F-C-F	—	107.5 ± 2.0	A-3786 (31)

Chemical Name Trifluoromethane

Empirical Formula CF₃H

Structural Formula

$$\begin{array}{c} \text{F} \\ | \\ \text{F} - \text{C} - \text{H} \\ | \\ \text{F} \end{array}$$

Molecular Weight 70.0

Formula Composition 17.1% C, 81.5% F, 1.4% H

Boiling Point, °C

-82.2

A-3786 (90)

Bond Measurements

Bond	Bond distance, Å	Bond angle, °	
C-F	1.35 ± 0.03	_____	A-3786 (79)
F-C-F	_____	108 ± 1.5	A-3786 (28)

9

Chemical Name	Dichlorodifluoromethane
Empirical Formual	CF ₂ Cl ₂
Structural Formual	$\begin{array}{c} \text{Cl} \\ \\ \text{F} - \text{C} - \text{F} \\ \\ \text{Cl} \end{array}$
Molecular Weight	120.9
Formula Composition	9.9% C, 31.4% F, 58.7% Cl

Melting Point, °C

-158.0

Kellex Data Book
(A 500.00)Boiling Point, °C

-29.44

ibid

Density, g/cc

Temperature, °C

15.6
37.81.346 for liquid
0.00474 for vapor at 760 mm

See Figure 143

ibid

Vapor Pressure, mm Hg

Temperature, °C

-17.8
65.61231
12770

See Figure 144

ibid

220 39

Viscosity, cp

Temperature, °C

-17.8

0.335 for liquid

See Figure 145

Kellex Data Book
(A 500.00)Critical Temperature, °C

111.5

ibid

Critical Pressure, psia

582.0

ibid

Critical Density, g/cc

0.556

ibid

Heat of Vaporization, cal/mol

Temperature, °C

-29.44

4826

ibid

Entropy of Vaporization

See Figure 146

Enthalpy of Vaporization

See Figure 147

Compressibility Factor (Cp/Cv)

Temperature, °C

15.6
98.91.141
1.114Kellex Data Book
(A 500.00)Bond Distance, Å

Bond

C-F
C-Cl1.35 ± 0.03
1.74 ± 0.03

A-3786 (8)

Toxicity

Non-toxic and non-irritating

M-2149 (44)

12

Chemical Name	Difluoromethane
Empirical Formula	CF ₂ H ₂
Structural Formula	$\begin{array}{c} \text{H} \\ \\ \text{F} - \text{C} - \text{F} \\ \\ \text{H} \end{array}$
Molecular Weight	52.0
Formula Composition	23.1% C, 73.1% F, 3.8% H

Bond Distance, Å

Bond

C-F

1.36 ± 0.02

A-3786 (8)

13

Chemical Name	Carbonyl fluoride
Empirical Formula	CF ₂ O
Structural Formula	$\begin{array}{c} \text{F} \\ \diagdown \\ \text{C} = \text{O} \\ \diagup \\ \text{F} \end{array}$
Molecular Weight	66.0
Formula Composition	18.2% C, 57.6% F, 24.2% O

Preparation

A-1507 (18)

Same reaction gave 54% yield

A-1969 (6)

Melting Point, °C

-114

A-1969 (6)

-107

Toxicity

Concentration

1 in 500

No small animals killed. M-2149 (49)

220 43

14

Chemical Name Trichlorofluoromethane

Empirical Formula CFC1₃

Structural Formula

$$\begin{array}{c} \text{F} \\ | \\ \text{Cl} - \text{C} - \text{Cl} \\ | \\ \text{Cl} \end{array}$$

Molecular Weight 137.4

Formula Composition 8.7% C, 13.8 % F, 77.5% Cl

Melting Point, °C

-111.0

Kellex Data Book
(A 500.00)Boiling Point, °C

23.7 at 760 mm

ibid

Density, g/cc

Temperature, °C

15.6
37.81.482 for liquid
0.00553 for vapor at 760 mm

See Figure 148

ibid

Vapor Pressure, mm Hg

Temperature, °C

-17.8
65.6130.8
2715

See Figure 149

ibid

16

Mass Spectrometer Data

Mass 101 = 100.0

Mass	Probable fragment	Ratio*
19	F	0.42
20	HF	0.21
24	C ₂	0.03
31	CF	18.6
35	Cl	19.2
37	Cl	7.2
42	—	0.83
47	CCl	0.12
49	CCl	5.6
51	CF ₂ H	4.3
60	C ₂ ClH	0.32
69	CClFH, CF ₃	15.1
85	CCl ₂ H	3.7
101	CFCl ₂	100.0
119	CCl ₃	1.5
150	C ₂ FCl ₃	0.03
274	—	0.02

*Av of 3 runs

Letter from S. S. Stief, Process Engineering Department, 10-3-47

Compressibility Factor (Cp/Cv)

Temperature, °C

15.6	1.142
98.9	1.117

Kellex Data Book
(A-500.00)Bond Distance, Å

Bond

C-F	1.40 ± 0.04
C-Cl	1.76 ± 0.02

A-3786 (8)

Toxicity

Toxicity of very low order.

M-2149 (44) -

220 46

17

Chemical Name	Fluoromethane
Empirical Formula	CFH ₃
Structural Formula	$\begin{array}{c} \text{H} \\ \\ \text{H} - \text{C} - \text{F} \\ \\ \text{H} \end{array}$
Molecular Weight	34.0
Formula Composition	35.3% C, 55.9% F, 8.8% H

Bond Distance, Å

Bond

C-F

1.42 ± 0.02

A-3786 (8)

220 47

Chemical Name Methyl difluoroarsine

Empirical Formula CF₂AsH₃

Molecular Weight 127.9

Formula Composition 9.4% C, 29.7% F, 58.6% As, 2.3% H

Preparation

2. By modification of Meyer reaction.

M-2149 (20)

Boiling Point, °C

74

M-2149 (20)

Toxicity

Concentration

0.375 mg/L
1 in 2800
4.5 mg/L

MLC mice
0/4 rats
0/10 mice

M-2149 (14)

220 48

Chemical Name Chlorodifluoromethane

Empirical Formula CF₂ClH

Structural Formula

$$\begin{array}{c} \text{Cl} \\ | \\ \text{F} - \text{C} - \text{F} \\ | \\ \text{H} \end{array}$$

Molecular Weight 86.5

Formula Composition 13.9% C, 43.9% F, 41.0% Cl, 1.2% H

Melting Point, °C

-160.0

Kellex Data Book
(A 500.00)

Boiling Point, °C

-40.8

ibid

Density, g/cc

Temperature, °C

15.6
37.8

1.239 for liquid
0.00343 for vapor at 760 mm

See Figure 153

ibid

Vapor Pressure, mm Hg

Temperature, °C

-17.8
65.6

2010
2224.0

See Figure 154

ibid

Viscosity, cp

Temperature, °C

-17.8

0.241

See Figure 155

ibid

20

Critical Temperature, °C

96.0

Kellex Data Book
(A 500.00)Critical Pressure, psia

716.0

ibid

Critical Density, g/cc

0.510

ibid

Heat of Vaporization, cal/mol

Temperature, °C

-40.8

4917

ibid

Entropy of Vaporization

See Figure 156

Enthalpy of Vaporization

See Figure 157

Compressibility Factor (Cp/Cv)

Temperature, °C

15.6
98.91.191
1.150

ibid

Bond Distance, Å

Bond

C-F
C-Cl1.36 ± 0.03
1.73 ± 0.03

A-3786 (8)

220 50

21

Chemical Name Dichlorofluoromethane

Empirical Formula CFC1₂H

Structural Formula
$$\begin{array}{c} \text{Cl} \\ | \\ \text{F} - \text{C} - \text{H} \\ | \\ \text{Cl} \end{array}$$

Molecular Weight 102.9

Formula Composition 11.7% C, 18.4% F, 68.9% Cl, 1.0% H

Melting Point, °C

-135.0

Kellex Data Book
(A 500.00)Boiling Point, °C

8.9

ibid

Density, g/cc

Temperature, °C

15.6
37.81.386 for liquid
0.00493 for vapor at 760 mm

See Figure 158

ibid

Vapor Pressure, mm Hg

Temperature, °C

-17.8
65.6235.3
4500

See Figure 159

ibid

220 51

22

Viscosity, cp

Temperature, °C

-17.8

0.482

See Figure 160

Kellex Data Book
(A 500.00)Critical Temperature, °C

178.5

ibid

Critical Pressure, psia

750.0

ibid

Critical Density, g/cc

0.522

ibid

Heat of Vaporization, cal/mol

Temperature, °C

8.9

5954

ibid

Entropy of Vaporization

See Figure 161

Enthalpy of Vaporization

See Figure 162

Compressibility Factor (Cp/Cv)

Temperature, °C

15.6
98.91.178
1.148

ibid

220 52

23

Bond Distance, Å

Bond

C-F 1.41 ± 0.03
C-Cl 1.73 ± 0.04

A-3786 (8)

Mass Spectrometer Data

Mass 69 = 100.0

Mass	Probable fragment	Ratio*
19	F	0.50
20	HF	0.28
24	C ₂	0.13
25	C ₂ H	0.06
31	CF	10.9
32	CFH	12.1
35	Cl	10.7
37	Cl	4.3
46	(CCl -47)	0.35
51	CF ₂ H	15.4
69	CClFH	100.0
85	CCl ₂ H	5.3
100	(CFCl ₂ - 101)	6.2
126	(C ₃ FCI ₂ -125)	0.02

*Av of 3 runs

Letter from S. S. Stief, Process Engineering Department, 10-3-47

This Company

Toxicity

Non-toxic and non-irritating

M-2149 (44)

24

Chemical Name Chlorofluoromethane

Empirical Formula CFC1H₂

Molecular Weight 68.5

Formula Composition 17.5% C, 27.8% F, 51.8% Cl, 2.9% H

Bond Distance, Å

Bond

C-F	1.40 ± 0.03
C-Cl	1.76 ± 0.02

A-3786 (8)

220 54

25

Chemical Name Carbonyl chlorofluoride
Empirical Formula CFC10
Structural Formula $\begin{array}{c} \text{F} \\ \diagdown \\ \text{C} = \text{O} \\ \diagup \\ \text{Cl} \end{array}$
Molecular Weight 82.5
Formula Composition 14.6% C, 23.0% F, 43.0% Cl, 19.4% O

Boiling Point, °C

-42

M-2149 (50)

ToxicityLC₅₀ Concentration, mg/L

0.27 mg/L

guinea pig

0.27 mg/L

rats

0.12 mg/L

mice

M-2149 (49)

220

55

26

Chemical Name Hexafluoroethane

Empirical Formula C₂F₆

Structural Formula

```

      F   F
      |   |
F — C — C — F
      |   |
      F   F
  
```

Molecular Weight 138.0

Formula Composition 17.4% C, 82.6% F

Preparation Melting Point, °C

-100.6 A-312 (3)

-100.6

-179.1 transition point BR-319 (7)

Boiling Point, °C

-78.2 A-312 (3)

-78.2 BR-319 (7)

-78 A-3786 (90)

Density, g/cc

Temperature, °C

-78 1.85 (liquid) A-312 (3)

-100.6 1.85 (solid)

Equation: $d = 2.399 - 0.00406 T$ (liquid) BR-319 (7)

Vapor Pressure, mm Hg

Equation: $\log p = 7.376 - \frac{875.7}{T}$ BR-319 (8)

220 56

27

Heat of Vaporization, cal/mol

Temperature, °C

100.6

4004.6

Trouton's constant = 20.5

BR-319 (7)

Dielectric Constant (ε)

Pressure, mm Hg

711

1.00197

608

1.00169

509

1.00140

411

1.00114

307

1.00086

201

1.00056

110

1.00031

61

1.00017

See Figure 163

BR-319 (7)

Polarization, cc

17.2 (6.5 atomic)

BR-319 (8)

Bond Measurement

Bond

Bond distance, Å

Bond angle, °

C-C

1.45 ± 0.06

—

C-F

1.35 ± 0.03

—

F-C-F

—

107.5 ± 1.5

A-3786 (79)

A-3786 (38)

220 57

28

Chemical Name	Tetrafluoroethylene
Empirical Formula	C ₂ F ₄
Structural Formula	<pre> F F C = C F F </pre>
Molecular Weight	100.0
Formula Composition	24.0% C, 76.0% F

Preparation Freezing Point, °C

-142.5 ibid

Boiling Point, °C

-78.4 ibid
 -76 A-3786 (90)

Bond Measurements

Bond	Bond distance, Å	Bond angle, °	
C-C	1.27 ± 0.02	—	
C-F	1.32 ± 0.02	—	A-3786 (80)
F-C-F	—	110 ± 2	A-3786 (44)

Reactions

1. Polymerizes in solution with peroxide catalyst.
2. Copolymerizes with CF₂=CFCl.
3. Pyrolysis at 550-700°C yields C₃ and C₄ compounds.
4. Reacts with sodium methoxide and methyl alcohol to form CH₃-O-CF₂-CF₂H.
M-3113 (130)

220 58

29

Chemical Name Tetrafluoroethylene polymer

Empirical Formula $(C_2F_4)_x$

Structural Formula
$$\left(\begin{array}{c} F & F \\ | & | \\ C & = C \\ | & | \\ F & F \end{array} \right)_n$$

Reactions

1. $(C_2F_4)_n + F_2 \xrightarrow{CaF_2}$ Normally resistant but will burn under certain conditions.
MDDC-208 (7)

2. $(C_2F_4)_n \xrightarrow[260 \text{ mm}]{535^\circ C}$

- a. 22% white waxy solid
- b. 78% of the following:
 - (1) C_2F_4
 - (2) C_3F_6
 - (3) C_4F_8

M-3113 (91)

220 59

30

Chemical Name	1,1-Dichloro-1,2,2,2-tetrafluoroethane
Empirical Formula	C ₂ F ₄ Cl ₂
Structural Formula	<pre> Cl F F - C - C - F Cl F </pre>
Molecular Weight	170.9
Formula Composition	14.0% C, 44.5% F, 41.5% Cl

Preparation

Boiling Point, °C

3.78 A-3786 (90)

31

Chemical Name 1,2-Dichloro-1,1,2,2-tetrafluoroethane

Empirical Formula C₂F₄Cl₂

Molecular Weight 170.9

Formula Composition 14.0% C, 44.5% F, 41.5% Cl

Preparation

M-3113 (22)

Freezing Point, °C

-94.0

Kellex Data Book
(A 500.00)Boiling Point, °C

3.56

ibid

Density, g/cc

1. Liquid:

Temperature, °C

15.6

1.479
12.34 lb/gal

See Figure 164

ibid

2. Vapor:

Temperature, °C

37.8

Lbs/cu ft

0.428*

ibid

* 14.7 lbs/sq inch abs

220 61

32

Vapor Pressure, mm Hg

Temperature, °C

-17.8	308
65.6	5042

Kellex Data Book
(A 500.00)

See Figure 165

Viscosity, cp

Temperature, °C

-17.8	0.336
-------	-------

See Figure 166

ibid

Critical Temperature, °C

145.7

ibid

Critical Pressure, psia

474.0

ibid

Critical Density, g/cc

0.588

ibid

Heat of Vaporization, btu/lb

Temperature, °C

3.56	59.0	ibid
------	------	------

Entropy of Vaporization

See Figure 167

Enthalpy of Vaporization

See Figure 168

220 62

33

Mass Spectrometer Data

Mass 85 = 100.0

Mass	Probable fragment	Ratio*
19	F	0.27
24	C ₂	0.47
31	CF	33.6
35	Cl	4.4
37	Cl	1.6
47	CCl	0.40
51	CF ₂ H	10.5
59	C ₂ Cl	0.66
62	C ₂ F ₂	0.44
64	(CFC1-66)	5.0
69	CF ₃	9.1
78	C ₂ FC1	0.26
82	CCl ₂	0.28
85	CF ₂ Cl	100.0
101	CFC1 ₂ (C ₂ F ₄ -100)	14.9
126	(C ₃ FC1 ₂ -125)	2.3
131	C ₃ F ₅	40.0
148	(C ₃ F ₄ Cl-149)	3.2
168		0.09

*Av of 3 runs

Letter - S. S. Stief, Process Engineering Department, 10/3/47.

220 63

34

 $C_2F_4H_2$

Chemical Name 1,1,2,2-Tetrafluoroethane

Empirical Formula $C_2F_4H_2$

Structural Formula

```

      F   F
      |   |
H - C - C - H
      |   |
      F   F

```

Molecular Weight 102.0

Formula Composition 23.5% C, 74.5% F, 2.0% H

Boiling Point, °C

-23

A-3786 (90)

Bond Measurements

Bond	Bond distance, Å	Bond angle, °	
C-C	1.46 ± 0.05	—	
C-F	1.33 ± 0.03	—	A-3786 (79)
F-C-F	—	108 ± 2	A-3786 (36)

220 64

35

Chemical Name	Bromotrifluoroethylene
Empirical Formula	C ₂ F ₃ Br
Structural Formula	$\begin{array}{c} \text{F} \quad \text{F} \\ \quad \\ \text{F} - \text{C} = \text{C} - \text{Br} \end{array}$
Molecular Weight	161.0
Formula Composition	14.9% C, 35.4% F, 49.7% Br

Reactions

Readily oxidized by air or oxygen.

M-3113 (5)

220 65

36

Chemical Name 1,1,1-Trichloro-2,2,2-trifluoroethane

Empirical Formula C₂F₃Cl₃

Structural Formula

$$\begin{array}{c} \text{Cl} \quad \text{F} \\ | \quad | \\ \text{Cl} - \text{C} - \text{C} - \text{F} \\ | \quad | \\ \text{Cl} \quad \text{F} \end{array}$$

Molecular Weight 187.4

Formula Composition 12.8% C, 30.4% F, 56.8% Cl

Preparation

1. CH₃-CF₃ + Cl₂ $\longrightarrow$ CCl₃-CF₃ M-3113 (129)
2. CFCl₂-CF₂Cl $\xrightarrow{\text{AlCl}_3, 50-60^\circ\text{C}}$ CCl₃-CF₃ ibid

Freezing Point, °C

13.8-14.2
14.2

ibid
J. Am. Chem. Soc., 62, 2051 (1940)

Boiling Point, °C

45
45.9
46.4

A-3786 (90)
J. Am. Chem. Soc., 62, 2051 (1940)
M-3113 (129)

Refractive Index (n_D)

Temperature, °C

20

1.3602
1.3610

ibid

25.5

J. Am. Chem. Soc., 62, 2051 (1940)
1.3568 M-3113 (129)

220 66

Molecular Refraction (MR_D)AR_F (calculated)

26.18

1.15

J. Am. Chem. Soc., 62, 2051 (1940)

26.24

1.17

M-3113 (129)

Bond Distance, Å

Bond

C-C

<1.55

C-F

1.34

C-Cl

1.76

F-F

2.18 ± 0.03

Cl-Cl

2.93 ± 0.03

Cl-F

3.88 ± 0.04

2.94 ± 0.03

A-3786 (41)

220 67

38

Chemical Name 1,1,2-Trichloro-1,2,2-trifluoroethane

Empirical Formula C₂F₃Cl₃

Molecular Weight 187.4

Formula Composition 12.8% C, 30.4% F, 56.8% Cl

Preparation Freezing Point, °C

-36.4
-35

J. Am. Chem. Soc., 56, 1726 (1934)
Kellex Data Book
(A 500.00)

Boiling Point, °C

46
47.55

47.7

47.8

MDDC-142 (4)
Kellex Data Book
(A 500.00)
A-1575 (2)
J. Am. Chem. Soc., 56, 1726 (1934)
M-3113 (130)

Density, g/cc

1. Liquid

Temperature, °C

-10	1.646	M-3113 (130)
+15.6	1.603	Kellex Data Book (A 500.00)
25	1.56354	J. Am. Chem. Soc., <u>56</u> , 1726 (1934)

See Figure 169

2. Vapor

Temperature, °C

47.55	0.465 lb/cu ft*	Kellex Data Book (A 500.00)
* 14.7 lbs/sq inch abs		

Refractive Index (n_D)

Temperature, °C

25	1.35572	J. Am. Chem. Soc., <u>56</u> , 1726 (1934)
25.5	1.3552	M-3113 (30)

Molecular Refraction (MR_D)AR_F (calculated)

26.170	1.144	M-3113 (130)
--------	-------	--------------

Vapor Pressure, mm Hg

Temperature, °C

-17.8	43.34	Kellex Data Book (A 500.00)
65.6	1339	

See Figure 170

40
Viscosity, cp

Temperature, °C

-17.78

0.745

Kellex Data Book
(A 500.00)

See Figure 171

ibid

Critical Temperature, °C

214.1

ibid

Critical Pressure, psia

499.0

ibid

Critical Density, g/cc

0.575

ibid

Heat of Vaporization, btu/lb

Temperature, °C

47.55

63.12

ibid

Entropy of Vaporization

See Figure 172

Enthalpy of Vaporization

See Figure 173

Compressibility Factor (cp/cv)

Temperature, °C

15.6
98.91.136
1.073

ibid

220 70

41

Mass Spectrometer Data

Mass	Probable fragment	Sample
12	C	219
13	CH	7
14	CH ₂ , N	9
15	CH ₃	10
16	O	11
17	OH	5
18	H ₂ O	17
19	F	31
22	HF	2
24	C ₂	102
26	C ₂ H ₂	3
27	C ₂ H ₃	2
28	N ₂	295
31	CF	3169
32	O ₂	35
35	Cl	780
36	Cl	126
37	HCl	247
44	CO ₂	34
47	CCl	1165
50	CF ₂	43
59	C ₂ Cl	64
62	C ₂ F ₂	76
66	CFC1	1066
78	C ₂ FC1	116
85	CF ₂ Cl	2168
101	CFC1 ₂	5434
116	C ₂ F ₃ Cl	572
132	C ₂ F ₂ Cl ₂	98
151	C ₂ F ₃ Cl ₂	2761
167	C ₂ F ₂ Cl ₃	24

Spectrum Library, Special Analyses Department, Report No. 165, by H. H. Rappaport

This Laboratory

Uses

As a solvent in the AgF₂ liquid phase fluorination of hydrocarbon oils to product C₂₁F₄₄. With solvent to oil ratio of 5:1, a product of good properties was obtained in 65-75% yield.

A-2550 (6)

220 71

42

Code Name	P-539
Chemical Name	Chlorotrifluoroethylene
Empirical Formula	C ₂ F ₃ Cl
Structural Formula	$\begin{array}{c} \text{F} \quad \text{F} \\ \quad \\ \text{Cl} - \text{C} = \text{C} - \text{F} \end{array}$
Molecular Weight	116.5
Formula Composition	20.6% C, 48.9% F, 30.5% Cl

See Section I (K-220) Page 111.

43

Chemical Name 1,1,1-Trifluoroethane

Empirical Formula C₂F₃H₃

Structural Formula

$$\begin{array}{c} \text{F} \quad \text{H} \\ | \quad | \\ \text{F} - \text{C} - \text{C} - \text{H} \\ | \quad | \\ \text{F} \quad \text{H} \end{array}$$

Molecular Weight 84.0

Formula Composition 28.6% C, 67.8% F, 3.6% H

Boiling Point, °C

-49.8

A-3786 (90)

Bond Measurements

Bond	Bond distance, Å	Bond angle, °	
C-C	1.45 ± 0.05	—	
C-F	1.33 ± 0.03	—	A-3786 (79)
F-C-F	—	108.5 ± 2	A-3786 (35)

220 73

44

C₂F₃H

14

Chemical Name Trifluoroethylene
Empirical Formula C₂F₃H
 H F
 | |
Structural Formula F - C = C - F
Molecular Weight 82.0
Formula Composition 29.3% C, 69.5% F, 1.2% H

Boiling Point, °C

-37

A-3786 (90)

Bond Measurements

Bond	Bond distance, Å	Bond angle, °	
C-C	1.28 ± 0.03	—	
C-F	1.35 ± 0.03	—	
F-C-C	—	122.5	
F-C-F	—	110	A-3786 (48)

220 74

45

Chemical Name 1,1,2,2-Tetrachloro-1,2-difluoroethane

Empirical Formula C₂F₂Cl₄

Structural Formula

$$\begin{array}{c} \text{Cl} \quad \text{Cl} \\ | \quad | \\ \text{Cl} - \text{C} - \text{C} - \text{Cl} \\ | \quad | \\ \text{F} \quad \text{F} \end{array}$$

Molecular Weight 203.9

Formula Composition 11.8% C, 18.6% F, 69.6% Cl

Preparation

CCl₂=CCl₂ + SbF₅ $\longrightarrow$ CFCl₂-CFCl₂ (yield 19 mol %) M-3113 (27)

Boiling Point, °C

91-92 MDDC-162 (28)
92.8 A-1575 (2)

Density, g/cc

Temperature, °C

20 1.6488 MDDC-162 (28)

Refractive Index (n_D)

Temperature, °C

20 1.4070 MDDC-162 (28)

220 75

46

Chemical Name 1,1-Dichloro-2,2-difluoroethylene

Empirical Formula C₂F₂Cl₂

Structural Formula $\begin{array}{c} \text{Cl} \quad \text{F} \\ | \quad | \\ \text{Cl} - \text{C} = \text{C} - \text{F} \end{array}$

Molecular Weight 132.9

Formula Composition 18.1% C, 28.6% F, 53.3% Cl

Preparation Freezing Point, °C

-127.1 to -126.7 M-3113 (129)

Boiling Point, °C

19.0 A-3786 (90)
 20.4 at 764.3 mm M-3113 (129)

Bond Measurements

Bond	Bond distance, Å	Bond angle, °	
C-C	1.30 ± 0.04	—	
C-F	1.32	—	
C-Cl	1.70 ± 0.02	—	A-3786 (80)
F-C-F	—	110	
Cl-C-Cl	—	115 ± 2	A-3786 (46)

Reactions

It was found that CF₂=CCl₂ added methyl alcohol exothermically at low temperatures (0° to room temperature) in the presence of sodium methylate to give essentially quantitative yields of saturated ethers. M-3113 (6)

220 76

note - pg 76A
ballons

47

Chemical Name	1,2-Dichloro-1,2-difluoroethylene
Empirical Formula	C ₂ F ₂ Cl ₂
Structural Formula	$\begin{array}{c} \text{Cl} \quad \text{Cl} \\ \quad \\ \text{F} - \text{C} = \text{C} - \text{F} \end{array}$
Molecular Weight	132.9
Formula Composition	18.1% C, 28.6% F, 53.3% Cl

Preparation

M-3113 (129)

Freezing Point, °C

1. Cis isomer

-130.5

J. Am. Chem. Soc., 56, 1726 (1934)

2. Trans isomer

-110.5

ibid

Boiling Point, °C

1. Cis isomer

21.1

ibid

2. Trans isomer

22.0

ibid

Density, g/cc

1. Cis isomer

Temperature, °C

0

1.4950

ibid

2. Trans isomer

Temperature, °C

0

1.4936

ibid

220 76A

48

Refractive Index (n_D)

1. Cis isomer

Temperature, °C

0

1.3777

J. Am. Chem. Soc., 56, 1726 (1934)

2. Trans isomer

Temperature, °C

0

1.3798

ibid

Molecular Refraction (M_R)

1. Cis isomer

 AR_F (calculated)

20.48

0.99

ibid

2. Trans isomer

 AR_F (calculated)

20.60

1.03

ibid

Reaction

Fluorinated in liquid phase at -60-0°C to give normal fluorination products.
M-3113 (129)

220 77

49

Chemical Name 1,1-Difluoroethylene

Empirical Formula C₂F₂H₂

Structural Formula

```

  F   H
  |   |
  C = C
  |   |
  F   H

```

Molecular Weight 64.0

Formula Composition 37.5% C, 59.4% F, 3.1% H

Boiling Point, °C

< -70

A-3786 (90)

Bond Measurements

Bond	Bond distance, Å	Bond angle, °	
C-C	< 1.34	—	A-3786 (80)
F-C-F	—	111.5 ± 1.5	A-3786 (51)

220 78

50

Chemical Name	Trichlorofluoroethylene
Empirical Formula	C ₂ FCl ₃
Structural Formula	$\begin{array}{c} \text{Cl} \quad \text{Cl} \\ \quad \\ \text{F} - \text{C} - \text{C} - \text{Cl} \end{array}$
Molecular Weight	149.4
Formula Composition	16.1% C, 12.7% F, 71.2% Cl

Reactions

Trichlorofluoroethylene reacts readily with methyl alcohol at low temperatures (0°C to room temperature) in the presence of sodium methylate to give essentially a quantitative yield of the saturated ether with some loss of HX so that a pure product was difficult to obtain.

M-3113 (6)

220 79

51

Chemical Name 1,2-Dibromo-1-chloro-1,2,2-trifluoroethane

Empirical Formula C₂F₃Br₂Cl

Structural Formula

$$\begin{array}{c} \text{Cl} \quad \text{F} \\ | \quad | \\ \text{Br} - \text{C} - \text{C} - \text{Br} \\ | \quad | \\ \text{F} \quad \text{F} \end{array}$$

Molecular Weight 276.4

Formula Composition 8.6% C, 20.7% F, 57.8% Br, 12.9% Cl

Preparation Freezing Point, °C

-72.8 to -72.6

ibid

Boiling Point, °C92.9
93.5J. Am. Chem. Soc., 56, 1726 (1934)
M-3113 (128)Density, g/cc

Temperature, °C

20

2.2318

J. Am. Chem. Soc., 56, 1726 (1934)Refractive Index, (n_D)

Temperature, °C

20

1.4272

ibid

Molecular Refraction (MR_D)AR_F (calculated)

28.53

1.09

ibid

220 80

52

Chemical Name 2-Bromo-1,1,1-trifluoroethane
Empirical Formula C₂F₃BrH₂
Structural Formula

$$\begin{array}{c}
 \text{F} \quad \text{H} \\
 | \quad | \\
 \text{F} - \text{C} - \text{C} - \text{Br} \\
 | \quad | \\
 \text{F} \quad \text{H}
 \end{array}$$

Molecular Weight 163.0
Formula Composition 14.7% C, 35.0% F, 49.1% Br, 1.2% H

Preparation Boiling Point, °C

25.5-26.5

A-1969 (8)

220 81

53

Chemical Name 2-Chloro-1,1,1-trifluoroethane

Empirical Formula C₂F₃ClH₂

Structural Formula

```

      F   Cl
      |   |
F - C - C - H
      |   |
      F   H
  
```

Molecular Weight 118.5

Formula Composition 20.3% C, 48.1% F, 29.9% Cl, 1.7% H

Boiling Point, °C

6.2 at 747 mm

A-3786 (90)

Bond Measurements

Bond	Bond distance, Å	Bond angle, °	
C-C	1.47 ± 0.03	—	
C-F	1.34	—	
C-Cl	1.72 ± 0.03	—	A-3786 (79)
C-C-Cl	—	119 ± 2	
F-C-F	—	108.0 ± 1.5	A-3786 (40)

220 82

54

 $C_2F_3H_3O$

Chemical Name 2,2,2-Trifluoroethanol

Empirical Formula $C_2F_3H_3O$

Structural Formula

$$\begin{array}{ccccccc} & F & & H & & & \\ & | & & | & & & \\ F & - C & - & C & - O & - H \\ & | & & | & & & \\ & F & & H & & & \end{array}$$

Molecular Weight 100.0

Formula Composition 24.0% C, 57.0% F, 3.0% H, 16.0% O

Preparation

Two-step hydrogenation of trifluoroacetamide at 90°C and initially 1500 psi with hydrogen and platinum oxide catalyst. Purification of product gave total of 76.5% yield of trifluoroethanol, 10% unreacted trifluoroacetamide, and 10% ammonium trifluoroacetate. A-1748 (1)

Boiling Point, °C

75-77 at 740 mm

A-1748 (1)

220 83

55

Chemical Name Trifluoromethyl methyl ether

Empirical Formula C₂F₃H₃O

Structural Formula
$$\begin{array}{ccccccc} & \text{F} & & & \text{H} & & \\ & | & & & | & & \\ \text{F} & - \text{C} & - & \text{O} & - & \text{C} & - \text{H} \\ & | & & & | & & \\ & \text{F} & & & \text{H} & & \end{array}$$

Molecular Weight 100.0

Formula Composition 24.0% C, 57.0% F, 3.0% H, 16.0% O

Density, g/cc

Temperature, °C

20	1.332	BR-645 (12)
----	-------	-------------

Molecular Volume, cc

Temperature, °C

20	72.9	BR-645 (12)
----	------	-------------

220

84

56

Chemical Name Trifluoroacetic acid

Empirical Formula C₂F₃HO₂

Structural Formula
$$\begin{array}{ccccccc} & & \text{F} & & \text{O} & & \\ & & | & & || & & \\ \text{F} & - & \text{C} & - & \text{C} & - & \text{O} - \text{H} \\ & & | & & & & \\ & & \text{F} & & & & \end{array}$$

Molecular Weight 114.0

Formula Composition 21.1% C, 49.9% F, 0.9% H, 28.1% O

Preparation

Acidified with H₂SO₄, CF₃-COOH extracted with ether, and purified as sodium salt with later addition of concentrated H₂SO₄. Net yield was 90%.

A-2104 (18)

220 85

57

Chemical Name Sodium trifluoroacetate

Empirical Formula $C_2F_3NaO_2$

Structural Formula

$$\begin{array}{c}
 \text{F} \quad \text{O} \\
 | \quad || \\
 \text{F} - \text{C} - \text{C} - \text{O} - \text{Na} \\
 | \\
 \text{F}
 \end{array}$$

Molecular Weight 136.0

Formula Composition 17.7% C, 41.9% F, 16.9% Na, 23.5% O

Preparation

58

Chemical Name Ethyldifluoroarsine

Empirical Formula C₂F₂AsH₅

Molecular Weight 141.9

Formula Composition 16.9% C, 26.8% F, 52.8% As, 3.5% H

Preparation

3. By modified Meyers reaction.

M-2149 (17)

Boiling Point, °C

96

ibid

Toxicity

MLC, mg/l

Animal

Time, min

0.2

mice

10

0.1

dog

30

M-2149 (11)

220

87

59

C₂FCl₄H

Chemical Name 1,1,2,2-Tetrachloro-1-fluoroethane

Empirical Formula C₂FCl₄H

Structural Formula

$$\begin{array}{c}
 \text{Cl} \quad \text{Cl} \\
 | \quad | \\
 \text{F} - \text{C} - \text{C} - \text{H} \\
 | \quad | \\
 \text{Cl} \quad \text{Cl}
 \end{array}$$

Molecular Weight 185.9

Formula Composition 12.9% C, 10.2% F, 76.4% Cl, 0.5% H

Preparation

A-2104 (4)
J. Am. Chem. Soc., 58, 402 (1936)

Melting Point, °C

-82.6

ibid

Boiling Point, °C

116.6

ibid

Density, g/cc

Temperature, °C

20

1.62232

ibid

Refractive Index (n_D)

Temperature, °C

20

1.44873

ibid

220 88

60

Chemical Name 1-Chloro-1-fluoroethylene

Empirical Formula C₂FC1H₂

Structural Formula

```

      F   H
      |   |
      C = C
      |   |
      Cl  H
  
```

Molecular Weight 80.5

Formula Composition 29.8% C, 23.6% F, 44.1% Cl, 2.5% H

Boiling Point, °C

-23

A-3786 (90)

Bond Distance, Å

Bond

C-Cl

1.70 ± 0.03

A-3786 (80)

F-Cl

2.55 ± 0.03

A-3786 (52)

220 89

61

Chemical Name 2-Fluoroethanol

Empirical Formula C₂FH₅O

Structural Formula

$$\begin{array}{ccccccc} & & \text{H} & & \text{H} & & \\ & & | & & | & & \\ \text{F} & - & \text{C} & - & \text{C} & - & \text{O} - \text{H} \\ & & | & & | & & \\ & & \text{H} & & \text{H} & & \end{array}$$

Molecular Weight 64.1

Formula Composition 37.5% C, 29.7% F, 7.8% H, 25.0% O

Preparation

CClH₂-CH₂OH + KF $\xrightarrow[5-6 \text{ hours in autoclave}]{130-135^\circ}$ CFH₂-CH₂OH (45% yield) M-2149 (36)

Boiling Point, °C

103.5 M-2149 (36)

Vapor Pressure

Equation: $\log P = 9.060 - 2304/T$ M-2149 (37)

Toxicity

LC ₅₀ , mg/l	Animal
0.005	dog
0.025 - 0.050	cat
0.2 - 0.4	goat
0.025	rabbit
> 0.3	rat
0.15	guinea pig
> 1.0	monkey

0.29 mg/l produced 62% mortality in an assortment of small animals excluding mice. M-2149 (31)

220 90

62

Chemical Name Dimethylfluorophosphate

Empirical Formula C₂FH₆O₃P

Structural Formula

$$\begin{array}{ccccccc}
 & \text{H} & & \text{O} & & \text{H} & \\
 & | & & || & & | & \\
 \text{H} & - \text{C} & - \text{O} & - \text{P} & - \text{O} & - \text{C} & - \text{H} \\
 & | & & | & & | & \\
 & \text{H} & & \text{F} & & \text{H} &
 \end{array}$$

Molecular Weight 128.0

Formula Composition 18.8% C, 14.8% F, 4.7% H, 37.5% O, 24.2% P

Boiling Point, °C

149

M-2149 (18)

Volatility, mg/l

Temperature, °C

-10	3.17
0	6.47
10	12.4
20	22.9
25	30.5
30	50.8
40	68.5

See Figure 174

M-2149 (18)

ToxicityCT₅₀, mg/min/m³

Animal

1200	mouse
2000	rat
2500	cat
7000	dog
8000	guinea pig
24000	goat
125000	rabbit

M-2149 (21)

63

LD₅₀, mg/kilo

3-4 (intraperitoneal injection) mouse
0.4-0.5 (intravenous injection) mouse
0.72 mg/mouse (skin absorption)

M-2149 (21)

LC₅₀, mg/l

0.25 mouse
0.30 (approximately) rat
Less toxic to guinea pigs and rabbits
Median detectable concentration for
humans, 0.18 mg/l.

M-2149 (6)

M-2149 (19)

220 92

64

Chemical Name Octafluoropropane

Empirical Formula C₃F₈

Structural Formula

$$\begin{array}{ccccccc}
 & & \text{F} & & \text{F} & & \text{F} \\
 & & | & & | & & | \\
 \text{F} & - & \text{C} & - & \text{C} & - & \text{C} & - & \text{F} \\
 & & | & & | & & | \\
 & & \text{F} & & \text{F} & & \text{F}
 \end{array}$$

Molecular Weight 188.0

Formula Composition 19.2% C, 80.8% F

Preparation Melting Point, °C

-183

A-312 (3)
A-3649 (428)

Boiling Point, °C

-38

-36

A-312 (3)
A-3649 (428)
A-3786 (91)

Density, g/cc

Temperature, °C

0.2

1.45

A-312 (3)

Vapor PressureEquation: $\log p = -1070/T + 7.43$

BR-319 (8)

220 93

65

Heat of Vaporization, cal/mol

4920

A-3649 (428)

Bond Measurements

Bond	Bond distance, Å	Bond angle, °	
C-C	1.47 ± 0.03	—	
C-F	1.34 ± 0.02	—	A-3786 (79)
F-C-F	—	107 ± 2	A-3786 (57)

220 94

66

Chemical Name	Hexafluoropropene
Empirical Formula	C ₃ F ₆
Structural Formula	$ \begin{array}{c} \text{F} \quad \text{F} \quad \text{F} \\ \quad \quad \\ \text{F} - \text{C} - \text{C} = \text{C} - \text{F} \\ \\ \text{F} \end{array} $
Molecular Weight	150.0
Formula Composition	24.0% C, 76.0% F

Preparation

1. $\text{CF}_2=\text{CF}_2 \xrightarrow{750^\circ\text{C}} \text{CF}_2=\text{CF}-\text{CF}_3$	M-2544 (2)
M-3113 (138)												
2. $\text{CF}_2\text{Br}-\text{CFBr}-\text{CF}_3 \xrightarrow{\text{Zn}} \text{CF}_2=\text{CF}-\text{CF}_3$	M-3113 (138)												
3. $\text{CF}_2\text{Cl}-\text{CFCl}-\text{CF}_3 \xrightarrow{\text{Zn}} \text{CF}_2=\text{CF}-\text{CF}_3$	M-3113 (138)
A-2104 (6)
A-770 (3)												
<table style="width: 100%; border-collapse: collapse;"> <tr> <td style="width: 60%;">a. $\text{CH}_2=\text{CCl}-\text{CH}_2\text{Cl} \xrightarrow{\text{HF}} \text{CH}_3-\text{CClF}-\text{CH}_2\text{Cl}$</td> <td style="width: 40%;"></td> </tr> <tr> <td>b. $\text{CH}_3-\text{CClF}-\text{CH}_2\text{Cl} \xrightarrow{\text{Cl}_2} \text{CHCl}_2-\text{CClF}-\text{CCl}_3$</td> <td></td> </tr> <tr> <td>c. $\text{CHCl}_2-\text{CClF}-\text{CCl}_3 \xrightarrow{\text{Zn}} \text{CCl}_2=\text{CF}-\text{CCl}_3$</td> <td></td> </tr> <tr> <td>d. $\text{CCl}_2=\text{CF}-\text{CCl}_3 \xrightarrow{\text{SbF}_3} \text{CCl}_2=\text{CF}-\text{CF}_3$</td> <td></td> </tr> <tr> <td>e. $\text{CCl}_2=\text{CF}-\text{CF}_3 \xrightarrow{\text{Cl}_2} \text{CCl}_3-\text{CClF}-\text{CF}_3$</td> <td></td> </tr> <tr> <td>f. $\text{CCl}_3-\text{CClF}-\text{CF}_3 \xrightarrow{\text{SbF}_3} \text{CF}_2\text{Cl}-\text{CClF}-\text{CF}_3$</td> <td style="vertical-align: top;">A-2104 (6)
A-770 (3)</td> </tr> </table>		a. $\text{CH}_2=\text{CCl}-\text{CH}_2\text{Cl} \xrightarrow{\text{HF}} \text{CH}_3-\text{CClF}-\text{CH}_2\text{Cl}$		b. $\text{CH}_3-\text{CClF}-\text{CH}_2\text{Cl} \xrightarrow{\text{Cl}_2} \text{CHCl}_2-\text{CClF}-\text{CCl}_3$		c. $\text{CHCl}_2-\text{CClF}-\text{CCl}_3 \xrightarrow{\text{Zn}} \text{CCl}_2=\text{CF}-\text{CCl}_3$		d. $\text{CCl}_2=\text{CF}-\text{CCl}_3 \xrightarrow{\text{SbF}_3} \text{CCl}_2=\text{CF}-\text{CF}_3$		e. $\text{CCl}_2=\text{CF}-\text{CF}_3 \xrightarrow{\text{Cl}_2} \text{CCl}_3-\text{CClF}-\text{CF}_3$		f. $\text{CCl}_3-\text{CClF}-\text{CF}_3 \xrightarrow{\text{SbF}_3} \text{CF}_2\text{Cl}-\text{CClF}-\text{CF}_3$	A-2104 (6)
A-770 (3)
a. $\text{CH}_2=\text{CCl}-\text{CH}_2\text{Cl} \xrightarrow{\text{HF}} \text{CH}_3-\text{CClF}-\text{CH}_2\text{Cl}$													
b. $\text{CH}_3-\text{CClF}-\text{CH}_2\text{Cl} \xrightarrow{\text{Cl}_2} \text{CHCl}_2-\text{CClF}-\text{CCl}_3$													
c. $\text{CHCl}_2-\text{CClF}-\text{CCl}_3 \xrightarrow{\text{Zn}} \text{CCl}_2=\text{CF}-\text{CCl}_3$													
d. $\text{CCl}_2=\text{CF}-\text{CCl}_3 \xrightarrow{\text{SbF}_3} \text{CCl}_2=\text{CF}-\text{CF}_3$													
e. $\text{CCl}_2=\text{CF}-\text{CF}_3 \xrightarrow{\text{Cl}_2} \text{CCl}_3-\text{CClF}-\text{CF}_3$													
f. $\text{CCl}_3-\text{CClF}-\text{CF}_3 \xrightarrow{\text{SbF}_3} \text{CF}_2\text{Cl}-\text{CClF}-\text{CF}_3$	A-2104 (6)
A-770 (3)												

Chemical Name 2-Chloro-1,1,1,2,3,3,3-heptafluoropropane

Empirical Formula C₃F₇Cl

Molecular Weight 204.5

Formula Composition 17.6% C, 65.1% F, 17.3% Cl

Preparation

1. $\text{CF}_2=\text{CCl}-\text{CF}_3 + \text{F}_2 \longrightarrow \text{CF}_3-\text{CClF}-\text{CF}_3$ M-3113 (134)
2. $\text{CF}_2=\text{CCl}-\text{CF}_3 + \text{HF} + \text{PbO}_2 \longrightarrow \text{CF}_3-\text{CClF}-\text{CF}_3$ ibid

Boiling Point, °C

-1

-2

ibid

Reactions

Vapor phase reaction with fluorine and cobalt trifluoride at 340°C yielded C₃F₈.

ibid

68

Chemical Name 1,2-Dibromo-1,1,2,3,3,3-hexafluoropropane

Empirical Formula C₃F₆Br₂

Structural Formula

```

      F   F   F
      |   |   |
F - C - C - C - F
      |   |   |
      Br  Br  F
  
```

Molecular Weight 310.0

Formula Composition 11.6% C, 36.8% F, 51.6% Br

Preparation

1. CF₃-CF=CF₂ + Br₂ $\longrightarrow$ CF₃-CFBr-CF₂Br M-3113 (132)
2. CF₃-CFH-CF₂H + Br₂ $\xrightarrow{600^{\circ}\text{C}}$ CF₃-CFBr-CF₂Br ibid

Freezing Point, °C

-95.0 to -94.6

ibid

Boiling Point, °C

71-71.5
72-73

J. Am. Chem. Soc., 68, 968 (1946)
M-3113 (132)

Density, g/cc

Temperature, °C

20

2.1693

ibid

Refractive Index (n_D)

Temperature, °C

20

1.3588

ibid

220 97

69

Molecular Refraction (MR_D)

AR_F (calculated)

31.43

1.07

M-3113 (132)

Reactions

Debrominated readily with zinc.

ibid

220 98

70

Chemical Name 1,2-Dichloro-1,1,2,3,3,3-hexafluoropropane

Empirical Formula C₃F₆Cl₂

Structural Formula

$$\begin{array}{ccccccc}
 & & \text{Cl} & & \text{Cl} & & \text{F} \\
 & & | & & | & & | \\
 \text{F} & - & \text{C} & - & \text{C} & - & \text{C} & - & \text{F} \\
 & & | & & | & & | \\
 & & \text{F} & & \text{F} & & \text{F}
 \end{array}$$

Molecular Weight 221.0

Formula Composition 16.3% C, 51.6% F, 32.1% Cl

Preparation

1. $\text{CF}_2=\text{CF}-\text{CF}_3 + \text{Cl}_2 \longrightarrow \text{CF}_2\text{Cl}-\text{CFCl}-\text{CF}_3$ M-3113 (135)
2. $\text{CCl}_3-\text{CFCl}-\text{CF}_3 + \text{SbF}_3\text{Cl}_2 \longrightarrow \text{CF}_2\text{Cl}-\text{CFCl}-\text{CF}_3$ ibid
3. $\text{CCl}_3-\text{CFCl}-\text{CF}_3 + \text{SbF}_3 \longrightarrow \text{CF}_2\text{Cl}-\text{CFCl}-\text{CF}_3$
- a. $\text{CH}_2\text{Cl}-\text{CHCl}-\text{CH}_2\text{Cl} \xrightarrow[\text{NaOH}]{\text{C}_2\text{H}_5\text{OH}} \text{CH}_2=\text{CCl}-\text{CH}_2\text{Cl}$
- b. $\text{CH}_2=\text{CCl}-\text{CH}_2\text{Cl} \xrightarrow{\text{HF}} \text{CH}_3-\text{CClF}-\text{CH}_2\text{Cl}$
- c. $\text{CH}_3-\text{CClF}-\text{CH}_2\text{Cl} \xrightarrow{\text{Cl}_2} \text{CHCl}_2-\text{CClF}-\text{CCl}_3$
- d. $\text{CHCl}_2-\text{CClF}-\text{CCl}_3 \xrightarrow{\text{Zn}} \text{CCl}_2=\text{CF}-\text{CCl}_3$
- e. $\text{CCl}_2=\text{CF}-\text{CCl}_3 \xrightarrow{\text{SbF}_3} \text{CCl}_2=\text{CF}-\text{CF}_3$
- f. $\text{CCl}_2=\text{CF}-\text{CF}_3 \xrightarrow{\text{Cl}_2} \text{CCl}_3-\text{CClF}-\text{CF}_3$ A-770 (3)
A-709 (3)

Freezing Point, °C

-136

M-3113 (135)

Boiling Point, °C

33.9 - 34.1
34.7

ibid

71

Density, g/cc

Temperature, °C

20	1.5896	M-3113 (135)
----	--------	--------------

Refractive Index (n_D)

Temperature, °C

20	1.3029	ibid
----	--------	------

Molecular Refraction (MR_D)

AR_F (calculated)

26.21	1.17	ibid
-------	------	------

Reactions

Dechlorinated with Zn to yield hexafluoropropene.	ibid
---	------

220 100

72

 $C_3F_6H_2$

Chemical Name 1,1,1,3,3,3-Hexafluoropropane

Empirical Formula $C_3F_6H_2$

Structural Formula

$$\begin{array}{ccccccc} & F & & H & & F & \\ & | & & | & & | & \\ F & - C & - & C & - & C & - F \\ & | & & | & & | & \\ & F & & H & & F & \end{array}$$

Molecular Weight 152.0

Formula Composition 23.7% C, 75.0% F, 1.3% H

Boiling Point, °C

-0.7

A-3786 (91)

220 101

73

Chemical Name 1,1,1,3,3,3-Hexafluoro-2-propanone

Empirical Formula C₃F₆O

Molecular Weight 166.0

Formula Composition 21.7% C, 68.7% F, 9.6% O

PreparationPolychloroacetone $\xrightarrow{\text{SbF}_5}$ polychloropolyfluoroacetonePolychloropolyfluoroacetone $\xrightarrow{\text{AgF}_2}$ a product containing some hexafluoroacetone
A-1969 (1)Boiling Point, °C

-28

A-1509 (9)

A-1969 (5)

220 102

74

Chemical Name 1,1,2-Trichloro-1,2,3,3,3-pentafluoropropane

Empirical Formula C₃F₅Cl₃

Structural Formula

```

      Cl  Cl  F
      |   |   |
F - C - C - C - F
      |   |   |
      Cl  F   F
  
```

Molecular Weight 237.4

Formula Composition 15.2% C, 40.0% F, 44.8% Cl

Preparation

1. CF₃-CCl=CCl₂ + F₂ $\longrightarrow$ CF₃-CClF-CCl₂F M-3113 (137)
2. CF₃-CCl=CCl₂ + HF + PbO₂ $\longrightarrow$ CF₃-CClF-CCl₂F ibid

Boiling Point, °C

73
73.5

ibid
J. Am. Chem. Soc., 67, 1639 (1945)

Density, g/cc

Temperature, °C

20

1.6614
1.6643

M-3113 (137)

J. Am. Chem. Soc., 67, 1639 (1945)Refractive Index (n_D)

Temperature, °C

20

1.3529
1.3538

ibid
M-3113 (137)

Molecular Refraction (MR_D)AR_F (calculated)

31.04

1.18

ibid

220 103

75

Chemical Name 1,2,2-Trichloro-1,1,3,3,3-pentafluoropropane

Empirical Formula C₃F₅Cl₃

Structural Formula

```

      Cl  Cl  F
      |  |  |
F - C - C - C - F
      |  |  |
      F  Cl F

```

Molecular Weight 237.4

Formula Composition 15.2% C, 40.0% F, 44.8% Cl

Preparation

M-3113 (133)

Freezing Point, °C

-4.30

J. Am. Chem. Soc., 63, 3478, (1941)Boiling Point, °C

72.0

ibid

Density, g/ml

Temperature, °C

20

1.6681

ibid

Refractive Index (n_D)

Temperature, °C

20

1.3519

ibid

Molecular Refraction (MR_D)AR_F (calculated)

30.77

1.12

ibid

220 104

76

Chemical Name 1,2,3-Trichloro-1,1,2,3,3-pentafluoropropane

Empirical Formula C₃F₅Cl₃

Structural Formula

```

      Cl  Cl  Cl
      |   |   |
F - C - C - C - F
      |   |   |
      F   F   F

```

Molecular Weight 237.4

Formula Composition 15.2% C, 40.0% F, 44.8% Cl

Preparation

M-3113 (136)

Boiling Point, °C

73.7

ibid

Density, g/ml

Temperature, °C

20

1.6562

ibid

Refractive Index (n_D)

Temperature, °C

20

1.3503

25.5

1.3480

ibid

Molecular Refraction (MR_D)AR_F (calculated)

30.87

1.14

ibid

Reactions

Dechlorinated readily with zinc..

ibid

220 105

77

Chemical Name 1-Chloro-1,2,3,3,3-pentafluoropropene

Empirical Formula C₃F₅Cl

Structural Formula

$$\begin{array}{ccccccc}
 & & \text{F} & & \text{F} & & \text{Cl} \\
 & & | & & | & & | \\
 \text{F} & - & \text{C} & - & \text{C} & = & \text{C} & - & \text{F} \\
 & & | & & & & & & \\
 & & \text{F} & & & & & &
 \end{array}$$

Molecular Weight 166.5

Formula Composition 21.6% C, 57.1% F, 21.3% Cl

Preparation

CF₃-CFC1-CFC1₂ chlorine removal → CF₃-CF=CFCl A-2104 (5)

Boiling Point, °C

7.9 M-3113 (133)

220 106

Chemical Name 2-Chloro-1,1,3,3,3-pentafluoropropene

Empirical Formula C₃F₅Cl

Molecular Weight 166.5

Formula Composition 21.6% C, 57.1% F, 21.3% Cl

Preparation

Freezing Point, °C

-130.4

ibid

Boiling Point, °C

6.7 at 764.3 mm
6.8

M-3113 (134)
J. Am. Chem. Soc., 63, 3478 (1941)

Density, g/cc

Temperature, °C

-20

1.592

M-3113 (134)

77

 C_3F_5Cl Refractive Index (n_D)

Temperature, °C

-20

1.314

M-3113 (134)

Molecular Refraction (MR_D) AR_F (calculated)

20.39

1.09

ibid

Reactions

Liquid phase reaction with fluorine gave $CF_3-CClF-CF_3$ and $(CF_3)_2CCl-CCl(CF_3)_2$.

Pyrolysis

It is more stable than $CF_2=CF-CF_2Cl$.

M-2534 (2)

220 108

80

Chemical Name 3-Chloro-1,1,2,3,3-pentafluoropropene

Empirical Formula C₃F₅Cl

Structural Formula

$$\begin{array}{ccccccc}
 & & \text{F} & & \text{F} & & \text{F} \\
 & & | & & | & & | \\
 \text{F} & - & \text{C} & - & \text{C} & = & \text{C} & - & \text{F} \\
 & & | & & & & & & \\
 & & \text{Cl} & & & & & &
 \end{array}$$

Molecular Weight 166.5

Formula Composition 21.6% C, 57.1% F, 21.3% Cl

Preparation

1. By fluorination of CFCl₂-CF=CF₂ A-2104 (5)
2. By pyrolysis of CF₂=CFCl M-3113 (133)

Boiling Point, °C

8.3 at 764.3 mm

ibid

Density, g/cc

Temperature, °C

-20

1.582

ibid

Refractive Index (n_D)

Temperature, °C

-20

1.318

ibid

Molecular Refraction (MR_D)AR_F (calculated)

20.76

1.16

ibid

220 109

81

Reactions

1. Readily brominated.
2. Readily chlorinated.
3. Gave positive permanganate unsaturation test.
4. Reacted with ammonia.
5. Reacted with aniline.
6. Hot tube reaction gave a mixture of CF₂=CFCl and hexafluorocyclobutene.

M-3113 (133)

M-2534 (2)

Pyrolysis

CF₂Cl-CF=CF₂ is less stable than CF₃-CCl=CF₂.

ibid

220 110

82

Chemical Name	Tetrachlorotetrafluoropropane (mixture of isomers)
Empirical Formula	C ₃ F ₄ Cl ₄
Molecular Weight	253.9
Formula Composition	14.2% C, 29.9% F, 55.9% Cl

Preparation

- $$\text{C}_3\text{H}_8 + \text{Cl}_2 \xrightarrow[\text{phase}]{\text{liquid}} \text{Highly chlorinated propane}$$

$$\text{Highly chlorinated propane} + \text{HF} \xrightarrow{\text{SbCl}_5} \text{C}_3\text{F}_4\text{Cl}_4 \quad \text{MDDC-162 (24)}$$
- $$\text{CF}_2=\text{CFCI} \xrightarrow[\text{hot tube}]{550-600^\circ\text{C}} \text{C}_3\text{Cl}_2\text{F}_4$$

$$\text{C}_3\text{Cl}_2\text{F}_4 + \text{Cl}_2 \longrightarrow \text{C}_3\text{Cl}_4\text{F}_4 \quad \text{M-3113 (137)}$$

Boiling Point, °C

111.1	MDDC-162 (28)
114	M-3113 (137)

Density, g/cc

Temperature, °C

20	1.7138	M-3113 (137)
	1.7155	MDDC-162 (28)

Refractive Index (n_D)

Temperature, °C

20	1.3959	M-3113 (137)
	1.3960	MDDC-162 (28)

Reactions

Dechlorinated with zinc to C₃Cl₂F₄. M-3113 (137)

Chemical Name 2,3-Dichloro-1,1,3,3-tetrafluoropropene

Empirical Formula C₃F₄Cl₂

Structural Formula

$$\begin{array}{c} \text{Cl} \quad \text{Cl} \quad \text{F} \\ | \quad | \quad | \\ \text{F} - \text{C} - \text{C} = \text{C} - \text{F} \\ | \\ \text{F} \end{array}$$

Molecular Weight 183.0

Formula Composition 19.7% C, 41.5% F, 38.8% Cl

Preparation

CF₂Cl-CCl₂-CF₂Cl + Zn ethanol → CF₂=CCl-CF₂Cl J. Am. Chem. Soc., 63, 3478 (1941)

Freezing Point, °C

-121.2

ibid

Boiling Point, °C

43
44.7

A-3786 (91)
J. Am. Chem. Soc., 63, 3478 (1941)

Density, g/cc

Temperature, °C

20

1.5406

ibid

Refractive Index (n_D)

Temperature, °C

20

1.3484

ibid

Molecular Refraction (MR_D)

AR_F (calculated)

25.45

1.13

ibid

220 112

84

Chemical Name	Dichlorotetrafluoropropene (mixture of isomers)
Empirical Formula	C ₃ F ₄ Cl ₂ (for the 2,3 isomer see page 208)
Molecular Weight	183.0
Formula Composition	19.7% C, 41.5% F, 38.8% Cl

Preparation

CF₂=CFCl $\xrightarrow[\text{hot tube}]{550-600^\circ}$ mixture containing some C₃F₄Cl₂ M-3113 (135)

Boiling Point, °C

47.2 ibid

Density, g/cc

Temperature, °C

20 1.5350 ibid

Refractive Index (n_D)

Temperature, °C

20 1.3509 ibid

Reactions

1. Chlorinated to C₃F₄Cl₄.
2. Partially brominated to C₃F₄Br₂Cl₂.
3. Gave positive permanganate unsaturation test.
4. Reacted with KI or NaI in acetone to yield chloride ion. ibid

85

Chemical Name 1,1,1,2,2-Pentachloro-3,3,3-trifluoropropane

Empirical Formula C₃F₃Cl₅

Structural Formula

$$\begin{array}{ccccccc} & & \text{F} & & \text{Cl} & & \text{Cl} \\ & & | & & | & & | \\ \text{F} & - & \text{C} & - & \text{C} & - & \text{C} & - & \text{Cl} \\ & & | & & | & & | \\ & & \text{F} & & \text{Cl} & & \text{Cl} \end{array}$$

Molecular Weight 270.3

Formula Composition 13.3% C, 21.1% F, 65.6% Cl

Preparation

1. $\text{CCl}_2=\text{CCl}-\text{CF}_3 + \text{Cl}_2 \longrightarrow \text{CCl}_3-\text{CCl}_2-\text{CF}_3$ M-3113 (137)
2. $\text{CF}_2\text{Cl}-\text{CFCI}-\text{CF}_2\text{Cl} + \text{AlCl}_3 \xrightarrow[5 \text{ hr}]{80-90^\circ\text{C}} \text{CCl}_3-\text{CCl}_2-\text{CF}_3$ (30% yield) ibid

Freezing Point, °C

108.9-109.2
109.1

ibid
J. Am. Chem. Soc., 63, 3478 (1941)

Boiling Point, °C

152
152.5-152.8
153.1

M-3113 (137)
Ind. Eng. Chem., 39, 313 (1947)
J. Am. Chem. Soc., 63, 3478 (1941)

Density, g/cc

Temperature, °C

20

1.7660

Ind. Eng. Chem., 39, 313 (1947)

Refractive Index (n_D)

Temperature, °C

20

1.4392

ibid

220 114

86

Chemical Name	1,1,2-Trichloro-3,3,3-trifluoropropene
Empirical Formula	C ₃ F ₃ Cl ₃
Structural Formula	$ \begin{array}{ccccccc} & & \text{F} & & \text{Cl} & & \text{Cl} \\ & & & & & & \\ \text{F} & - & \text{C} & - & \text{C} & = & \text{C} & - & \text{Cl} \\ & & & & & & & & \\ & & \text{F} & & & & & & \end{array} $
Molecular Weight	199.4
Formula Composition	18.1% C, 28.6% F, 53.3% Cl

Preparation

1.	CCl ₂ =CCl-CCl ₃ + SbF ₃	$\xrightarrow{150^\circ\text{C}}$	CCl ₂ =CCl-CF ₃	M-3113 (136)
2.	CCl ₃ -CCl ₂ -CF ₃ + Zn	$\longrightarrow$	CCl ₂ =CCl-CF ₃	ibid

Freezing Point, °C

-114.7	ibid
--------	------

Boiling Point, °C

88.3	ibid
------	------

Density, g/cc

Temperature, °C

20	1.6188	ibid
----	--------	------

Refractive Index (n_D)

Temperature, °C

20	1.4095	ibid
----	--------	------

Molecular Refraction (MR_D)

220 115

AR_F (calculated)

30.48	1.20	ibid
-------	------	------

Reactions

Liquid phase reaction with F₂ at 0°C yielded 25 mol % CF₃-CFCl-CCl₂F, 16 mol % C₃F₄Cl₄ and 15 mol % C₆F₈Cl₆.
 ibid

87

C₃F₃H₅

Chemical Name 1,1,1-Trifluoropropane

Empirical Formula C₃F₃H₅

Molecular Weight 98.0

Formula Composition 36.8% C, 58.1% F, 5.1% H

Boiling Point, °C

-13
-15.6 at 741 mm

A-3786 (91)

Bond Measurements

Bond	Bond distance, Å	Bond angle, °	
C-C (C-CF ₃)	1.48 - 1.51	—	
C-C (C-CH ₃)	1.50 - 1.57	—	
C-F	1.33 ± 0.02	—	A-3786 (79)
F-C-F	—	108	A-3786 (56)

220 116

88

Chemical Name 2,2-Difluoropropane

Empirical Formula C₃F₂H₆

Structural Formula

```

      H   F   H
      |   |   |
H - C - C - C - H
      |   |   |
      H   F   H
  
```

Molecular Weight 80.0

Formula Composition 45.0% C, 47.5% F, 7.5% H

Boiling Point, °C

0.3 at 758 mm

A-3786 (91)

Bond Measurements

Bond	Bond distance, Å	Bond angle, °
C-C	1.51 ± 0.02	—
C-F	1.34 ± 0.02	—
F-C-F	—	112 ± 3

A-3786 (79)

220 117

89

C₃F₂H₄

Chemical Name	1,1-Difluoropropene
Empirical Formula	C ₃ F ₂ H ₄
Structural Formula	$\begin{array}{ccccc} \text{F} & & & & \text{H} \\ & & & & \\ \text{C} & = & \text{C} & - & \text{C} & - & \text{H} \\ & & & & \\ \text{F} & & \text{H} & & \text{H} \end{array}$
Molecular Weight	78.0
Formula Composition	46.2% C, 48.7% F, 5.1% H

Boiling Point, °C

-30
-32 at 741 mm

A-3786 (91)

220 118

90

Chemical Name 1,2-Dibromo-2-chloro-1,1,3,3,3-pentafluoropropane

Empirical Formula C₃F₅Br₂Cl

Structural Formula

$$\begin{array}{ccccccc}
 & & \text{Br} & & \text{Br} & & \text{F} \\
 & & | & & | & & | \\
 \text{F} & - & \text{C} & - & \text{C} & - & \text{C} & - & \text{F} \\
 & & | & & | & & | \\
 & & \text{F} & & \text{Cl} & & \text{F}
 \end{array}$$

Molecular Weight 326.4

Formula Composition 11.0% C, 29.1% F, 49.0% Br, 10.9% Cl

Preparation

M-3113 (130)

Boiling Point, °C

111

ibid

220 119

Chemical Name 1,2-Dibromo-3-chloro-1,1,2,3,3-pentafluoropropane

Empirical Formula C₃F₅Br₂Cl

Structural Formula

```

      F   F   F
      |   |   |
F - C - C - C - F
      |   |   |
      Br  Br  Cl
  
```

Molecular Weight 326.4

Formula Composition 11.0% C, 29.1% F, 49.0% Br, 10.9% Cl

Preparation

CF₂=CF-CF₂Cl + Br₂ $\longrightarrow$ CF₂Br-CFBr-CF₂Cl M-3113 (131)

Freezing Point, °C

-123.7 to -123.1 ibid

Boiling Point, °C

55-57 at 105 mm. ibid

Density, g/cc

Temperature, °C

20 2.2050 ibid

Refractive Index (n_D)

Temperature, °C

20 1.4029 ibid

Molecular Refraction (MR_D)

AR_F (calculated)

36.11 1.03 ibid

220 120

92

C₃F₄Br₂Cl₂

Chemical Name	Dibromodichlorotetrafluoropropane
Empirical Formula	C ₃ F ₄ Br ₂ Cl ₂
Molecular Weight	342.9
Formula Composition	10.5% C, 22.2% F, 46.6% Br, 20.7% Cl

Preparation

M-3113 (131)

Boiling Point, °C

55-58 at 25 mm

ibid

Density, g/cc

Temperature, °C

20

2.2414

ibid

Refractive Index (n_D)

Temperature, °C

20

1.4472

ibid

Reactions

Debrominated with Zn to C₃F₄Cl₂.

ibid

220 121

Chemical Name 1,1,2,2-Tetrafluoro-1-methoxyethane

Empirical Formula C₃F₄H₄O

Structural Formula

$$\begin{array}{ccccccc}
 & \text{H} & & \text{F} & \text{F} & & \\
 & | & & | & | & & \\
 \text{H} & - \text{C} & - \text{O} & - \text{C} & - \text{C} & - \text{H} \\
 & | & & | & | & & \\
 & \text{H} & & \text{F} & \text{F} & &
 \end{array}$$

Molecular Weight 132.0

Formula Composition 27.3% C, 57.6% F, 3.0% H, 12.1% O

Preparation

M-3113 (139)

Freezing Point, °C

-107

ibid

Boiling Point, °C

36.5

ibid

Density, g/cc

Temperature, °C

20

1.2939

ibid

220 122

94

C₃F₃Cl₄H

Chemical Name 1,1,1,2-Tetrachloro-3,3,3-trifluoropropane

Empirical Formula C₃F₃Cl₄H

Molecular Weight 235.9

Formula Composition 15.3% C, 24.2% F, 60.1% Cl, 0.4% H

Boiling Point, °C

127.5-129

MDDC-168 (11)

Density, g/cc

Temperature, °C

20

1.6792

MDDC-162 (28)

Refractive Index (n_D)

Temperature, °C

20

1.4175

ibid

220 123

95

 $C_3F H_5O_2$

Chemical Name Methyl fluoroacetate

Empirical Formula $C_3F H_5O_2$

Molecular Weight 92.0

Formula Composition 39.2% C, 20.6% F, 5.4% H, 34.8% O

Preparation

M-2149 (36)

Freezing Point, °C

-35

ibid

Boiling Point, °C

104.5

ibid

Vapor PressureEquation: $\log p = 8.568 - 2141.5/T$

ibid

ToxicityApprox LC_{50} , mg/l

Animal

0.010

dog

0.025 = 0.050

rabbit

0.10

guinea pig

> 2.6

mouse

> 1.0

monkey

 LC_{50} for rabbits, guinea pigs and rats is 0.15 mg/l. Much less toxic to mice.

220 124

96

Concentration, mg/l	Fatalities, mice
---------------------	------------------

1.0	3/10
2.0	4/10
3.0	5/10

M-2149 (27)

By intravenous injection	0.25 mg/kilo for mice
By skin absorption	0.25 mg/kilo for mice

Toxic concentrations not detected by smell. The odor is faint and not characteristic.

Concentration

50 mg/m ³	faint, fruity smell
400 mg/l	odor not appreciable

M-2149 (40)

Absorption

Charcoal penetration - A concentration of 1 in 200 causes an incipient breakdown of the gas mask canister after 2.5 to 3 hours. Complete breakdown occurs after 9 to 10 hours. A toxic concentration passes canister after 5 hours.

M-2149 (37)

220 125

Chemical Name 2-Chloro-1,1,2-trifluoro-1-methoxyethane

Empirical Formula C₃F₃ClH₄O

Structural Formula

$$\begin{array}{ccccccc}
 & \text{H} & & \text{F} & & \text{H} & \\
 & | & & | & & | & \\
 \text{H} & - \text{C} & - & \text{O} & - & \text{C} & - \text{C} - \text{F} \\
 & | & & | & & | & \\
 & \text{H} & & \text{F} & & \text{Cl} &
 \end{array}$$

Molecular Weight 148.5

Formula Composition 24.2% C, 38.4% F, 23.9% Cl, 2.7% H, 10.8% O

Preparation Freezing Point*, °C

-109.4 to -109.0
- 92.6 to - 92.0

ibid

*Exists in two forms

Boiling Point, °C

70.6

ibid

Density, g/cc

Temperature, °C

20

1.3636

ibid

Refractive Index, (n_D)

Temperature, °C

20

1.3340

ibid

98

Molecular Refraction (MR_D)

AR_F (calculated)

22.46

1.01

M-3113 (138)

Solubility

Insoluble in cold concentration H_2SO_4 .

ibid

220 127

Chemical Name 2,2-Dichloro-1,1-difluoro-1-methoxyethane

Empirical Formula C₃F₂Cl₂H₄O

Molecular Weight 165.0

Formula Composition 21.8% C, 23.0% F, 43.1% Cl, 2.4% H, 9.7% O

Preparation

M-3113 (139)

Freezing Point, °C

-35

ibid

Boiling Point, °C

105

ibid

Density, g/cc

Temperature, °C

20

1.4262

ibid

Refractive Index (n_D)

Temperature, °C

20

1.3861

ibid

100

Molecular Refraction (MR_D)

AR_F (calculated)

27.18

0.97

M-3113 (139)

Reactions

Heating with alcoholic KOH gave a strong fluoride and a very weak chloride test.
ibid

220 129

DECLASSIFIED

Chemical Name Decafluorobutane

Empirical Formula C₄F₁₀

Molecular Weight 238.0

Formula Composition 20.2% C, 79.8% F

Preparation

Melting Point, °C

Solidifies as a "glass"

BR-319 (8)
A-312 (4).

Boiling Point, °C

-4.7 at 760 mm
 (assumed to be the iso-compound)
 -2 (approximately)
 -1.5 (approximately)
 -1.4 ± 0.2 at 769 mm
 +3.0 (normal)

A-312 (4)
 M-3113 (154)
 MDDC-600 (48)
 A-3468 (85)
 M-530 (1)
 M-3113 (154)

220 130

Density, g/cc

1. Liquid:

Temperature, °C

0.2	1.53	
8.8	1.49	
20.8	1.47	Br-319 (8)
20	1.47	A-312 (4)
45	1.47	
55	1.43	
65	1.40	
75	1.36	
85	1.30	A-3648 (143)

Temperature, °C

Orthobaric density

45	1.41
55	1.36
65	1.32
75	1.25
85	1.19
113.3	0.63*

*extrapolated

See Figure 175

MDDC-213 (18)

2. Vapor:

Temperature, °C

Orthobaric density

45	0.053
55	0.063
65	0.084
75	0.110
85	0.147
113.3	0.63*

*extrapolated

See Figure 175

ibid

Vapor Pressure

Temperature, °C	Atmosphere*
-28.3	0.35
-20.0	0.50
0.0	1.11
+10.10	1.62
20.00	2.29
29.85	3.14
40.34	4.21
50.00	5.61
60.51	7.24
64.95	7.98
70.37	9.17
82.15	12.19
90.00	13.66

*For sample having b p -1.4 ± 0.2 at 769 mm

See Figure 176

A-3468 (133)

Equations:

a. For sample having b p -4.7° , possible the iso-compound,
 $\log p = 7.43 - 1217/T$.

b. For sample having b p $+3.0$, $\log p = 7.44 - 1260/T$.

BR-319 (8)

Critical Temperature, °C

113.3 ± 0.2

A-3468 (142)

Critical Pressure, atm

22.5

ibid

Critical Density, g/cc

0.5098 ± 0.006

ibid

220 132

104

C₄F₁₀

Heat of Vaporization, cal/mol

5557

5600 (uncertain of sample)

5800 (uncertain of sample)

A-3468 (136)

BR-319 (8)

Entropy of Vaporization

20.5

A-3468 (136)

220 133

Chemical Name Octafluoro-1-butene

Empirical Formula C₄F₈

Molecular Weight 200.0

Formula Composition 24.0% C, 76.0% F

Preparation

M-3113 (154)

Boiling Point, °C

4.8 at 764.3 mm

ibid

Density, g/cc

Temperature, °C

-20

1.615

ibid

Reactions

1. May be chlorinated.
2. Liquid phase reaction with fluorine yields C₄F₁₀ and C₈F₁₈.
3. Gives positive permanganate unsaturation test.

ibid

106

Chemical Name	Octafluoro-2-butene
Empirical Formula	C ₄ F ₈
Structural Formula	$ \begin{array}{ccccccc} & \text{F} & & & \text{F} & & \\ & & & & & & \\ \text{F} & - \text{C} & - & \text{C} & = & \text{C} & - \text{C} - \text{F} \\ & & & & & & \\ & \text{F} & & \text{F} & & \text{F} & \end{array} $
Molecular Weight	200.0
Formula Composition	24.0% C, 76.0% F

Preparation

1. $\text{CF}_3\text{-CFCI-CFCI-CF}_3 + \text{Zn} \longrightarrow \text{CF}_3\text{-CF=CF-CF}_3$
2. $\text{CF}_2\text{Cl-CF=CF-CF}_2\text{Cl} + \text{HF} \xrightarrow{\text{HgO}} \text{CF}_3\text{-CF=CF-CF}_3$

M-3113 (153)

Melting Point, °C

-136 to -134

ibid

Boiling Point, °C

1.2 at 764.3 mm

ibid

Density, g/cc

Temperature, °C

-20

1.601

ibid

Reactions

1. Readily chlorinated.
2. Readily brominated.
3. Gives positive permanganate unsaturation test.

ibid

220 135

107

Chemical Name Octafluorocyclobutane

Empirical Formula C₄F₈

Molecular Weight 200.0

Formula Composition 24.0% C, 76.0% F

Preparation

M-3113 (155)

Boiling Point, °C

-4.0 at 764.3 mm
-5 (approx)

ibid
A-3786 (91)

Density, g/cc

Temperature, °C

-20

1.654

M-3113 (155)

220 136

108

Chemical Name Hexafluoro-1,3-butadiene

Empirical Formula C₄F₆

Structural Formula

$$\begin{array}{ccccccc} & & \text{F} & & \text{F} & & \text{F} & & \text{F} \\ & & | & & | & & | & & | \\ \text{F} & - & \text{C} & = & \text{C} & - & \text{C} & = & \text{C} & - & \text{F} \end{array}$$

Molecular Weight 162.0

Formula Composition 29.6% C, 70.4% F

Preparation

1. $\text{CF}_2\text{Cl}-\text{CFCl}-\text{CFCl}-\text{CF}_2\text{Cl} + \text{Zn} \longrightarrow \text{CF}_2=\text{CF}-\text{CF}=\text{CF}_2$
2. $\text{CF}_2\text{Cl}-\text{CFCl}-\text{CF}=\text{CF}_2 + \text{Zn} \longrightarrow \text{CF}_2=\text{CF}-\text{CF}=\text{CF}_2$

M-3113 (151)

Freezing Point, °C

-132.4 to -132.1

ibid

Boiling Point, °C

6.6

ibid

Density, g/cc

Temperature, °C

-20

1.553

ibid

Refractive Index (n_D)

Temperature, °C

-20

1.378

ibid

220 137

109

Molecular Refraction (MR_D)AR_F (calculated)

24.06

1.58

M-3113 (151)

Reactions

1. Brominated to yield C₄Br₂F₆ and C₄Br₄F₆.
2. Chlorinated to yield C₄Cl₄F₆.
3. Reacts in liquid phase with fluorine to form addition compound, dimer and high polymers.
4. Forms C₈F₁₂ and C₁₂F₁₈ when heated in bomb at 120-200°C.
5. Pyrolyzed at 400-650°C to form CF₂-CF=CF-CF₂.
6. Polymerized by benzoyl peroxide. ibid

220 138

110

Chemical Name	Hexafluorocyclobutene
Empirical Formula	C ₄ F ₆
Structural Formula	$ \begin{array}{c} \text{F} - \text{C} = \text{C} - \text{F} \\ \quad \\ \text{F} - \text{C} - \text{C} - \text{F} \\ \quad \\ \text{F} \quad \text{F} \end{array} $
Molecular Weight	162.0
Formula Composition	29.6% C, 70.4% F

Preparation

Freezing Point, °C

-61.1 to -60.9
-60.37

ibid
Ind. Eng. Chem., 39, 367 (1947)

Boiling Point, °C

0.0 at 764.3 mm
1.13

M-3113 (152)
Ind. Eng. Chem., 39, 367 (1947)

Density, g/cc

Temperature, °C

-20

1.602

M-3113 (152)

Refractive Index (n_D)

Temperature, °C

-20

1.298

M-3113 (152)

Molecular Refraction (MR_D)AR_F (calculated)

18.80

1.15

ibid

Reactions

1. Readily chlorinated.
2. Readily brominated.
3. Reacts in liquid phase with fluorine to yield octafluorocyclobutane as the main product.
4. Pyrolyzed at 750° to higher boiling products. ibid

220 140

112

Chemical Name 2,3-Dibromo-1,1,1,2,3,4,4,4-octafluorobutane

Empirical Formula C₄F₈Br₂

Structural Formula

```

      F   F   F   F
      |   |   |   |
F - C - C - C - C - F
      |   |   |   |
      F   Br  Br  F
  
```

Molecular Weight 359.9

Formula Composition 13.3% C, 42.3% F, 44.4% Br

Preparation Boiling Point, °C

96 ibid

Refractive Index (n_D)

Temperature, °C

20 1.3574 ibid

220 141

*May be a mixture of $\text{CF}_2\text{Br}-\text{CF}=\text{CF}-\text{CF}_2\text{Br}$ and $\text{CF}_2\text{Br}-\text{CFBr}-\text{CF}=\text{CF}_2$

Formula Composition 14.9% C, 35.4% F, 49.7% Br

M-3113 (139)

ibid

ibid

ibid

ibid

114

Chemical Name 1,2-Dichloro-1,1,2,3,3,4,4,4-octafluorobutane

Empirical Formula C₄F₈Cl₂

Structural Formula

```

      F   F   F   F
      |   |   |   |
F - C - C - C - C - F
      |   |   |   |
      Cl  Cl  F   F
  
```

Molecular Weight 271.0

Formula Composition 17.7% C, 56.1% F, 26.2% Cl

Preparation Freezing Point, °C

28-29 ibid

Boiling Point, °C

64 ibid

Reaction

Dechlorinated with Zn to CF₂=CF-CF₂-CF₃. ibid

115

Chemical Name 1,4-Dichloro-1,1,2,2,3,3,4,4-octafluorobutane

Empirical Formula C₄F₈Cl₂

Structural Formula

```

      Cl  F  F  Cl
      |  |  |  |
F - C - C - C - C - F
      |  |  |  |
      F  F  F  F

```

Molecular Weight 271.0

Formula Composition 17.7% C, 56.1% F, 26.2% Cl

Preparation Boiling Point, °C

64.0

ibid

220 144

116

Chemical Name 2,3-Dichloro-1,1,1,2,3,4,4,4-octafluorobutane

Empirical Formula C₄F₈Cl₂

Structural Formula

```

      F   F   F   F
      |   |   |   |
F - C - C - C - C - F
      |   |   |   |
      F   Cl  Cl  F
  
```

Molecular Weight 271.0

Formula Composition 17.7% C, 56.1% F, 26.2% Cl

Preparation

M-3113 (145)

Boiling Point, °C

64

ibid

117

Chemical Name	Trichloroheptafluorobutane
Empirical Formula	C ₄ F ₇ Cl ₃
Molecular Weight	287.4
Formula Composition	16.7% C, 46.3% F, 37.0% Cl

Preparation

M-3113 (146)

Boiling Point, °C

99

ibid

Density, g/cc

Temperature, °C

20

1.7249

ibid

Refractive Index, (n_D)

Temperature, °C

20

1.3467

ibid

Molecular Refraction (MR_D)AR_F (calculated)

35.45

1.14

ibid

220 145A

118

Chemical Name	Trichloroheptafluorobutane
Empirical Formula	C ₄ F ₇ Cl ₃
Molecular Weight	287.4
Formula Composition	16.7% C, 46.3% F, 37.0% Cl

Preparation Boiling Point, °C

100		ibid
-----	--	------

Density, g/cc

Temperature, °C

20	1.7350	ibid
----	--------	------

Refractive Index (n_D)

Temperature, °C

20	1.3509	ibid
----	--------	------

Molecular Refraction (M_R)AR_F (calculated)

35.73	1.16	ibid
-------	------	------

220 146

119

Chemical Name	Chloroheptafluorobutene
Empirical Formula	C ₄ F ₇ Cl
Molecular Weight	216.5
Formula Composition	22.2% C, 61.4% F, 16.4% Cl

Preparation

M-3113 (140)

Boiling Point, °C

34-35

ibid

ReactionChlorinated to C₄F₇Cl₃.

ibid

220 147

120

Chemical Name 2-Chloro-1,1,1,3,4,4,4-heptafluoro-2-butene

Empirical Formula C₄F₇Cl

Structural Formula

$$\begin{array}{ccccccc}
 & \text{F} & & \text{Cl} & & \text{F} & & \text{F} \\
 & | & & | & & | & & | \\
 \text{F} & - \text{C} & - & \text{C} & = & \text{C} & - & \text{C} & - & \text{F} \\
 & | & & & & & & | \\
 & \text{F} & & & & & & \text{F}
 \end{array}$$

Molecular Weight 216.5

Formula Composition 22.2% C, 61.4% F, 16.4% Cl

Preparation Boiling Point, °C

33-35

ibid

Density, g/cc

Temperature, °C

17

1.487

ibid

Refractive Index (n_D)

Temperature, °C

17

1.3115

ibid

220 148

121

Chemical Name 1,2,3,4-Tetra~~bro~~mo-1,1,2,3,4,4-hexafluorobutane

Empirical Formula C₄F₆Br₄

Structural Formula

```

      F   F   F   F
      |   |   |   |
F - C - C - C - C - F
      |   |   |   |
      Br  Br  Br  Br
  
```

Molecular Weight 481.7

Formula Composition 10.0% C, 23.7% F, 66.3% Br

Preparation Boiling Point, °C

118-122 at 60 mm

ibid

Density, g/cc

Temperature, °C

25

2.588

ibid

Refractive Index, (n_D)

Temperature, °C

20

1.467

ibid

220 149

122

Chemical Name 1,2,3,4-Tetrachloro-1,1,2,3,4,4-hexafluorobutane

Empirical Formula C₄F₆Cl₄

Structural Formula

$$\begin{array}{ccccccc}
 & \text{F} & & \text{F} & & \text{F} & & \text{F} \\
 & | & & | & & | & & | \\
 \text{F} & - \text{C} & - & \text{C} & - & \text{C} & - & \text{C} & - & \text{F} \\
 & | & & | & & | & & | \\
 & \text{Cl} & & \text{Cl} & & \text{Cl} & & \text{Cl}
 \end{array}$$

Molecular Weight 303.9

Formula Composition 15.8% C, 37.5% F, 46.7% Cl

Preparation

1. $\text{CCl}_2=\text{CCl}-\text{CCl}=\text{CCl}_2 + 3 \text{ F}_2 \longrightarrow \text{CF}_2\text{Cl}-\text{CFCI}-\text{CFCI}-\text{CF}_2\text{Cl}$ M-2544 (2)
(30% yield)
2. $2 \text{ CFCI}=\text{CFCI} + 2 \text{ F}_2 \longrightarrow \text{CF}_2\text{Cl}-\text{CFCI}-\text{CFCI}-\text{CF}_2\text{Cl}$
3. $\text{CF}_2=\text{CF}-\text{CFCI}-\text{CF}_2\text{Cl} + \text{Cl}_2 \longrightarrow \text{CF}_2\text{Cl}-\text{CFCI}-\text{CFCI}-\text{CF}_2\text{Cl}$ M-3113 (147)

Boiling Point, °C

134.1
134.5-134.6

ibid

Density, g/cc

Temperature, °C

20

1.7812

ibid

Refractive Index, (n_D)

Temperature, °C

20

1.3853

20.5

1.3850

ibid

220 150

123

Molecular Refraction (M_R) M_R (calculated)

40.01

1.08

M-3113 (147)

Reactions

1. Dechlorinated by Zn in alcohol to $CF_2=CF=CF_2$.
2. Dechlorinated by Zn in dioxane to $CF_2Cl-CF=CF-CF_2Cl$. *ibid*

220 151

124

Chemical Name	1,2-Dichloro-1,2,3,3,4,4-hexafluorocyclobutane
Empirical Formula	C ₄ F ₆ Cl ₂
Structural Formula	<pre> Cl Cl F - C - C - F F - C - C - F F F </pre>
Molecular Weight	233.0
Formula Composition	20.6% C, 49.0% F, 30.4% Cl

Preparation

1. Passing CF₂=CFCl through a tube at 500-550°C.
2. Heating CF₂=CFCl in a bomb at 100°C or higher.

M-3113 (144)

Freezing Point, °C

-17
-20.7 to -20.0

ibid

Boiling Point, °C

56
60.4

ibid

Density, g/cc

Temperature, °C

20

1.6448

ibid

Refractive Index (n_D)

Temperature, °C

20
25.5

1.3340
1.3310

ibid

220 152

125

Molecular Refraction (M_R) AR_F (calculated)

29.21

1.19

M-3113 (144)

Reactions

1. Dechlorinated with Zn to form $CF_2-CF=CF-CF_2$.
2. Pyrolyzed at 550° to yield $CFCl=CF_2$.
3. Negligible thermal vapor phase chlorinolysis under conditions where pyrolysis did not occur. ibid

220 153

12.6

Chemical Name 1,4-Dichloro-1,1,2,3,4,4-hexafluoro-2-butene

Empirical Formula C₄F₆Cl₂

Molecular Weight 233.0

Formula Composition 20.6% C, 49.0% F, 30.4% Cl

Preparation Boiling Point, °C

64-66

ibid

Reactions

1. Liquid phase reaction with fluorine at 0° yields 27 mol % CF₂Cl-CF₂-CF₂-CF₂Cl, 9 mol % C₄Cl₃F₇, and 12 mol % CF₂Cl-CF₂-CF(CF₂Cl)-CF(CF₂Cl)-CF₂-CF₂Cl.
2. Forms precipitate with pyridine, piperidine, and ammonia.
3. Reacts with HgO + HF to form CF₃-CF=CF-CF₃. ibid

220 154

127

Chemical Name 2,3-Dichloro-1,1,1,4,4,4-hexafluoro-2-butene

Empirical Formula C₄F₆Cl₂

Structural Formula

$$\begin{array}{ccccccc}
 & \text{F} & & & \text{F} & & \\
 & | & & & | & & \\
 \text{F} & - \text{C} & - & \text{C} & = & \text{C} & - \text{C} - \text{F} \\
 & | & & | & & | & \\
 & \text{F} & & \text{Cl} & & \text{Cl} & \text{F}
 \end{array}$$

Molecular Weight 233.0

Formula Composition 20.6% C, 48.9% F, 30.5% Cl

Preparation Boiling Point, °C

66-68

ibid

Density, g/cc

Temperature, °C

25

1.600

ibid

Refractive Index, (n_D)

Temperature, °C

20

1.3480

ibid

220 155

128

Chemical Name 3,4-Dichloro-1,1,2,3,4,4-hexafluoro-1-butene

Empirical Formula C₄F₆Cl₂

Structural Formula

$$\begin{array}{ccccccc}
 & \text{F} & & \text{F} & & \text{F} & & \text{F} \\
 & | & & | & & | & & | \\
 \text{C} & = & \text{C} & - & \text{C} & - & \text{C} & - & \text{F} \\
 & | & & & & | & & | \\
 & \text{F} & & & & \text{Cl} & & \text{Cl}
 \end{array}$$

Molecular Weight 233.0

Formula Composition 20.6% C, 49.0% F, 30.4% Cl

Preparation

1. $\text{CF}_2=\text{CFCl} \xrightarrow{550-600^\circ} \text{CF}_2=\text{CF}-\text{CFCl}-\text{CF}_2\text{Cl}$
2. $\text{CF}_2\text{Br}-\text{CFBr}-\text{CFCl}-\text{CF}_2\text{Cl} + \text{Zn} \longrightarrow \text{CF}_2=\text{CF}-\text{CFCl}-\text{CF}_2\text{Cl} \quad \text{M-3113 (143)}$

Boiling Point, °C

65-66

ibid

Density, g/cc

Temperature, °C

20

1.5764

ibid

Refractive Index (n_D)

Temperature, °C

20

1.3391

ibid

220 156

137

Molecular Refraction (MR_D)AR_F (calculated)

30.90

1.09

M-3113 (143)

Reactions

1. Brominated to C₄Br₂Cl₂F₆.
2. Chlorinated to C₄Cl₄F₆.
3. Gives positive permanganate unsaturation test.
4. Oxidized by alkaline permanganate to CF₂ClCOOH.
5. Reacts with aluminum chloride to form C₄Cl₃F₅.
6. Dechlorinated to CF₂=CF=CF=CF₂.

ibid

220 157

130

Chemical Name	Pentachloropentafluorobutane
Empirical Formula	C ₄ F ₅ Cl ₅
Molecular Weight	320.3
Formula Composition	15.0% C, 29.6% F, 55.4% Cl

Preparation

1. Liquid phase fluorination of CFCl=CFCl.
2. Liquid phase fluorination of CCl₂=CCl-CCl=CCl₂. M-3113 (148)

Boiling Point, °C

90-92 at 78 mm	
104.5 at 100 mm	ibid

Density, g/cc

Temperature, °C		
20	1.7961	ibid

Refractive Index (n_D)

Temperature, °C		
20	1.4203	ibid

Molecular Refraction (MR_D)

	AR _F (calculated)	
45.16	1.13	ibid

220 158

131

Chemical Name 3,3,4-Trichloro-1,1,2,4,4-pentafluoro-1-butene

Empirical Formula C₄F₅Cl₃

Structural Formula

$$\begin{array}{ccccccc}
 & & & & \text{F} & & \text{Cl} & & \text{F} \\
 & & & & | & & | & & | \\
 \text{C} & = & \text{C} & - & \text{C} & - & \text{C} & - & \text{F} \\
 & & & & | & & | & & | \\
 & & & & \text{F} & & \text{F} & & \text{Cl} & & \text{Cl}
 \end{array}$$

Molecular Weight 249.5

Formula Composition 19.2% C, 38.1% F, 42.7% Cl

Preparation Boiling Point, °C

102-103

ibid

220 159

132

Chemical Name 1,1,2,3,4,4-Hexachloro-1,2,3,4-tetrafluorobutane

Empirical Formula C₄F₄Cl₆

Structural Formula

```

      Cl  F  F  Cl
      |  |  |  |
F - C - C - C - C - F
      |  |  |  |
      Cl Cl Cl Cl

```

Molecular Weight 336.8

Formula Composition 14.2% C, 22.6% F, 63.2% Cl

Preparation Boiling Point, °C

133-134 at 100 mm ibid

Density, g/cc

Temperature, °C

20 1.8302 ibid

Refractive Index (n_D)

Temperature, °C

20 1.4568 ibid

Molecular Refraction (MR_D)AR_F (calculated)

50.10 1.16 ibid

Reactions

Dechlorinated with Zn to CFCl=CF=CF=CFCl. ibid

220 160

133

Chemical Name	1,2,2,3,3,4-Hexachloro-1,1,4,4-tetrafluorobutane
Empirical Formula	C ₄ F ₄ Cl ₆
Structural Formula	$ \begin{array}{ccccccc} & \text{F} & & \text{Cl} & & \text{Cl} & & \text{F} \\ & & & & & & & \\ \text{F} & - \text{C} & - & \text{C} & - & \text{C} & - & \text{C} & - \text{F} \\ & & & & & & & \\ & \text{Cl} & & \text{Cl} & & \text{Cl} & & \text{Cl} \end{array} $
Molecular Weight	336.8
Formula Composition	14.2% C, 22.6% F, 63.2% Cl

Preparation Boiling Point, °C

125-126 at 76 mm

ibid

Density, g/cc

Temperature, °C

20

1.8276

ibid

Refractive Index (n_D)

Temperature, °C

20

1.4579

ibid

Molecular Refraction (MR_D)MR_F (calculated)

50.28

1.15

ibid

ReactionsDechlorinated with Zn to C₄F₄Cl₂.

ibid

220 161

134

Chemical Name 1,4-Dichloro-1,2,3,4-tetrafluoro-1,3-butadiene

Empirical Formula C₄F₄Cl₂

Structural Formula

$$\begin{array}{ccccccc} & & \text{F} & & \text{F} & & \\ & & | & & | & & \\ \text{F} & - & \text{C} & = & \text{C} & - & \text{C} & = & \text{C} & - & \text{F} \\ & & | & & & & | & & & & \\ & & \text{Cl} & & & & \text{Cl} & & & & \end{array}$$

Molecular Weight 195.0

Formula Composition 24.6% C, 39.0% F, 36.4% Cl

Preparation

M-3113 (141)

Boiling Point, °C

78

ibid

Density, g/cc

Temperature, °C

20

1.5579

ibid

Refractive Index (n_D)

Temperature, °C

20

1.4019

ibid

Molecular Refraction (MR_D)AR_F (calculated)

30.46

0.99

ibid

220 162

135

Reactions

1. Forms $C_4F_4Cl_6$ by chlorination.
2. Reacts with bromine.
3. Gives positive permanganate unsaturation test.

M-3113 (141)

220 163

136

Chemical Name 2,3-Dichloro-1,1,4,4-tetrafluoro-1,3-butadiene

Empirical Formula C₄F₄Cl₂

Structural Formula

$$\begin{array}{ccccccc} & \text{F} & & & \text{F} & & \\ & | & & & | & & \\ \text{F} - & \text{C} = & \text{C} - & \text{C} = & \text{C} - & \text{F} \\ & & | & & | & & \\ & & \text{Cl} & & \text{Cl} & & \end{array}$$

Molecular Weight 195.0

Formula Composition 24.6% C, 39.0% F, 36.4% Cl

Preparation Boiling Point, °C

69-70

ibid

Density, g/cc

Temperature, °C

20

1.5525

ibid

Refractive Index (n_D)

Temperature, °C

20

1.3832

ibid

Molecular Refraction (MR_D)AR_F (calculated)

29.30

0.72

ibid

220 164

137

Reactions

1. Forms $C_4F_4Cl_6$ by chlorination.
2. Reacts with bromine.
3. Gives positive permanganate unsaturation test.

M-3113 (141)

220 165

138

Chemical Formula	Heptachlorotrifluorobutane
Empirical Formula	C ₄ F ₃ Cl ₇
Molecular Weight	353.3
Formula Composition	13.6% C, 16.1% F, 70.3% Cl

Preparation

Formed in the reaction of C₄Cl₆ with fluorine.

M-3113 (150)

Boiling Point, °C

124-125 at 25 mm

ibid

Density, g/cc

Temperature, °C

20

1.8649

ibid

Refractive Index (n_D)

Temperature, °C

20

1.4910

ibid

Molecular Refraction (MR_D)

AR_F (calculated)

54.86

1.12

ibid

220 166

139

Chemical Name 1,1,1-Trifluorobutane

Empirical Formula C₄F₃H₇

Structural Formula

$$\begin{array}{ccccccc} & \text{F} & \text{H} & \text{H} & \text{H} & & \\ & | & | & | & | & & \\ \text{F} & - \text{C} & - \text{C} & - \text{C} & - \text{C} & - \text{H} & \\ & | & | & | & | & & \\ & \text{F} & \text{H} & \text{H} & \text{H} & & \end{array}$$

Molecular Weight 112.0

Formula Composition 42.9% C, 50.9% F, 6.2% H

Melting Point, °C

-114.79

A-3786 (91)

220 167

140

Chemical Name 1,1,2,2,3,3,4,4-Octachloro-1,4-difluorobutane

Empirical Formula C₄F₂Cl₈

Structural Formula

```

      Cl  Cl  Cl  Cl
      |   |   |   |
F - C - C - C - C - F
      |   |   |   |
      Cl  Cl  Cl  Cl

```

Formula Composition 13.0% C, 10.3% F, 76.7% Cl

Preparation Boiling Point, °C

133 at 10 mm
152.5 at 20 mm
203 at 100 mm

ibid
J. Am. Chem. Soc., 62, 341 (1940)
M-3113 (150)

Density, g/cc

Temperature, °C

20

1.9272

J. Am. Chem. Soc., 62, 341 (1940)Refractive Index (n_D)

Temperature, °C

20

1.5256

ibid

Molecular Refraction (MR_D)AR_F (calculated)

58.83

0.71

ibid

220 168

141

Reactions

220 169

142

Chemical Name 1,2,3,4-Tetrachloro-1,4-difluoro-1,3-butadiene

Empirical Formula C₄F₂Cl₄

Structural Formula

$$\begin{array}{ccccccc} \text{F} & - & \text{C} & = & \text{C} & - & \text{C} & = & \text{C} & - & \text{F} \\ & & | & & | & & | & & | & & \\ & & \text{Cl} & & \text{Cl} & & \text{Cl} & & \text{Cl} & & \end{array}$$

Molecular Weight 227.9

Formula Composition 21.1% C, 16.7% F, 62.2% Cl

Preparation Melting Point, °C

-78

ibid

Boiling Point, °C131
139ibid
M-3113 (146)Density, g/cc

Temperature, °C

20

1.5192
1.5913M-2567 (2)
M-3113 (146)Refractive Index (n_D)

Temperature, °C

20

1.4710

ibid
M-2567 (2)

220 170

143

Molecular Refraction (MR_D) ΔR_F (calculated)

40.01	0.78	M-3113 (146)
41.26 (calculated)	—	
41.92	—	M-2567 (2)

Reactions

1. Forms $C_4F_2Cl_8$ by chlorination.
2. Reacts with bromine.
3. Gives positive permanganate unsaturation test. M-3113 (146)

220 171

144

Chemical Name 2,2-Difluorobutane

Empirical Formula C₄F₂H₈

Structural Formula

```

      H   F   H   H
      |   |   |   |
H - C - C - C - C - H
      |   |   |   |
      H   F   H   H

```

Molecular Weight 94.1

Formula Composition 51.1% C, 40.4% F, 8.5% H

Preparation

PCl₅ used to substitute keto group of 2-butanone to give the dichloride which is fluorinated with SbF₃ to give the difluoride. B-97 (11)

Density, g/cc

Temperature, °C

20

0.903

BR-645 (12)

Molecular Volume, cc

Temperature, °C

20

104.2

ibid

220 172

145

Chemical Name 1,1-Difluoro-1-butene

Empirical Formula C₄F₂H₆

Structural Formula

$$\begin{array}{ccccccc} & & & & \text{F} & & \text{H} & & \text{H} \\ & & & & | & & | & & | \\ \text{C} & = & \text{C} & - & \text{C} & - & \text{C} & - & \text{H} \\ & & | & & | & & | & & | \\ & & \text{F} & & \text{H} & & \text{H} & & \text{H} \end{array}$$

Molecular Weight 92.0

Formula Composition 52.2% C, 41.3% F, 6.5% H

Boiling Point, °C

3.71

A-3706 (91)

220 173

146

Chemical Name 1,2-Dibromo-3,4-dichloro-1,1,2,3,4,4-hexafluorobutane

Empirical Formula C₄F₆Br₂Cl₂

Structural Formula

```

      F   F   F   F
      |   |   |   |
F - C - C - C - C - F
      |   |   |   |
      Br  Br  Cl  Cl

```

Molecular Weight 392.9

Formula Composition 12.2% C, 29.0% F, 40.7% Br, 18.1% Cl

Preparation Boiling Point, °C

63 at 14 mm

ibid

Density, g/cc

Temperature, °C

20

2.2132

ibid

Refractive Index (n_D)

Temperature, °C

20

1.4267

ibid

Molecular Refraction (MR_F)AR_F (calculated)

45.54

1.03

ibid

ReactionDebrominated with Zn to CF₂=CF-CFCl-CF₂Cl.

ibid

220 174

147

Chemical Name	Dichlorohexafluorobutane
Empirical Formula	C ₄ F ₆ Cl ₂ H ₂
Molecular Weight	235.0
Formula Composition	20.4% C, 48.5% F, 30.2% Cl, 0.9% H

Boiling Range, °C

67.3-71.0

MDDC-162 (28)

Density, g/cc

Temperature, °C

20

1.5391

ibid

Refractive Index, (n_D)

Temperature, °C

20

1.3442

ibid

220 175

148

Chemical Name	Chlorohexafluorobutene
Empirical Formula	C ₄ F ₆ ClH
Molecular Weight	198.5
Formula Composition	24.2% C, 57.4% F, 17.9% Cl, 0.5% H

Boiling Point, °C

38.0-38.3

MDDC-162 (28)

MDDC-168 (11)

Density, g/cc

Temperature, °C

20

1.4666

MDDC-162 (28)

Refractive Index (n_D)

Temperature, °C

20

1.3012

ibid

220 176

149

Chemical Name	Trichlorotetrafluorobutene
Empirical Formula	$C_4F_4Cl_3H$
Molecular Weight	231.4
Formula Composition	20.8% C, 32.8% F, 46.0% Cl, 0.4% H

Boiling Point, °C

109-110

MDDC-162 (28)

Density, g/cc

Temperature, °C

20

1.6500

ibid

Refractive Index (n_D)

Temperature, °C

20

1.3865

ibid

220 177

150

Chemical Name Ethyl trifluoroacetate

Empirical Formula C₄F₃H₅O₂

Molecular Weight 142.0

Formula Composition 33.8% C, 40.2% F, 3.5% H, 22.5% O

Preparation

MDDC-784 (1)

Boiling Point, °C

62 at 760 mm

ibid

Refractive Index (n_D)

Temperature, °C

19

1.3074

ibid

220 178

151

Chemical Name 2-Fluoroethyl fluoroacetate

Empirical Formula C₄F₂H₆O₂

Structural Formula

$$\begin{array}{ccccccc}
 & \text{H} & \text{H} & & \text{O} & \text{H} & \\
 & | & | & & || & | & \\
 \text{F} & - \text{C} & - \text{C} & - \text{O} & - \text{C} & - \text{C} & - \text{F} \\
 & | & | & & & | & \\
 & \text{H} & \text{H} & & & \text{H} &
 \end{array}$$

Molecular Weight 124.0

Formula Composition 38.7% C, 30.7% F, 4.8% H, 25.8% O

Boiling Point, °C

85 at 48 mm
90.5-91 at 58 mm

M-2149 (41)

Toxicity

LC ₅₀ , mg/l	Animal	
0.05	rabbit	
0.07	guinea pig	
0.14	rat	
0.45	mouse	
LD ₅₀ (subcutaneous)		
8.5 mg/kilo	mouse	
0.4 mg/kilo	rabbit	ibid
Concentration, mg/l		
0.092	69% mortality in an assortment of small animals excluding mice.	
0.10	6/6 guinea pigs	
0.05	2/5 guinea pigs	M-2149 (28)

Saturation concentration at 25°C is 7.5 mg/l which is considerably higher than lethal dose. M-2149 (42)

220 179

152

Chemical Name	Ethyl dichlorofluoroacetate
Empirical Formula	C ₄ FC ₂ H ₅ O ₂
Structural Formula	$ \begin{array}{ccccccc} & \text{Cl} & \text{O} & & \text{H} & \text{H} & \\ & & & & & & \\ \text{F} & - \text{C} & - \text{C} & - \text{O} & - \text{C} & - \text{C} & - \text{H} \\ & & & & & & \\ & \text{Cl} & & & \text{H} & \text{H} & \end{array} $
Molecular Weight	175.0
Formula Composition	27.4% C, 10.9% F, 40.5% Cl, 2.9% H, 18.3% O

Preparation

LRG-50 (14)

220 180

153

Chemical Name	2-Chloroethyl fluoroacetate
Empirical Formula	C ₄ FClH ₆ O ₂
Structural Formula	$ \begin{array}{ccccccc} & \text{H} & \text{H} & & \text{O} & \text{H} & \\ & & & & & & \\ \text{Cl} - & \text{C} & - \text{C} & - \text{O} & - \text{C} & - \text{C} & - \text{F} \\ & & & & & & \\ & \text{H} & \text{H} & & & \text{H} & \end{array} $
Molecular Weight	140.5
Formula Composition	34.1% C, 13.5% F, 25.3% Cl, 4.3% H, 22.8% O

Preparation

1. $\text{CH}_2\text{Cl}-\text{CH}_2\text{OH} + \text{CH}_2\text{F}-\text{COCl} \longrightarrow \text{CH}_2\text{F}-\text{COO}-\text{CH}_2-\text{CH}_2\text{Cl}$
2. $\text{CH}_2\text{Cl}-\text{CH}_2\text{OH} + \text{CH}_2\text{F}-\text{COO}-\text{CH}_3 \longrightarrow \text{CH}_2\text{F}-\text{COO}-\text{CH}_2-\text{CH}_2\text{Cl}$

M-2149 (41)

Boiling Point, °C

67-68 at 7 mm
78.5 at 15 mm

ibid

Toxicity

Concentration, mg/l

0.1	0/4 mice
	1/4 guinea pigs
0.3	2/2 guinea pigs
	0/4 rats
0.7	0/10 mice
	2/2 guinea pigs
0.10	54% mortality in small animals excluding mice.

M-2149 (27)

220 181

154

Chemical Name Diethylfluorophosphate

Empirical Formula C₄FH₁₀O₃P

Structural Formula

$$\begin{array}{ccccccc}
 & \text{H} & \text{H} & & \text{F} & & \text{H} & \text{H} \\
 & | & | & & | & & | & | \\
 \text{H} & - \text{C} & - \text{C} & - \text{O} & - \text{P} & - \text{O} & - \text{C} & - \text{C} & - \text{H} \\
 & | & | & & | & & | & | \\
 & \text{H} & \text{H} & & \text{O} & & \text{H} & \text{H}
 \end{array}$$

Molecular Weight 156.0

Formula Composition 30.8%, 12.2% F, 6.4% H, 30.8% O, 19.8% P

Boiling Point, °C

170-171

M-2149 (21)

Volatility, mg/l

Temperature, °C

-10	0.893
0	1.97
10	4.13
20	8.18
25	11.3
30	15.5
40	28.1

See Figure 177

ibid

Toxicity

LC ₅₀ (inhalation), mg/l	LD ₆₀ (absorption) mg/l	Animal
0.41	0.72	mouse
0.8	—	mouse

Median detectable concentration (humans) is 0.15 mg/l.

ibid

220 182

155

Chemical Name Dodecafluoropentane

Empirical Formula C₅F₁₂

Molecular Weight 288.1

Formula Composition 20.8% C, 79.2% F

Preparation A-3468 (85)
MDDC-600 (47)Boiling Point, °C29.4
29.4-29.5A-3468 (85)
MDDC-600 (48)

220 183

156

Chemical Name 1,1,1,2,3,3,4,4,4-Nonafluoro-2-trifluoromethylbutane

Empirical Formula C₅F₁₂

Molecular Weight 288.1

Formula Composition 20.8% C, 79.2% F

Preparation

A-585 (74)

Boiling Range

24.2-29.3 (first plateau)
 39.0-47.0 (second plateau)

A-585 (75)

220 184

157

Chemical Name Decafluorocyclopentane

Empirical Formula C₅F₁₀

Molecular Weight 250.1

Formula Composition 24.0% C, 76.0% F

Preparation

MDDC-600 (47)

Melting Point, °C

-12

A-312 (4)

Boiling Point, °C

20.5

22

23.5

23.5-23.7

Ind. Eng. Chem., 39, 354 (1947)

A-312 (4)

A-3468 (85)

A-3786 (91)

MDDC-600 (48)

Density, g/cc

Temperature, °C

0.2

8.8

20.8

30

1.72

1.69

1.67

1.64

BR-319 (8)

A-312 (4)

220 185

158

Refractive Index (n_D)

Temperature, °C

30

1.24

A-199 (5)

Vapor PressureEquation: $\log p = 7.43 - 1350/T$

BR-319 (8)

Heat of Vaporization, cal/mol

Temperature, °C

23

6200

ibid

220 186

159

Chemical Name	Chloroundecafluoropentane
Empirical Formula	C ₅ F ₁₁ Cl
Molecular Weight	304.5
Formula Composition	19.7% C, 68.6% F, 11.7% Cl

Boiling Point, °C

57-58

MDDC-162 (29)

Density, g/cc

Temperature, °C

20

1.682

ibid

Refractive Index (n_D)

Temperature, °C

20

1.2785

ibid

220 187

160

Chemical Name	Dichlorodecafluoropentane
Empirical Formula	C ₅ F ₁₀ Cl ₂
Molecular Weight	321.0
Formula Composition	18.7% C, 59.2% F, 22.1% Cl

Boiling Point, °C

87.5-88.0

MDDC-162 (29)

Density, g/cc

Temperature, °C

20

1.735

ibid

Refractive Index (n_D)

Temperature, °C

20

1.3122

ibid

220 188

161

Chemical Name	Trichlorononafluoropentane
Empirical Formula	C ₅ F ₉ Cl ₃
Molecular Weight	337.4
Formula Composition	17.8% C, 50.6% F, 31.6% Cl

Boiling Point, °C

118-119

MDDC-162 (29)

Density, g/cc

Temperature, °C

20

1.776

ibid

Refractive Index (n_D)

Temperature, °C

20

1.3630

ibid

220 189

162

Chemical Name 1,2-Dichloro-3,3,4,4,5,5-hexafluorocyclopentene

Empirical Formula C₅F₆Cl₂

Structural Formula

Molecular Weight 245.0

Formula Composition 24.5% C, 46.5% F, 29.0% Cl

Preparation

1.
$$\text{C}_5\text{Cl}_8 \xrightarrow{\text{SbF}_3} \text{C}_5\text{F}_6\text{Cl}_2$$

(cyclopentene)

 - a. $\text{CHCl}_3 + \text{CCl}_2=\text{CCl}_2 \xrightarrow{\text{AlCl}_3} \text{CHCl}_2-\text{CCl}_2-\text{CCl}_3$
 - b. $\text{CHCl}_2-\text{CCl}_2-\text{CCl}_3 \xrightarrow{\text{NaOH}} \text{CCl}_2=\text{CCl}-\text{CCl}_3$
 - c. $\text{CCl}_2=\text{CCl}-\text{CCl}_3 + \text{CHCl}=\text{CCl}_2 \xrightarrow{\text{AlCl}_3} \text{CCl}_2=\text{CCl}-\text{CCl}_2-\text{CHCl}-\text{CCl}_3$
 - d. $\text{CCl}_2=\text{CCl}-\text{CCl}_2-\text{CHCl}-\text{CCl}_3 \xrightarrow{\text{NaOH}} \text{CCl}_2=\text{CCl}-\text{CCl}=\text{CCl}-\text{CCl}_3$
 - e. $\text{CCl}_2=\text{CCl}-\text{CCl}=\text{CCl}-\text{CCl}_3 \xrightarrow{\text{AlCl}_3} \text{C}_5\text{Cl}_8$

(cyclopentene) A-770 (2)
2.
$$\text{C}_5\text{Cl}_8 \xrightarrow[5-10\% \text{ SbF}_3\text{Cl}_2]{\text{SbF}_3} \text{C}_5\text{F}_6\text{Cl}_2$$

(cyclopentene) A-2104 (5)

Reactions

C₅F₆Cl₂ was oxidized to hexafluoroglutaric acid. ibid

163

Chemical Name	Dichlorohexafluoropentadiene
Empirical Formula	C ₅ F ₆ Cl ₂
Molecular Weight	245.0
Formula Composition	24.5% C, 46.5% F, 29.0% Cl

Boiling Point, °C

87.2-89.5

MDDC-162 (28)

Refractive Index (n_D)

Temperature, °C

20

1.3578

ibid

220 191

164

Chemical Name 2,2-Difluoropentane

Empirical Formula C₅F₂H₁₀

Structural Formula

```

      H   F   H   H   H
      |   |   |   |   |
H - C - C - C - C - C - H
      |   |   |   |   |
      H   F   H   H   H
  
```

Molecular Weight 108.1

Formula Composition 55.5% C, 35.2% F, 9.3% H

Density, g/cc

Temperature, °C

20

0.896

BR-645 (12)

Molecular Volume, cc

Temperature, °C

20

120.6

ibid

220 192

165

 $C_5F_2H_{10}$

Chemical Name 3,3-Difluoropentane

Empirical Formula $C_5F_2H_{10}$

Structural Formula

$$\begin{array}{ccccccc} & H & H & F & H & H & \\ & | & | & | & | & | & \\ H & - C & - C & - C & - C & - C & - H \\ & | & | & | & | & | & \\ & H & H & F & H & H & \end{array}$$

Molecular Weight 108.1

Formula Composition 55.5% C, 35.2% F, 9.3% H

Density, g/cc

Temperature, °C

20

0.911

BR-645 (12)

Molecular Volume, cc

Temperature, °C

20

118.7

ibid

220 193

166

Chemical Name 1-Fluoropentane

Empirical Formula C₅FH₁₁

Structural Formula

```

      H   H   H   H   H
      |   |   |   |   |
F - C - C - C - C - C - H
      |   |   |   |   |
      H   H   H   H   H

```

Molecular Weight 90.1

Formula Composition 66.7% C, 21.1% F, 12.2% H

Density, g/cc

Temperature, °C

20

0.788

BR-645 (12)

Molecular Volume, cc

Temperature, °C

20

114.3

ibid

220 194

167

Chemical Name Dichlorononafluoropentane
Empirical Formula C₅F₉Cl₂H
Molecular Weight 303.0
Formula Composition 19.8% C, 56.5% F, 23.4% Cl, 0.3% H

Boiling Point, °C

31.0-31.7

MDDC-162

Refractive Index, (n_D)

Temperature, °C

20

1.3415

ibid

220 195

168

C₅F₈ClH

Chemical Name Chlorooctafluoropentene
Empirical Formula C₅F₈ClH
Molecular Weight 248.5
Formula Composition 24.1% Cl, 61.2% F, 14.3% Cl, 0.4% H

Preparation

Polychloropentanes $\xrightarrow[\text{Antimony pentahalides}]{\text{HF}}$ mixture containing C₅F₈ClH
MDDC-162 (24)

Boiling Point, °C

54.8-56.3

MDDC-162 (28)

Refractive Index (n_D)

Temperature, °C

20

1.3030

ibid

220 196

169

Chemical Name Trichlorohexafluoropentene
Empirical Formula C₅F₆Cl₃H
Molecular Weight 281.4
Formula Composition 21.3% C, 40.5% F, 37.8% Cl, 0.4% H

Preparation

Polychloropentanes $\xrightarrow[\text{Antimony pentahalides}]{\text{HF}}$ mixture containing C₅F₆Cl₃H
MDDC-162 (24)

Boiling Point, °C

110-112

MDDC-162 (28)

Refractive Index (n_D)

Temperature, °C

20

1.3768

ibid

220 197

170

Chemical Name 1,1,1,5,5,5-Hexafluoro-2,4-pentanedione

Empirical Formula C₅F₆H₂O₂

Structural Formula

$$\begin{array}{ccccccc} & \text{F} & & \text{H} & & \text{F} & \\ & | & & | & & | & \\ \text{F} & - \text{C} & - & \text{C} & - & \text{C} & - & \text{C} & - & \text{C} & - & \text{F} \\ & | & & || & & | & & || & & | & & \\ & \text{F} & & \text{O} & & \text{H} & & \text{O} & & \text{F} & & \end{array}$$

Molecular Weight 208.1

Formula Composition 28.8% C, 54.8% F, 1.0% H, 15.4% O

Preparation

By condensation of ethyltrifluoroacetate with trifluoroacetone.

A-2104 (6)

171

Chemical Name	Hexafluoroglutaric acid
Empirical Formula	C ₅ F ₆ H ₂ O ₄
Structural Formula	$\begin{array}{c} \text{CF}_2 \begin{cases} \text{--- COOH} \\ \text{--- COOH} \end{cases} \end{array}$
Molecular Weight	240.1
Formula Composition	25.0% C, 47.5% F, 0.8% H, 26.7% O

Preparation

By oxidation of 1,2-dichlorohexafluorocyclopentene.

M-3814 (2)
A-2104 (10)
A-709 (2)

Above preparation gives 90% yield.

Ind. Eng. Chem., 39, 416 (1947)

172

Chemical Name 1,1,1-Trifluoro-2,4-pentanedione

Empirical Formula C₅F₃H₅O₂

Molecular Weight 154.0

Formula Composition 38.9% C, 37.0% F, 3.3% H, 20.8% O

Preparation

1. By condensation of ethyltrifluoroacetate with acetone. A-2104 (24)
2. By condensation of ethylacetate with trifluoroacetone. LRG-50 (14)

220 200

173

Chemical Name Tetradecafluorohexane

Empirical Formula C₆F₁₄

Structural Formula

Molecular Weight 21.3% C, 78.7% F

Preparation

A-3468 (59)

2. Formed as impurity in C₇F₁₆ preparation.

A-3468 (112)

Boiling Point, °C

56-58

A-3468 (59)

57.0

A-3468 (112)

220 201

Chemical Name 2,3-Bis(trifluoromethyl)-1,1,1,4,4,4-hexafluoro-2-butene

Empirical Formula C₆F₁₂

Molecular Weight 300.1

Formula Composition 24.0% C, 76.0% F

Preparation

Boiling Point, °C

54.1 at 736
55

A-3786 (91)
M-3113 (156)

Reactions

Gave positive permanganate unsaturation test.

ibid

Chemical Name Dodecafluorocyclohexane

Empirical Formula C₆F₁₂

Structural Formula

Molecular Weight 300.1

Formula Composition 24.0% C, 76.0% F

Preparation

Prepared by direct fluorination of benzene. Ratio used, F₂:C₆H₆:N₂ was 9:1:9. Silver-plated copper gauge was used in the reaction zone which was kept at 130°C. The product was collected at -80°C at 4.5 g/hr with 35% of the product being C₆F₁₂.

M-3823 (1)

A-1991 (4)

Melting Point, °C

35
50
50
51-52
58.4-59.4
55.2-58.2

A-311 (3)

A-3649 (428)

MDDC-319 (29)

A-211 (5)

This Laboratory

J. Am. Chem. Soc., 69, 2503 (1947)

Boiling Point, °C

45.2-53.4
50
50.2
52
52
Sublimes

A-312 (18)

A-3786 (92)

MDDC-300 (10)

A-3649 (428)

A-199 (4)

This Laboratory

Density, g/cc

Temperature, °C

20
30

1.711
1.684

A-312 (13)

A-199 (4)

A-3649 (428)

220 203

176

Refractive Index (n_D)

Temperature, °C

30	1.2622	A-312 (18)
	1.2685	A-199 (4)
		A-3649 (428)

Specific Refraction

0.098		
0.0975 (calculated using AR _F = 1.23)		A-199 (4)

Vapor Pressure

Equation: $\log p = 7.51 - 1500/T$		BR-319 (9)
------------------------------------	--	------------

Heat of Vaporization, cal/mol

Temperature, °C

52	6900	ibid
----	------	------

Solubility

At 0°C, C₆F₁₂ is insoluble in methyl alcohol and water, completely miscible with benzotrifluoride, and soluble to the extent of 0.7% in carbon tetrachloride.

At 27°C, C₆F₁₂ is insoluble in methyl alcohol and water, completely miscible with benzotrifluoride, ethyl ether, and carbon tetrachloride. The following results were determined at 27°C:

Solvent	Solubility of C ₆ F ₁₂ , %
Acetone	8
Chloroform	19 ^a
Benzene	2 ^b
Trichloroethylene	0.2 ^a

^aCompletely miscible at 50°C.

^bSolubility increases on warming to 50°C; however, two layers remain.

A-312 (18)

220 204

177

SECRETUltraviolet Absorption

Transparent in ultraviolet region.

BR-497 (3)

Bond Distance, Å

Bond

C-C	1.50 ± 0.03
C-F	1.33 ± 0.02

A-3786 (61)

220 205

Chemical Name Hexafluorobenzene

Empirical Formula C₆F₆

Structural Formula

Molecular Weight 186.1

Formula Composition 38.7%, 61.3% F

Melting Point, °C

-13 to -11

Ind. and Eng. Chem., 39, 367 (1947)

Boiling Point, °C

81.0-82.0 at 743 mm

ibid

Density, g/cc

Temperature, °C

20

1.612

ibid

Refractive Index (n_D)

Temperature, °C

20

1.3664

ibid

220 206

SECRET

179

Chemical Name

Bis(heptafluoroisopropyl)ether

Empirical Formula

C₆F₁₄O

Structural Formula

Molecular Weight

354.1

Formula Composition

20.4% C, 75.1% F, 4.5% O

220 207

SECRET

150

Chemical Name	Chlorotridecafluorohexane
Empirical Formula	C ₆ F ₁₃ Cl
Molecular Weight	354.5
Formula Composition	20.3% Cl, 69.7% F, 10.0% Cl

Boiling Point, °C

81-84

MDDC-162 (29)

Density, g/ccTemperature, °C

20

1.728

ibid

Refractive Index (n_D)Temperature, °C

20

1.286

ibid

220 208

181

Chemical Name 2,3-Dichloro-2,3-bis(trifluoromethyl)-1,1,1,4,4,4-hexafluorobutane

Empirical Formula $C_6F_{12}Cl_2$

Molecular Weight 371.0

Formula Composition 19.4% C, 61.5% F, 19.1% Cl

Preparation

Melting Point, °C

91.5-93 ibid

Boiling Point, °C

116 ibid

Reactions

Dechlorinated with Zn to $(CF_3)_2C=C(CF_3)_2$. ibid

182

Chemical Name Dichlorododecafluorohexane
Empirical Formula C₆F₁₂Cl₂
Molecular Weight 371.0
Formula Composition 19.4% C, 61.5% F, 19.1% Cl

Boiling Point, °C

110±1-110.2

MDDC-162 (29)

Density, g/cc

Temperature, °C

20

1.767

Ind. Eng. Chem., 29, 313 (1947)Refractive Index (n_D)

Temperature, °C

20

1.3150

MDDC-162 (29)

220 210

183

Chemical Name Dichlorodecafluorocyclohexane
Empirical Formula $C_6F_{10}Cl_2$
Molecular Weight 333.0
Formula Composition 21.6% C, 57.1% F, 21.3% Cl

Boiling Point, °C

105-106

MDDC-162 (29)

Refractive Index (n_D)

Temperature, °C

20

1.3328

ibid

220 211

184

Chemical Name Hexachlorooctafluorohexane (mixture of isomers)
 Empirical Formula C₆F₈Cl₆
 Molecular Weight 436.8
 Formula Composition 16.5% C, 34.8% F, 48.7% Cl

Preparation

CF₃-CCl=CCl₂ + F₂ ————— C₆F₈Cl₆ M-3113 (156)

Boiling Point, °C

115 at 20 mm ibid

Density, g/cc

Temperature, °C

20 1.9415 ibid

Refractive Index (n_D)

Temperature, °C

20 1.4387 ibid

Molecular Refraction (MR_D)

AR_F (calculated)

59.14 1.10 ibid

220 212

185

Chemical Name 1,2,4-Trifluorobenzene

Empirical Formula C₆F₃H₃

Structural Formula

Molecular Weight 132.1

Formula Composition 54.5% C, 43.2% F, 2.3% H

Bond Distance, Å

Bond

C-C	1.35 ± 0.02
C-F	1.38 ± 0.04

A-3786 (81)

220 213

186

Chemical Name 2,2-Difluoro-4-methyl pentane

Empirical Formula C₆F₂H₁₂

Molecular Weight 122.1

Formula Composition 59.1% C, 31.1% F, 9.8% H

Density, g/cc

Temperature, °C

20

0.883

BR-645 (12)

Molecular Volume, cc

Temperature, °C

20

137.6

ibid

220 214

187

Chemical Name p-Difluorobenzene

Empirical Formula C₆F₂H₄

Structural Formula

Molecular Weight 114.1

Formula Composition 63.2% C, 33.3% F, 3.5% H

Preparation

N-2037 (4)

Boiling Point, °C

86-88

87.4 at 738 mm

ibid

A-3786 (92)

Bond Distance, Å

Bond

C-C 1.35 ± 0.02

C-F 1.36 ± 0.04

A-3786 (81)

188

Chemical Name Fluorobenzene

Empirical Formula C₆H₅F

Structural Formula

Molecular Weight 96.1

Formula Composition 75.0% C, 19.8% F, 5.2% H

Boiling Point, °C

50.1 at 236 mm

A-3786 (92)

Density, g/cc

Temperature, °C

20

1.024

BR-645 (12)

Molecular Volume, cc

Temperature, °C

20

93.8

ibid

Bond Distance, Å

Bond

C-C

1.38 ± 0.02

A-3786 (81)

Toxicity

17 mg/l for mice

M-2149 (46)

220 216

189

Chemical Name 2,5-Difluoroaniline

Empirical Formula C₆F₂H₅N

Structural Formula

Molecular Weight 129.1

Formula Composition 55.8% C, 29.4% F, 3.9% H, 10.9% N

Preparation

N-2037 (5)

Boiling Point, °C

89.5-91 at 26 mm

ibid

220 217

190

Chemical Name 1-Chloro-2-fluorobenzene

Empirical Formula C₆FC1H₄

Structural Formula

Molecular Weight 130.5

Formula Composition 55.2% C, 14.5% F, 27.2% Cl, 3.1% H

Boiling Point, °C

136

A-3786 (92)

Bond Distance, Å

Bond

C-C 1.38 ± 0.02

C-Cl 1.72 ± 0.03

A-3786 (81)

220 218

191

Chemical Name 1-Chloro-3-fluorobenzene

Empirical Formula C_6FClH_4

Molecular Weight 130.5

Formula Composition 55.2% C, 14.5% F, 27.2% Cl, 3.1% H

Boiling Point. °C

124

A-3786 (92)

Bond Distance. Å

Bond

C-C	1.38 ± 0.02
C-F	1.34 ± 0.03
C-Cl	1.73 ± 0.03

A-3786 (81)

192

Chemical Name 4-Fluoroaniline

Empirical Formula C₆FH₆N

Molecular Weight 111.1

Formula Composition 64.9% C, 17.1% F, 5.4% H, 12.6% N

Preparation

N-2037 (4)

Boiling Point, °C

184.5-186.5

ibid

220 220

193

Chemical Name 1,4-Difluoro-3-nitrobenzene

Empirical Formula C₆F₂H₃NO₂

Structural Formula

Molecular Weight 159.1

Formula Composition 45.3% C, 23.9% F, 1.9% H, 8.8% N, 20.1% O

Preparation

N-2037 (4)

Boiling Point, °C

204

ibid

220 221

194

Chemical Name 1-Fluoro-4-nitrobenzene

Empirical Formula C₆H₄NO₂

Structural Formula

Molecular Weight 141.1

Formula Composition 51.1% C, 13.5% F, 2.8% H, 9.9% N, 22.7% O

Preparation

N-2037 (4)

Boiling Point, °C

86 at 14 mm

ibid

220 222

195

C₆F₃H₁₂O₃P

Chemical Name Tris(2-fluoroethyl)phosphite

Empirical Formula C₆F₃H₁₂O₃P

Structural Formula

Molecular Weight 220.0

Formula Composition 32.7% C, 25.9% F, 5.5% H, 21.8% O, 14.1% P

Preparation

M-2149 (42)

Boiling Point, °C

100 at 0.5 mm

ibid

Toxicity

Concentration, mg/l

Animals

1.0

4/20 mice

0.5

4/4 guinea pigs

0/10 mice

2/5 rats

4/4 guinea pigs

2/2 cats

0.2

2/4 guinea pigs

2/2 cats

1/1 dog

0.15

4/4 rabbits

0/1 goat

0.10

2/2 dogs

2/2 cats

1/6 guinea pigs

M-2149 (34)

220 223

176

Chemical Name Di-isopropylfluorophosphate

Empirical Formula C₆H₁₄O₃P

Structural Formula

$$\begin{array}{ccccccc}
 & \text{H} & & \text{H} & & \text{F} & & \text{H} & & \text{H} \\
 & | & & | & & | & & | & & | \\
 \text{H} & - \text{C} & - & \text{C} & - & \text{O} & - & \text{P} & - & \text{O} & - & \text{C} & - & \text{C} & - & \text{H} \\
 & | & & | & & & & | & & | & & | & & | \\
 & \text{H} & \text{H} & \text{C} & \text{H} & & \text{O} & & \text{H} & \text{C} & \text{H} & \text{H} \\
 & & & | & & & & & & | & & \\
 & & & \text{H} & & & & & & \text{H} & &
 \end{array}$$

Molecular Weight 184.0

Formula Composition 39.2% C, 10.3% F, 7.6% H, 26.1% O, 16.8% P

Boiling Point, °C

183

M-2149 (21)

Volatility, mg/l

Temperature, °C

-10	0.595
0	1.35
10	2.88
20	5.84
25	8.16
30	11.25
40	20.9

See Figure 179

ibid

Toxicity

Concentration, mg/l

0.036	Median detectable concentration - humans	
0.55	LC ₅₀ mice inhalation	
1.45 mg/mouse	LD ₅₀ mice skin absorption	M-2149 (22)
0.62	LC ₅₀ mice	
0.82	2/3 rabbits	
	0/4 guinea pigs	
	6/6 rats	
	10/10 mice	M-2149 (10)

197

Chemical Name 1,1,1,3,4,4,4-Heptafluoro-2,2,3-tris(trifluoromethyl)butane

Empirical Formula C₇F₁₆

Structural Formula

Molecular Weight 388.1

Formula Composition 21.7% C, 78.3% F

Preparation

Boiling Point, °C

82

A-199 (4)
A-312 (3)

Density, g/cc

Temperature, °C

30

1.7535

A-199 (4)
A-312 (3)

Refractive Index (n_D)

Temperature, °C

30

1.2676

ibid

Specific Refraction

Temperature, °C

30

0.0959

A-199 (4)

198

Chemical Name Hexadecafluoroheptane

Empirical Formula C₇F₁₆

Structural Formula

$$\begin{array}{ccccccccccc} & \text{F} & \text{F} & \text{F} & \text{F} & \text{F} & \text{F} & \text{F} & & & \\ & | & | & | & | & | & | & | & & & \\ \text{F} & - \text{C} & - \text{C} & - \text{C} & - \text{C} & - \text{C} & - \text{C} & - \text{C} & - & \text{F} & \\ & | & | & | & | & | & | & | & & & \\ & \text{F} & \text{F} & \text{F} & \text{F} & \text{F} & \text{F} & \text{F} & & & \end{array}$$

Molecular Weight 388.1

Formula Composition 21.7% C, 78.3% F

See Section I

Page 57

220 225

199

Chemical Name 1,1,1,2,3,4,4,5,5,5-Decafluoro-2,3-bis(trifluoromethyl)pentane

Empirical Formula C₇F₁₆

Structural Formula

Molecular Weight 388.1

Formula Composition 21.7% C, 78.3% F

Preparation

- Hydrocarbon input rate 10 to 20 g/hr in a reactor 6 inches in diameter and 3 feet long.
- 20 to 30% yield of crude with 60% of crude boiling in range 81-84°C.

- Hydrocarbon addition rate 10 to 40 g/hr in reactor 3 inches in diameter and 2 feet long containing 950 g of CoF₃.
- With reactor temperature of 200°C the crude yield averaged 30%.
BR-420 (3)

Boiling Point, °C

83.0

BR-527 (15)

Density, g/cc

Temperature, °C

20

1.730

ibid

220 226

SECRET200Refractive Index (n_D)

Temperature, °C

20

1.267

BR-527 (15)

Specific Refraction

Temperature, °C

20

0.0968

LRG-64 (III-3)

PurificationPurification steps for product C₇F₁₆:

- a. Aqueous extraction.
- b. Alcohol extraction - Azeotropism of the fluorocarbon and the starting material necessitates this step.
- c. Distillation.

BR-527 (2)

220 227

SECRET

201

Chemical Name Nonafluoro(pentafluoroethyl)cyclopentane

Empirical Formula C₇F₁₄

Structural Formula

Molecular Weight 350.1

Formula Composition 24.0% C, 76.0% F

Preparation A-3468 (110)
MDDC-600 (47)

A-730 (8)

A-1730 (2)

Boiling Point, °C75.064

A-770 (8)

75.06

A-3468 (128)

75.1-75.2

MDDC-600 (48)

Density, g/cc

Temperature, °C

20

1.7707 ± 0.0002

A-3468 (128)

220 228

202

C₇F₁₄Refractive Index (n_D)

Temperature, °C

20

1.2772

A-3468 (128)

Specific Inductance Capacity

1.80

MDDC-278 (6)

Infrared Absorption

See Figure 180

220 229

204

Chemical Name Octafluorobis(trifluoromethyl)cyclopentane
 Empirical Formula C₇F₁₄

Structural Formula

and 1,3 isomer

Molecular Weight 350.1
 Formula Composition 24.0% C, 76.0% F

Preparation

MDDC-600 (48)
 A-3468 (110)

Boiling Point, °C71.67

A-770 (8)

71.5-71.8

MDDC-600 (48)

Density, g/cc

Temperature, °C

20

1.7660 ± 0.002

A-3468 (128)

Refractive Index (n_D)

Temperature, °C

20

1.2765

ibid

220 231

205

Chemical Name	Chloropentadecafluoroheptane
Empirical Formula	C ₇ F ₁₅ Cl
Structural Formula	(Probably a mixture of isomers)
Molecular Weight	404.5
Formula Composition	20.8% C, 70.4% F, 8.8% Cl

Preparation

1. C ₇ H ₄ F ₆ Cl ₆ + SbF ₅ → C ₇ F ₁₅ Cl	A-1510 (11)
2. C ₇ H ₂ F ₁₀ Cl ₂ + CoF ₃ → C ₇ F ₁₅ Cl	MDDC-162 (20)

Boiling Point, °C

99	(one isomer)	A-770 (7)
106	(a second isomer)	A-770 (7)
100		BR-690 (11)
101.3		A-3728 (6 of C ₇ F ₁₆)
106.6-107		MDDC-162 (22)
98-108	(du Pont sample)	
100-107	(Purdue sample)	M-255 (13)

Density, g/cc

Temperature, °C

25	1.7558	A-1510 (12)
	1.756	MDDC-162 (22)
30	1.74	(du Pont sample)
	1.75	(Purdue sample)
		M-255 (13)

Refractive Index (n_D)

Temperature, °C

25	1.295	MDDC-162 (22)
30	1.290	(Purdue sample)
	1.291	(du Pont sample)
		M-255 (13)

220 232

206

Specific Inductance Capacity

2.09 (Purdue sample)
2.15 (du Pont sample)

M-255 (13)

Analysis

Minimum concentration of 0.018% in air is detectable by halide lamp method.
MDDC-209 (19)

220 233

207

Chemical Name	Pentadecafluoroheptane
Empirical Formula	C ₇ F ₁₅ H
Molecular Weight	370.1
Formula Composition	22.7% C, 77.0% F, 0.3% H

Preparation

Pentadecafluoroheptane was obtained by an elaborate fractionation of residues from the preparation of C₇F₁₆. Three cuts (10, 12, 17) were taken and properties were determined. M-222 (5)

Boiling Point, °C

86.45-86.5 at 745 mm (cut 10)	M-222 (17)
86.7-86.7 at 745 mm (cut 12)	A-3728 (14 of C ₇ F ₁₆)
86.7	A-3959 (6)
87	M-215 (28)
87 (isomer 1)	A-3500 (4)
87.39 (isomer 1)	M-222 (17)
88.9-91.1 at 745 mm (cut 17)	M-215 (28)
91 (isomer 2)	A-3500 (4)
91.92 (isomer 2)	

Density, g/cc

Temperature, °C

20	1.7052 (cut 10)	
	1.7061 (cut 12)	
	1.7082 (cut 17)	M-222 (17)

Refractive Index (n_D)

Temperature, °C

20	1.2681 (cut 10)	
	(cut 12)	ibid
	(isomer 1)	
	1.2703 (isomer 2)	A-3500 (4)
	1.2706 (cut 17)	M-222 (17)

220 234

208

C₇F₁₅HSECRETSpecific Inductance Capacity

2.47 (isomer 1)
2.746 (cut 10)
2.75 (isomer 1)
2.756 (cut 12)
2.92 (isomer 2)
2.93 (isomer 2)
2.954 (cut 17)

MDDC-278 (6)
M-222 (17)
A-3500 (4)
M-222 (17)
A-3500 (4)
MDDC-278 (6)
M-222 (17)

220 235

SECRET

207

Chemical Name Dichlorotetradecafluoroheptane
 Empirical Formula C₇F₁₄Cl₂
 Molecular Weight 421.0
 Formula Composition 20.0% C, 63.2% F, 16.8% Cl

Preparation

C₇H₂Cl₂F₁₀ was fluorinated with CoF₃ and the product was rectified. The fraction boiling 128-132°C was rectified again and was found to contain some C₇F₁₄Cl₂.

Boiling Point, °C

125-130	M-255 (13)
130	BR-690 (11)
131.3-132.2	MDDC-162 (23)

Density, g/cc

Temperature, °C		
23	1.792	ibid
30	1.80	M-255 (13)

Refractive Index (n_D)

Temperature, °C		
20	1.3188	MDDC-162 (23)
30	1.324	M-255 (13)

Specific Inductance Capacity

2.41	ibid
------	------

220 236

210

$C_7F_{14}H_2$

Chemical Name	Tetradecafluoroheptane
Empirical Formula	$C_7F_{14}H_2$
Molecular Weight	352.1
Formula Composition	23.9% C, 75.5% F, 0.6% H

Preparation

By-product in preparation of C_7F_{16}	A-2104 (3)
--	------------

Freezing Point, °C

-64.3	ibid
-------	------

Boiling Point, °C

91.3	ibid
95.71	MDDC-278 (6)
96	M-215 (28)

Specific Inductance Capacity

3.18	MDDC-278 (6)
------	--------------

220 237

211

 $C_7F_{13}Cl$

Chemical Name 3-Chloro-1-(trifluoromethyl)decafluorocyclohexane

Empirical Formula $C_7F_{13}Cl$

Structural Formula

Molecular Weight 366.5

Formula Composition 22.9% C, 67.4% F, 9.7% Cl

Preparation Boiling Point, °C

101.9-102.9

ibid

Density, g/cc

Temperature, °C

20

1.822

ibid

Refractive Index (n_D)

Temperature, °C

20

1.3104

ibid

220 238

212

Mass Spectrometer Data

Mass 69 = 100.0

Mass	Probable fragment	Ratio*
19	F	0.05
26	—	0.03
31	CF	13.8
35	Cl	33.9
37	Cl	0.18
47	CCl	0.26
50	CF ₂	1.5
55	—	0.29
63	—	0.23
66	CFC1	0.18
69	CF ₃	100.0
80	C ₂ FC1	0.57
85	CF ₂ Cl	0.73
93	C ₃ F ₃	7.0
100	C ₂ F ₄	11.3
112	C ₃ F ₄	12.1
120	(C ₂ F ₅ - 119)	3.3
124	C ₄ F ₄	1.4
131	C ₃ F ₅	31.7
142	(C ₄ F ₅ - 143)	1.8
148	(C ₃ F ₄ Cl - 149)	2.1
154	C ₂ F ₅ Cl	0.93
162	C ₄ F ₆	2.7
181	C ₄ F ₇	16.3
232	(C ₅ F ₉ - 231)	1.8
244	(C ₆ F ₉ - 243)	2.1
262	C ₆ F ₁₀	1.8
282	(C ₆ F ₁₁ - 281)	1.0
338	(C ₆ F ₁₂ Cl - 337)	1.4

*Av of three runs

Letter from S. S. Stief, Process Engineering Department, 10-3-47.

220 239

213

Chemical Name (Chlorodifluoromethyl)undecafluorocyclohexane

Empirical Formula C₇F₁₃Cl

Structural Formula

Molecular Weight 366.5

Formula Composition 22.9% C, 67.4% F, 9.7% Cl

Boiling Point, °C

102.2-103.2

MDDC-162 (23)

Density, g/cc

Temperature, °C

20

1.824

ibid

Refractive Index (n_D)

Temperature, °C

20

1.3122

ibid

220 240

214

Chemical Name	Chlorotridecafluoroheptene
Empirical Formula	C ₇ F ₁₃ Cl
Molecular Weight	366.5
Formula Composition	22.9% C, 67.4% F, 9.7% Cl

Boiling Point, °C

99.5-100.0

MDDC-162 (23)

Density, g/cc

Temperature, °C

20

1.79

ibid

Refractive Index (n_D)

Temperature, °C

20

1.3044

ibid

220 241

215

 $C_7F_{13}H_3$

Chemical Name Tridecafluoroheptane
Empirical Formula $C_7F_{13}H_3$
Molecular Weight 334.1
Formula Composition 25.2% C, 73.9% F, 0.9% H

Preparation

By-product in preparation of C_7F_{16} .

MDDC-278 (6)

Boiling Point, °C

122-130

ibid

220 242

216

 $C_7F_{13}H$

Chemical Name Tridecafluoroheptene
 Empirical Formula $C_7F_{13}H$
 Molecular Weight 332.1
 Formula Composition 25.3% C, 74.4% F, 0.3% H

Preparation Ind. Eng. Chem., 39, 346 (1947)Boiling Point, °C

64-65

ibid

Density, g/cc

Temperature, °C

20

1.66

ibid

Refractive Index (n_D)

Temperature, °C

20

1.282

ibid

Specific Refraction

0.1064

ibid

220 243

217

Chemical Name	Dichlorododecafluoroheptene
Empirical Formula	C ₇ F ₁₂ Cl ₂
Molecular Weight	383.0
Formula Composition	22.0% C, 59.5% F, 18.5% Cl

Boiling Point, °C

126.6-128.8

MDDC-162 (23)

Density, g/cc

Temperature, °C

20

1.804

ibid

Refractive Index (n_D)

Temperature, °C

20

1.333

ibid

220 244

218

Chemical Name	Dodecafluoroheptane
Empirical Formula	C ₇ F ₁₂ H ₄
Molecular Weight	316.1
Formula Composition	26.6% C, 72.1% F, 1.3% H

Boiling Point, °C

70-78

M-255 (3)

Density, g/cc

Temperature, °C

30

1.55

ibid

Refractive Index (n_D)

Temperature, °C

30

1.285

ibid

Specific Inductance Capacity

2.15

ibid

220 245

note - pg 245A
follows

219

Chemical Name Dodecafluoroheptene
 Empirical Formula C₇F₁₂H₂
 Molecular Weight 314.1
 Formula Composition 26.8% C, 72.6% F, 0.6% H

Preparation

1. $\text{C}_7\text{H}_2\text{Cl}_2\text{F}_{12} + \text{C}_2\text{H}_5\text{OH} \xrightarrow[\text{reflux}]{\text{Zn}} \text{C}_7\text{F}_{12}\text{H}_2$ MDDC-162 (11)
2. $\text{C}_7\text{H}_2\text{Cl}_3\text{F}_9 \xrightarrow[\text{SbCl}_5]{\text{HF}} \text{mixture containing C}_7\text{F}_{12}\text{H}_2$ MDDC-162 (1)

Boiling Point, °C

70.0-71.0	MDDC-162 (11)
70-72	A-1506 (2)
70.5-72.0	MDDC-162 (3)

Refractive Index (n_D)

Temperature, °C

20	1.282	MDDC-162 (4)
----	-------	--------------

220 245A

220

Chemical Name

1,4-Difluoro-2-(trifluoromethyl)benzene

Empirical Formula

C₇F₅H₃

Structural Formula

Molecular Weight

182.1

Formula Composition

46.2% C, 52.2% F, 1.6% H

Boiling Point, °C

108 at 744 mm

A-3786 (92)

220 246

221

Chemical Name 1-Fluoro-3-(trifluoromethyl)benzene

Empirical Formula C₇F₄H₄

Structural Formula

Molecular Weight 164.1

Formula Composition 51.2% C, 46.4% F, 2.4% H

Density, g/cc

Temperature, °C

20

1.297

BR-645 (12)

Molecular Volume, cc

Temperature, °C

20

126.5

ibid

Ultraviolet Absorption

Band maxima			
ν , cm ⁻¹	ϵ ^a	λ , Å	E ^b 1 cm
37060	1970	2698	120
38060	2070	2628	125
28910	1310	2570	80

^a Molecular extinction coefficient^b Extinction intensity

BR-497 (2)

220 247

222

Chemical Name 1-Fluoro-4-(trifluoromethyl)benzene

Empirical Formula C₇F₄H₄

Molecular Weight 164.1

Formula Composition 51.2% C, 46.4% F, 2.4% H

Ultraviolet Absorption

Band maxima			
ν , cm ⁻¹	ϵ ^a	λ , Å	E 1% ^b 1 cm
37700	230	2653	14
38610	262	2590	16
38980	297	2565	18
39890	279	2513	17

^aMolecular extinction coefficient^bExtinction intensity

BR-497 (2)

220 248

223

Chemical Name (Trifluoromethyl)benzene

Empirical Formula C₇F₃H₅

Structural Formula

Molecular Weight 146.1

Formula Composition 57.6% C, 39.0% F, 3.4% H

Preparation

1% benzalchloride in trichloromethylbenzene reduces the yield considerably.
BR-331 (8)

Freezing Point, °C

-29.3 (Johns Hopkins sample)

This Laboratory

Boiling Point, °C

100-102

100.2 at 752 mm

101-102

A-311 (3)

A-3786 (92)

Ind. Eng. Chem., 39, 302 (1947)

220 243

224

Density, g/cc

Temperature, °C

20

1.190

BR-645 (12)

Johns Hopkins sample

10

1.20222

20

1.18837

25

1.18150

30

1.17425

40

1.16030

50

1.14595

60

1.13123

70

1.11642

80

1.10100

See Figure 181

This Laboratory

Refractive Index (n_D)

Temperature, °C

Johns Hopkins sample

10

1.4200

20

1.4152

30

1.4101

40

1.4051

60

1.3945

$$\text{Equation: } n_D = 1.4253 - 0.00051 t$$

See Figure 182

ibid

220 250

225

Vapor Pressure, mm Hg

Temperature, °C	Johns Hopkins sample
-24.3	1.58
-24.0	1.60
-20.0	2.22
-14.8	3.30
-13.9	3.54
-12.4	3.95
-11.7	4.12
- 1.8	8.13
- 1.7	8.24
+ 1.3	9.89
1.5	9.96
22.9	34.3
23.1	34.7
44.7	95.5
45.5	99.3
77.8	350.8
100.8	734.9
101.0	744.3
111.6	996.1
131.8	1702.8

See Figure 183

This Laboratory

Viscosity, cp

Temperature, °C	Johns Hopkins sample
20	0.579
25	0.549
30	0.519
40	0.466
50	0.423
60	0.385
70	0.357

$$\text{Equation: } \log \eta = 427.805/T - 1.69683$$

See Figure 184

ibid

220 251

226

C₇F₃H₅Surface Tension, dynes/cm

Temperature, °C	Johns Hopkins sample
10	24.7
20	23.5
25	23.0
30	22.5
40	21.4
50	20.4
60	19.3
70	18.3

Equation: $\gamma^{1/4} = 1.865 d - 0.01348$, where d is density.

See Figures 185 and 186

This Laboratory

Parachor

Temperature, °C		
25	270	ibid

Molecular Volume, cc

Temperature, °C		
20	122.8	BR-645 (12)

Infrared Absorption

See Figure 187

This Laboratory

Ultraviolet Absorption

Band maxima			
ν , cm ⁻¹	ϵ ^a	λ , Å	$E_{1\%}^{1\text{cm}}$ ^b
37550	615	2663	42
38490	731	2598	50
39410	556	2538	38

^a Molecular extinction coefficient
^b Extinction intensity

BR-497 (2)

220 252

Bond Measurements

Bond	Bond distance, Å	Bond angle, °
C-C	1.39 ± 0.02	—
C-F (CF ₃)	1.34 ± 0.02	—
F-C-F	—	108.5 ± 1

A-3786 (70)

Reactions

1. $\text{C}_6\text{H}_5\text{CF}_3 + \text{Cl}_2 \xrightarrow{200^\circ\text{C}} \text{C}_6\text{Cl}_5\text{CF}_3$
Product purified by recrystallization from methanol. M-3811 (3)
A-503b (3)
2. $\text{C}_6\text{H}_5\text{CF}_3 + \text{Cl}_2 \xrightarrow[20-60^\circ\text{C}, 20 \text{ hr}]{\text{Fe} + \text{FeCl}_3} \text{C}_6\text{H}_3\text{Cl}_2\text{CF}_3$ (main product) + small amounts of more highly chlorinated material
M-3812 (3)
3. $\text{C}_6\text{H}_5\text{CF}_3 + \text{Cl}_2 \xrightarrow[20-60^\circ\text{C}, 17 \text{ hr}]{\text{Fe} + \text{FeCl}_3} \text{C}_6\text{H}_3\text{Cl}_2\text{CF}_3 + \text{C}_6\text{H}_4\text{ClCF}_3$ ibid

228

 $C_7F_2H_{14}$

Chemical Name 1,1-Difluoroheptane

Empirical Formula $C_7F_2H_{14}$

Structural Formula

```

      F   H   H   H   H   H   H
      |   |   |   |   |   |   |
H - C - C - C - C - C - C - C - H
      |   |   |   |   |   |   |
      F   H   H   H   H   H   H

```

Molecular Weight 136.1

Formula Composition 61.8% C, 27.9% F, 10.3% H

Boiling Point, °C

119.7

MDDC-319 (45)

Density, g/cc

Temperature, °C

20

0.8959

BR-645 (12)

Molecular Volume, cc

Temperature, °C

20

152.0

ibid

220 254

229

C₇F₂H₁₄

Chemical Name 2,2-Difluoroheptane

Empirical Formula C₇F₂H₁₄

Molecular Weight 136.1

Formula Composition 61.8% C, 27.9% F, 10.3% H

Boiling Point, °C

111.8

MDDC-319 (45)

220 255

230

Chemical Name (Difluoromethyl)benzene

Empirical Formula C₇F₂H₆

Structural Formula

Molecular Weight 128.7

Formula Composition 65.6% C, 29.7% F, 4.7% H

Density, g/cc

Temperature, °C

20

1.136

BR-645 (12)

Molecular Volume, cc

Temperature, °C

20

112.8

ibid

220 256

231

Chemical Name 2,4-Difluorotoluene

Empirical Formula C₇F₂H₆

Structural Formula

Molecular Weight 128.1

Formula Composition 65.6% C, 29.7% F, 4.7% H

Preparation

2-Amino-4-nitrotoluene will undergo Schiemann - Balz reaction to yield 2,4-difluorotoluene. LRG-19 (25)

Ultraviolet AbsorptionBand maxima

ν , cm ⁻¹	ϵ ^a	λ , Å	$E_{1\%}^{1\text{cm}}$ ^b
36930	1410	2708	110
37630	1660	2658	130
38490	1540	2598	120
38910	1150	2570	90

^aMolecular extinction coefficient^bExtinction intensity

BR-497 (2)

220 257

232

Chemical Name

1-Fluoroheptane

Empirical Formula

C₇H₁₅F

Structural Formula

Molecular Weight

118.1

Formula Composition

71.2% C, 16.1% F, 12.7% H

Boiling Point, °C

120.4

MDDC-319 (45)

220 258

233

Chemical Name (Fluoromethyl)benzene

Empirical Formula C₇H₇F

Structural Formula

Molecular Weight 110.1

Formula Composition 76.4% C, 17.3% F, 6.3% H

Density, g/cc

Temperature, °C

20

1.029

BR-645 (12)

Molecular Volume, cc

Temperature, °C

20

107.0

ibid

220 259

234

Chemical Name m-Fluorotoluene

Empirical Formula C₇H₇F

Structural Formula

Molecular Weight 110.1

Formula Composition 76.4% C, 17.3% F, 6.3% H

Preparation

M-3823 (3)

Density, g/cc

Temperature, °C

20

0.990

BR-645 (12)

Molecular Volume, cc

Temperature, °C

20

111.2

ibid

220 260

235

Ultraviolet Absorption

Band maxima			
ν , cm^{-1}	ϵ^a	λ , $\text{\AA}$	$E_{1\text{ cm}}^{1\% b}$
37130	1430	2693	130
37880	1210	2640	110
38100	1210	2625	110
38820	880	2575	80
39220	880	2550	80

^aMolecular extinction coefficient^bExtinction intensity

BR-497 (2)

220 261

236

Chemical Name p-Fluorotoluene

Empirical Formula C₇H₇F

Structural Formula

Molecular Weight 110.1

Formula Composition 76.4% C, 17.3% F, 6.3% H

Ultraviolet AbsorptionBand maxima

ν , cm ⁻¹	ϵ ^a	λ , Å	$E_{1\%}^{1\text{cm}}$ ^b
36650	1780	2728	180
37410	1760	2673	160
37910	1100	2638	100
38270	1100	2613	100
38640	990	2588	90

^aMolecular extinction coefficient
^bExtinction intensity

BR-497 (2)

220 262

237

Chemical Name Dichlorododecafluoroheptane
Empirical Formula $C_7F_{12}Cl_2H_2$
Molecular Weight 385.0
Formula Composition 21.8% C, 59.2% F, 18.5% Cl, 0.5% H

Preparation

MDDC-162 (11)

Boiling Point, °C

125.8-126.8

ibid

220 263

238

Chemical Name	Trichloroundecafluoroheptane
Empirical Formula	$C_7F_{11}Cl_3H_2$
Molecular Weight	401.5
Formula Composition	20.9% C, 52.1% F, 26.5% Cl, 0.5% H

Preparation

MDDC-162 (11)

Boiling Point, °C

147.9-152.8

MDDC-162 (14)

237

Chemical Name	Chloroundecafluoroheptane
Empirical Formula	C ₇ F ₁₁ ClH ₄
Molecular Weight	332.5
Formula Composition	25.2% C, 62.9% F, 10.7% Cl, 1.2% H

Boiling Point, °C

90-100

M-255 (3)

Density, g/cc

Temperature, °C

30

1.58

ibid

Refractive Index (n_D)

Temperature, °C

30

1.305

ibid

Specific Inductance Capacity

2.50

ibid

220 265

246

Chemical Name Chloroundecafluoroheptene
 Empirical Formula C₇F₁₁ClH₂
 Molecular Weight 330.5
 Formula Composition 25.4% C, 63.3% F, 10.7% Cl, 0.6% H

Preparation

C₇F₉Cl₃H₂ $\xrightarrow[\text{SbCl}_5 \text{ and SbF}_5]{\text{HF}}$ C₇F₁₁ClH₂ MDDC-162 (1)
 (mixture)

Boiling Point, °C

91-99.5 A-1506 (8)
 93.6-96.0 MDDC-162 (4)

Refractive Index (n_D)

Temperature, °C

20

1.3071

ibid

220 266

241

 $C_7F_{10}Cl_4H_2$

Chemical Name Tetrachlorodecafluoroheptane
Empirical Formula $C_7F_{10}Cl_4H_2$
Molecular Weight 417.9
Formula Composition 20.1% C, 45.5% F, 33.9% Cl, 0.5% H

Preparation

MDDC-162 (14)

Boiling Point, °C

174-178

ibid

220 267

242

Chemical Name Dichlorodecafluoroheptane
Empirical Formula $\text{C}_7\text{F}_{10}\text{Cl}_2\text{H}_4$
Molecular Weight 349.0
Formula Composition 24.1% C, 54.4% F, 20.4% Cl, 1.1% H

Boiling Point, °C

117-120

M-255 (3)

Density, g/cc

Temperature, °C

30

1.65

ibid

Refractive Index (n_D)

Temperature, °C

30

1.339

ibid

Specific Inductance Capacity

2.98

ibid

220 268

243

 $C_7F_{10}Cl_2H_2$

Chemical Name	Dichlorodecafluoroheptene
Empirical Formula	$C_7F_{10}Cl_2H_2$
Molecular Weight	347.0
Formula Composition	24.2% C, 54.8% F, 20.4% Cl, 0.6% H

Preparation

MDDC-162 (1)

Boiling Point, °C115-120
115.5-117.0A-1506 (2)
MDDC-162 (5)Refractive Index (n_D)

Temperature, °C

20

1.3423

ibid

220 269

244

Chemical Name	Trichlorononafluoroheptane
Empirical Formula	C ₇ F ₉ Cl ₃ H ₄
Molecular Weight	365.5
Formula Composition	23.0% C, 46.8% F, 29.1% Cl, 1.1% H

Boiling Point, °C

142-147

M-255 (3)

Density, g/cc

Temperature, °C

30

1.70

ibid

Refractive Index (n_D)

Temperature, °C

30

1.367

ibid

Specific Inductance Capacity

3.20

ibid

220 270

245

 $C_7F_9Cl_3H_2$

Chemical Name	Trichlorononafluoroheptene
Empirical Formula	$C_7F_9Cl_3H_2$
Molecular Weight	363.5
Formula Composition	23.1% C, 47.0% F, 29.3% Cl, 0.6% H

Preparation
$$C_7Cl_{12}H_4 \xrightarrow[220^\circ C]{HF + SbCl_5} \text{mixture containing some } C_7F_9Cl_3H_2$$

MDDC-162 (1)

Boiling Point, °C

142.0-146.3

MDDC-162 (5)

Refractive Index (n_D)

Temperature, °C

20

1.3717

ibid

220 271

246

Chemical Name Dichlorooctafluoroheptadiene
Empirical Formula $C_7F_8Cl_2H_2$
Molecular Weight 309.0
Formula Composition 27.2% C, 49.2% F, 23.0% Cl, 0.6% H

Preparation

Fluorination of polychloroheptanes with HF and $SbCl_5$ at about $110^\circ C$ produced a fraction boiling between $132-136^\circ C$, the analysis of which indicated $C_7F_8Cl_2H_2$.

MDDC-162 (5)

Boiling Point, $^\circ C$

134.4-135.3

MDDC-162 (7)

Refractive Index (n_D)

Temperature, $^\circ C$

20

1.3858

ibid

Reactions

May be converted to C_7F_{16} , $C_7F_{15}Cl$ and $C_7F_{14}Cl_2$ by treatment with AgF_2 .
MDDC-162 (5)

220 272

247

Chemical Name	Dichloro(trifluoromethyl)benzene
Empirical Formula	$\text{C}_7\text{F}_3\text{Cl}_2\text{H}_3$
Molecular Weight	215.0
Formula Composition	39.1% C, 26.5% F, 33.0% Cl, 1.4% H

Boiling Point, °C

170-173

Ind. Eng. Chem., 39, 303 (1947)

220 273

248

 $C_7F_3ClH_4$

Chemical Name

1-Chloro-4-(trifluoromethyl)benzene

Empirical Formula

 $C_7F_3ClH_4$

Structural Formula

Molecular Weight

180.5

Formula Composition

46.6% C, 31.6% F, 19.6% Cl, 2.2% H

Boiling Point, °C

138 at 757 mm.

A-3786 (92)

220 274

249

Chemical Name Octadecafluorooctane

Empirical Formula C₈F₁₈

Molecular Weight 438.1

Formula Composition 21.9% C, 78.1% F

Boiling Point, °C

104

LRG-64 (III-9)
A-312 (11)Density, g/cc

Temperature, °C

20

1.73

BR-319 (11)

Refractive Index (n_D)

Temperature, °C

20

1.279

21

1.284

LRG-64 (III-3)

Specific Refraction

Temperature, °C

20

0.101
0.0947ibid
BR-645 (5)

220 275

250

Molecular Refraction (MR_D)

41.49

BR-645 (5)

Vapor Pressure, mm HgEquation: $\log p = 7.58 - 1770/T$

LRG-64 (III-10)

Viscosity, cp

Temperature, °C

20

1.63

BR-319 (11)

Surface Tension, dynes/cm

Temperature, °C

20

15.7

22

15.3

ibid

Parachor

Temperature, °C

(Calculated)

20

501

ibid

502

LRG-64 (III-10)

251

C₈F₁₈

Chemical Name 2,2,4-Tris(trifluoromethyl)-1,1,1,3,3,4,5,5,5-nonafluoropentane

Empirical Formula C₈F₁₈

Structural Formula

Molecular Weight 438.1

Formula Composition 21.9% C, 78.1% F

Boiling Point, °C

103.0-105.0 at 753 mm
104

A-311 (4)
A-312 (3)

Density, g/cc

Temperature, °C

20 1.825
30 1.8002

BB-645 (13)
A-199 (4)
A-312 (3)

Refractive Index, (n_D)

Temperature, °C

30 1.2735
1.2738

ibid
A-199 (4)
A-311 (4)

220 277

252

Specific Refraction

Temperature, °C

30

0.0948

A-199 (4)

LRG-64 (III-3)

0.0957

A-199 (6)

Molecular Refraction (MR_D)

41.50

A-199 (6)

Molecular Volume, cc

Temperature, °C

20

240.1

BR-645 (13)

220 278

253

 C_8F_{16}

Code Name

C-816

Chemical Name

Decafluorobis(trifluoromethyl)cyclohexane

Empirical Formula

 C_8F_{16}

Structural Formula

mixed with ortho and meta isomers

Molecular Weight

400.1

Formula Composition

24.0% C, 76.0% F

See Section I

Page 1

220 279

Chemical Name	Hexafluoro-1,3-butadiene dimer
Empirical Formula	C ₈ F ₁₂
Molecular Weight	324.1
Formula Composition	29.6% C, 70.4% F

Preparation Boiling Point, °C

98-100 ibid

Density, g/cc

Temperature, °C

20 1.7075 ibid

Refractive Index (n_D)

Temperature, °C

20 1.3220 ibid

Reactions

1. Chlorinated to C₈F₁₂Cl₄ and C₈F₁₂Cl₆.
2. Brominated.
3. Liquid phase fluorination at 0° yields addition compounds, dimer, and higher boiling products.
4. Gives positive permanganate unsaturation test.
5. Saturated by vapor phase reaction with CoF₃ at 200°.
6. Partially rearranges at 200-500° to a higher melting saturated isomer.
7. Reacts with C₄F₆ to form C₁₂F₁₈. ibid

Chemical Name Hexafluoro-1,3-butadiene dimer
probably dodecafluorotricyclo(2.2.0.2^{2,3})octane

Empirical Formula C₈F₁₂

Molecular Weight 324.1

Formula Composition 29.6% C, 70.4% F

Preparation

M-3113 (158)

Freezing Point, °C

40.1

ibid

Boiling Point, °C

79.8-79.9

ibid

Reactions

Negative permanganate unsaturation test.

ibid

256

 $C_8F_{17}N$

Chemical Name Undecafluoro-N,N-bis(trifluoromethyl)cyclohexylamine

Empirical Formula $C_8F_{17}N$

Structural Formula

Molecular Weight 433.1

Formula Composition 22.2% C, 74.6% F, 3.2% N

Density, g/cc

Temperature, °C

20

1.247

BR-645 (13)

Molecular Volume, cc

Temperature, °C

20

234.5

ibid

220 282

257

C₈F₁₅Cl

Chemical Name Chlorononafluorobis(trifluoromethyl)cyclohexane
 Empirical Formula C₈F₁₅Cl
 Molecular Weight 416.5
 Formula Composition 23.1% C, 68.4% F, 8.5% Cl

PreparationObtained in preparation of C₈F₁₆ (Section I, Page 1)

MDDC-209 (11)

Boiling Point, °C

127.8-129.15

This Laboratory

Density, g/cc

Temperature, °C

10	1.90450
20	1.88224
25	1.87113
30	1.85995
40	1.83711
50	1.81471
60	1.79126
70	1.76717
80	1.74356

Equation: $d = 1.92607 - 2.1546 \times 10^{-3} t - 1.5911 \times 10^{-6} t^2$
 or simplified $d = 1.92851 - 2.2986 \times 10^{-3} t$

See Figure 188

ibid

Refractive Index (n_D)

Temperature, °C

10	1.3221
20	1.3183
30	1.3140
40	1.3107
50	1.3067
60	1.3021

Equation: $n_D = 1.3261 - 0.00040 t$

See Figure 189

ibid

220 283

258

Vapor Pressure, mm Hg
Temperature, °C

-32.3	0.16
-30.2	0.18
-28.2	0.22
-28.1	0.23
-25.6	0.31
-25.0	0.32
-25.0	0.32
-24.9	0.33
-22.5	0.36
-22.5	0.37
-19.8	0.48
-17.1	0.61
-16.9	0.63
-16.8	0.63
-13.7	0.82
-10.3	1.10
- 6.4	1.47
- 5.8	1.54
- 2.2	1.99
- 0.1	2.32
+ 4.4	3.20
9.3	4.44
14.4	6.20
19.7	8.66
20.3	8.92
22.0	9.88
22.3	10.12
22.9	10.44
45.1	34.4
50.8	45.7
51.2	46.8
68.1	98.0
70.0	106.5
102.0	342.3
108.5	418.0
127.6	736.9
139.6	1022.6
159.6	1668.0
159.6	1676.9

Equation: $\log p = 6.7396 - 1150.2/T - 160670$

See Figure 190

This Laboratory

220 284

257

C₈F₁₅Cl

Viscosity, cp

Temperature, °C

10	3.85
20	3.03
25	2.69
30	2.42
40	1.98
50	1.64
60	1.38
70	1.18

Equation: $\log \eta = \frac{831.420}{T} - 2.35628$

See Figure 191

This Laboratory

Surface Tension, dyne/cm

Temperature, °C

10	19.4
20	18.5
25	18.0
30	17.6
40	16.7
50	15.8
60	15.0
70	14.1

Equation: $\gamma^{1/4} = 1.187 d - 0.1610$, where d is density.

See Figures 192 and 193

ibid

Parachor

Temperature, °C

25	459	ibid
----	-----	------

Heat of Vaporization, cal/mol

Temperature, °C

(Calculated)

25	10191	
128.6	8920	ibid

220 285

260

Entropy of Vaporization, cal/mol/°C

Temperature, °C	(Calculated)	
25	34.18	
128.6	22.21	This Laboratory

Ultrasonic Velocity, m/sec

Temperature, °C	
20	691.8
30	663.1
40	635.5
50	608.6
60	582.3

Molecular sound velocity	1940
Molecular weight	414-418

See Figure 194

K-66 (7)

Infrared Absorption

See Figure 195

This Laboratory

220 286

261

Chemical Name 1,6-Dichloro-1,1,2,2,3,4,5,5,6,6 decafluoro-
3,4-bis(chlorodifluoromethyl)hexane

Empirical Formula C₈F₁₄Cl₄

Structural Formula

Molecular Weight 503.9

Formula Composition 19.1% C, 52.8% F, 28.1% Cl

Preparation

Boiling Point, °C

125-126 at 70 mm

ibid

220 287

262

Code Name	C-816 Cl_2
Chemical Name	Dichlorooctafluorobis(trifluoromethyl)cyclohexane
Empirical Formula	$C_8F_{14}Cl_2$
Structural Formula	$C_6F_8Cl_2(CF_3)_2$ (mixture of isomers)
Molecular Weight	433.0
Formula Composition	22.2% C, 61.4% F, 16.4% Cl

See Section I

Page 29

220 288

263

 $C_8F_{12}Cl_6$

Chemical Name Hexafluoro-1,3-butadiene dimer hexachloride
 Empirical Formula $C_8F_{12}Cl_6$
 Molecular Weight 536.8
 Formula Composition 17.9% C, 42.5% F, 39.6% Cl

Preparation

30% thermal dimer of $CF_2=CF=CF=CF_2$ adds chlorine to yield $C_8F_{12}Cl_6$.
 M-3113 (157)

Boiling Point, °C

139-140 at 20 mm
 261

ibid

Refractive Index (n_D)

Temperature, °C

20

1.4040

ibid

Reactions

Negative permanganate unsaturation test.

ibid

220 289

264

Chemical Name Hexafluoro-1,3-butadiene dimer tetrachloride
 Empirical Formula $C_8F_{12}Cl_4$
 Molecular Weight 465.9
 Formula Composition 20.6% C, 49.0% F, 30.4% Cl

Preparation

70% thermal dimer of $CF_2=CF-CF=CF_2$ adds chlorine to yield $C_8F_{12}Cl_4$
 $n_D^{20} = 1.3870$ (157)

Boiling Point, °C

94-95 at 20 mm
 203

ibid

Refractive Index (n_D)

Temperature, °C

20

1.3870

ibid

Reaction

Negative permanganate unsaturation test.

ibid

220 230

265

 $C_8F_6Cl_4$

Chemical Name	Tetrachlorobis(trifluoromethyl)benzene
Empirical Formula	$C_8F_6Cl_4$
Molecular Weight	351.9
Formula Composition	27.3% C, 32.4% F, 40.3% Cl

Preparation

A-879 (12)

220 231

266

Chemical Name Bis(trifluoromethyl)benzene

Empirical Formula $C_8F_6H_4$

Structural Formula

Molecular Weight 214.1

Formula Composition 44.9% C, 53.2% F, 1.9% H

See Section I

Page 41

267

 $C_8F_3Cl_7$

Chemical Name 1-Dichlorotrifluoroethyl-2,3,4,5,6-pentachlorobenzene

Empirical Formula $C_8F_3Cl_7$

Structural Formula

Molecular Weight 401.3

Formula Composition 23.9% C, 14.2% F, 61.9% Cl

Preparation Melting Point, °C

65-66

ibid

220 223

268

 $C_8F_2Cl_8$

Chemical Name 1-Trichlorodifluoroethyl-2,3,4,5,6-pentachlorobenzene
Empirical Formula $C_8F_2Cl_8$

Structural Formula

Molecular Weight 417.8
Formula Composition 23.0% C, 9.1% F, 67.9% Cl

Preparation Ind. Eng. Chem., 39, 384 (1947)Melting Point, °C

120-121

Ind. Eng. Chem., 39, 384 (1947)

220 204

269

C₈F₂H₁₆

Chemical Name 2,2-Difluorooctane

Empirical Formula C₈F₂H₁₆

Molecular Weight 150.1

Formula Composition 64.0% C, 25.3% F, 10.7% H

Density, g/cc

Temperature, °C

20

0.887

BR-645 (12)

Molecular Volume, cc

Temperature, °C

20

169.3

ibid

220 235

Preparation

Boiling Point, °C

Reactions

271

Chemical Name 1,2-Dichloro-3,5-bis(trifluoromethyl)benzene

Empirical Formula $\text{C}_8\text{F}_6\text{Cl}_2\text{H}_2$

Structural Formula

Molecular Weight 283.0

Formula Composition 33.9% C, 40.3% F, 25.1% Cl, 0.7% H

Boiling Point, °C

170.5 at 745 mm

A-3786 (92)

220 297

272

Chemical Name	Dichlorobis(trifluoromethyl)benzene
Empirical Formula	$C_8F_6Cl_2H_2$
Structural Formula	$C_6H_2Cl_2(CF_3)_2$
Molecular Weight	283.0
Formula Composition	33.9% C, 40.3% F, 25.1% Cl, 0.7% H

See Section I

Page 53

220 298

273

Chemical Name 1-Chloro-2,4-bis(trifluoromethyl)benzene
Empirical Formula $\text{C}_8\text{F}_6\text{ClH}_3$

Structural Formula

Molecular Weight 248.5
Formula Composition 38.6% C, 45.9% F, 14.3% Cl, 1.2% H

Boiling Point, °C

149.2

A-3786 (92)

220 229

274

C₈F₆ClH₃

Chemical Name 1-Chloro-3,5-bis(trifluoromethyl)benzene

Empirical Formula C₈F₆ClH₃

Structural Formula

Molecular Weight 248.5

Formula Composition 38.6% C, 45.9% F, 14.3% Cl, 1.2% H

Boiling Point, °C

138.2

A-3786 (92)

Bond Distance, Å

Bond

C-C 1.39 ± 0.03
C-Cl <1.71

A-3786 (81)

220 300

275

 $C_8F_6ClH_3$

Chemical Name	Chlorobis(trifluoromethyl)benzene
Empirical Formula	$C_8F_6ClH_3$
Structural Formula	$C_6H_3Cl(CF_3)_2$ (mixture of isomers)
Molecular Weight	248.5
Formula Composition	38.6% C, 45.9% F, 14.3% Cl, 1.2% H

See Section I

Page 51

220 301

276

 $C_8F_4Cl_5H$

Chemical Name (Chlorotetrafluoroethyl)tetrachlorobenzene
Empirical Formula $C_8F_4Cl_5H$
Molecular Weight 350.4
Formula Composition 27.4% C, 21.7% F, 50.6% Cl, 0.3% H

Preparation

Boiling Point, °C

89-92 at 1 mm

ibid

220 302

278

Chemical Name (Dichlorotrifluoroethyl)chlorobenzene
Empirical Formula $\text{C}_8\text{F}_3\text{Cl}_3\text{H}_4$
Molecular Weight 263.5
Formula Composition 36.5% C, 21.6% F, 40.4% Cl, 1.5% H

Preparation

Boiling Point, °C

52-56 at 1 mm

ibid

Density, g/cc

Temperature, °C

25

1.498

ibid

Refractive Index (n_D)

Temperature, °C

25

1.4818

ibid

220 304

279

Chemical Name (Trichlorodifluoroethyl)chlorobenzene
 Empirical Formula C₈F₂Cl₄H₄
 Molecular Weight 280.0
 Formula Composition 34.3% C, 13.6% F, 50.7% Cl, 1.4% H

Preparation Boiling Point, °C

72-73 at 1 mm

ibid

Density, g/cc

Temperature, °C

25

1.537

ibid

Refractive Index (n_D)

Temperature, °C

25

1.5140

ibid

220 305

280

Chemical Name 1,1,1-Trifluoro-3-thenoylpropanone

Empirical Formula C₈F₃H₅O₂S

Structural Formula

Molecular Weight 222.1

Formula Composition 43.3% C, 25.7% F, 2.2% H, 14.4% O, 14.4% S

Preparation

A-3962 (1)

220 306

281

C₉F₂₀

Chemical Name Eicosfluorononane

Empirical Formula C₉F₂₀

Structural Formula

```

      F   F   F   F   F   F   F   F   F
      |   |   |   |   |   |   |   |   |
F - C - C - C - C - C - C - C - C - C - F
      |   |   |   |   |   |   |   |   |
      F   F   F   F   F   F   F   F   F

```

Molecular Weight 488.1

Formula Composition 22.1% C, 77.9% F

Boiling Point, °C

123

LRG-64 (III-4)

Density, g/cc

Temperature, °C

20

1.80

BR-319 (12)
LRG-64 (III-3)Refractive Index (n_D)

Temperature, °C

20

1.278
1.283ibid
BR-319 (12)Specific RefractionAR_F (calculated)0.097
0.0953—
1.23

LRG-64 (III-3)

Viscosity, mp

Temperature, °C

20

20

BR-319 (12)

220 307

282

C₉F₂₀Surface Tension

Temperature, °C

20

15.5 (Ring method)

22

15.3 (Sugden & Ferguson method)
BR-319 (12)Parachor

Temperature, °C

20

545

ibid

220 308

283

 C_9F_{18}

Chemical Name Nonafluoro-1,2,4-tris(trifluoromethyl)cyclohexane

Empirical Formula C_9F_{18}

Structural Formula

Molecular Weight 450.1

Formula Composition 24.0% C, 76.0% F

Boiling Point, °C

125

BR-319 (12)

Density, g/cc

Temperature, °C

20

1.85

ibid

Refractive Index (n_D)

Temperature, °C

20

1.295

ibid

220 309

284

 C_9F_{18}

Chemical Name Nonafluoro-1,3,5-tris(trifluoromethyl)cyclohexane

Empirical Formula C_9F_{18}

Structural Formula

Molecular Weight 450.1

Formula Composition 24.0% C, 76.0% F

Preparation

1. $C_6H_3(CF_3)_3 \xrightarrow{CoF_3} C_6F_9(CF_3)_3$ (84% yield) A-3468 (59)
2. $C_6H_3(CF_3)_3 \xrightarrow{F_2} C_6F_9(CF_3)_3$
 - a. $C_6H_3(CH_3)_3 \xrightarrow{Cl_2} C_6H_3(CCl_3)_3$
 - b. $C_6H_3(CCl_3)_3 \xrightarrow{HF} C_6H_3(CF_3)_3$ A-208 (4)
3. $C_6F_3(CF_3)_3 \xrightarrow{CoF_3} C_6F_9(CF_3)_3$ (71% yield) A-3468 (59a)
4. Fluorination of 1,3,5-trimethyl-cyclohexane gives a 33% yield of C_9F_{18} .
LRG-49 (13)

Melting Point, °C

About -80

A-208 (4)

220 310

285

C₉F₁₈Boiling Point, °C

123
124.7-125.1
125.18

A-312 (4)
MDDC-600 (48)
A-770 (8)

Density, g/cc

Temperature, °C

20

1.891
1.893
1.9025
1.868
1.8876

BR-329 (9)
BR-645 (13)
A-3468 (128)
MDDC-319 (31)
LRG-64 (III-3)

30

0.28
35.7
62.2
94.6

1.9445
1.8630
1.8040
1.7300

See Figure 196

A-312 (16)

0.0
28.0
76.0

1.9484
1.8848
1.7710

See Figure 196

A-312 (15)

Refractive Index (n_D)

Temperature, °C

20
30

1.2995
1.2930

A-3468 (128)
LRG-64 (III-3)
A-312 (4)
MDDC-319 (31)
BR-319 (11)

Specific Refraction

Temperature, °C

30

0.0972
0.0975

AR_F (calculated)

1.23

LRG-64 (III-3)

220 311

286

C₉F₁₈Viscosity, mp

Temperature, °C

0.3
2037.49
25MDDC-319 (31)
BR-329 (15)0.28
35.7
62.2
94.637.49
17.27
11.25
7.32

See Figure 197

A-312 (16)

Molecular Volume, cc

Temperature, °C

20

237.7

BR-645 (13)

Analysis

F⁻ determined by Na fusion with titration of fluoride with thorium nitrate, Na alizarin indicator.

A-311 (1)

220 312

287

C₉F₁₆

Chemical Name Hexadecafluorooctahydroindene
 Empirical Formula C₉F₁₆

Structural Formula

Molecular Weight 412.1
 Formula Composition 26.2% C, 73.8% F

Preparation

C₉H₁₀ (Indan) $\xrightarrow{\text{CoF}_3}$ C₉F₁₆ (20% yield)

A-3468 (120)

Freezing Point, °C

-8 to -15

Ind. Eng. Chem., 39, 380 (1947)Boiling Point, °C

117.2-117.5
 117.83

MDDC-600 (8)
 A-3468 (128)
 A-770 (8)

Density, g/cc

Temperature, °C

20

1.8838

Ind. Eng. Chem., 39, 380 (1947)
 1.8948 A-3468 (128)

Refractive Index (n_D)

Temperature, °C

20

1.3033

Ind. Eng. Chem., 39, 380 (1947)
 1.3077 A-3468 (128)

220 313

288

 $C_9F_9H_3$

Chemical Name 1,3,5-Tris(trifluoromethyl)benzene

Empirical Formula $C_9F_9H_3$

Structural Formula

Molecular Weight 282.1

Formula Composition 38.3% C, 60.6% F, 1.1% H

Preparation

Temperature and pressure ranges of 110-235°C and 150-2200 psi for varying periods of time.

A-768 (17)

Melting Point, °C

9.0

Ind. Eng. Chem., 39, (1947)Boiling Point, °C

118.0 at 742.6 mm

118-121

119.6 at 750 mm

A-3786 (92)

A-768 (19)

Ind. Eng. Chem., 39, 394 (1947)Density, g/cc

Temperature, °C

25

1.5139

ibid

220 314

287

C9F9H3Refractive Index (np)

Temperature, °C

25

1.3558

A-3786 (74)

Ind. Eng. Chem., 39, 394 (1947)Bond Measurements

Bond

Bond distance, Å

Bond angle, °

C-C (ring)

 1.41 ± 0.02

—

C-C

 1.50 ± 0.02

—

C-F

 1.36 ± 0.02

—

 $\angle$ FCF 107.5 ± 1

A-3786 (75)

220 315

290

C₉F₃H₉

Chemical Name 2,4,6-Trifluoromesitylene

Empirical Formula C₉F₃H₉

Structural Formula

Molecular Weight 174.1

Formula Composition 62.1% C, 32.7% F, 5.2% H

Freezing Point, °C

68.7

A-3786 (64)

Boiling Point, °C

92 at 60 mm

A-3786 (92)

Bond Distance, Å

Bond

C-C	1.37
C-F	1.34

A-3786 (81)

220 316

291

 $C_9F_9Cl_2H$

Chemical Name 2,4-Dichloro-1,3,5-tris(trifluoromethyl)benzene
 Empirical Formula $C_9F_9Cl_2H$

Structural Formula

Molecular Weight 351.0
 Formula Composition 30.8% C, 48.7% F, 20.2% Cl, 0.3% H

Preparation

Fluorinated in autoclave at 220–280°C for 20 hours.

Ind. Eng. Chem., 39, 394 (1947)

Melting Point, °C

61.0

ibid

Boiling Point, °C

71.0 at 5 mm
 71.1 at 5 mm

A-3786 (93)
 Ind. Eng. Chem., 39, 394 (1947)

220 317

292

 $C_9F_9ClH_2$

Chemical Name 2-Chloro-1,3,5-tris(trifluoromethyl)benzene

Empirical Formula $C_9F_9ClH_2$

Structural Formula

Molecular Weight 316.6

Formula Composition 34.1% C, 54.0% F, 11.2% Cl, 0.7% H

Preparation

Fluorinated in autoclave at 220-280°C for 20 hours.

Ind. Eng. Chem., 39, 394 (1947)Melting Point, °C

-3.0

ibid

Boiling Point, °C152.4 at 750 mm
152.6 at 753.7 mm

A-3786 (93)

Density, g/cc

Temperature, °C

25

1.6316

Ind. Eng. Chem., 39, 394 (1947)

220 318

293

 $C_9F_9ClH_2$ Refractive Index (n_D)

Temperature, °C

25

1.3903

Ind. Eng. Chem., 39, 394 (1947)

Molecular Refraction (M_R)

Temperature, °C

25

46.027

 AR_F (calculated)

1.144

ibid

220 319

C₁₀F₂₀

294

Chemical Name

1-Trifluoromethyl-4-(heptafluoroisopropyl)decafluoro-
cyclohexane

Empirical Formula

C₁₀F₂₀

Structural Formula

Molecular Weight

500.1

Formula Composition

24.0% C, 76.0% F

Boiling Point, °C

144-147°

MDDC-209 (11)

220 320

295

Chemical Name Octadecafluorodecahydronaphthalene
 Empirical Formula C₁₀F₁₈

Structural Formula

Molecular Weight 462.1
 Formula Composition 26.0% C, 74.0% F

Melting Point, °C

-75

A-312 (20)

Boiling Point, °C

136-138
 138
 140
 140-144

A-312 (20)
 BR-319 (12)
 Ind. Eng. Chem., 39, 367 (1947)
 MDDC-209 (11)

Density, g/cc

Temperature, °C

20

1.92 BR-319 (12)
 1.932 BR-645 (13)
 1.9456
 Ind. Eng. Chem., 39, 367 (1947)
 1.9229 A-312 (20)
 1.923 MDDC-319 (31)
 1.92
 1.72 BR-329 (14)

23.5

24.6

99.3

270 321

276

C₁₀F₁₈Refractive Index (n_D)

Temperature, °C

19	1.314	BR-319 (12)
20	1.3118	
	Ind. Eng. Chem., 39, 367 (1947)	
23.5	1.3125	LRG-64 (III-3)
24.5	1.3125	A-312 (20)

Specific Refraction

Temperature, °C

20	0.103	
23.5	0.101	LRG-64 (III-3)
—	0.101	A-312 (20)

Molecular Refraction (M_R)46.32
46.71

A-312 (20)

Viscosity, mp

Temperature, °C

20	50.5	BR-329 (14)
24.6	53.39	
99.3	11.61	A-312 (20)

Surface Tension, dynes/cm

Temperature, °C

20	19.25	BR-319 (12)
----	-------	-------------

Parachor

Temperature, °C

20	511	BR-319 (12)
----	-----	-------------

220 322

C₁₀F₁₈

297

Molecular Volume, cc

Temperature, °C

20

239.1

BR-645 (13)

220 323

298

 $C_{10}F_{10}H_4$

Chemical Name

Bis(pentafluoroethyl)benzene

Empirical Formula

 $C_{10}F_{10}H_4$

Structural Formula

(mixture of isomers)

Molecular Weight

314.1

Formula Composition

38.2% C, 60.5% F, 1.3% H

Preparation

A-1525 (2)

220 324

299

C₁₀FH₇

Chemical Name 1-Fluoronaphthalene

Empirical Formula C₁₀FH₇

Structural Formula

Molecular Weight 146.1

Formula Composition 82.2% C, 13.0% F, 4.8% H

Density, g/cc

Temperature, °C

20

1.134

BR-645 (12)

Molecular Volume, cc

Temperature, °C

20

128.9

BR-645 (12)

220 325

300

 $C_{11}F_{20}$

Chemical Name Heptadecafluoro-1-(trifluoromethyl)decahydronaphthalene
 Empirical Formula $C_{11}F_{20}$

Structural Formula

Molecular Weight 512.0
 Formula Composition 25.8% C, 74.2% F

Melting Point, °C

<-75

Ind. Eng. Chem., 39, 367 (1947)Boiling Point, °C

161

ibid

Density, g/cc

Temperature, °C

20

1.9606

ibid

Refractive Index (n_D)

Temperature, °C

20

1.3168

ibid

220 326

301

 $C_{11}F_{20}$

Chemical Name Heptadecafluoro-2-(trifluoromethyl)decahydronaphthalene

Empirical Formula $C_{11}F_{20}$

Structural Formula

Molecular Weight 512.00

Formula Composition 25.8% C, 74.2% F

Melting Point, °C

< -60

Ind. Eng. Chem., 39, 367 (1947)

Boiling Point, °C

160-161

ibid

Density, g/cc

Temperature, °C

20

1.9632

ibid

Refractive Index (n_D)

Temperature, °C

20

1.3164

ibid

220 327

C₁₂F₂₂

302

Chemical Name Docosafluorodicyclohexyl

Empirical Formula C₁₂F₂₂

Structural Formula

Molecular Weight 562.1

Formula Composition 25.6% C, 74.4% F

Melting Point, °C

75

A-312 (4)

Boiling Point, °C

90 at 90 mm

J. Am. Chem. Soc., 63, 2793 (1941)

303

 $C_{12}F_{20}$

Chemical Name Eicosafuorododecahydroacenaphthylene

Empirical Formula $C_{12}F_{20}$

Structural Formula

Molecular Weight 620.0

Formula Composition 38.7% C, 61.3% F.

Freezing Point, °C

2 to 0

Ind. Eng. Chem., 39, 367 (1947)

Boiling Point, °C

173

ibid

Density, g/cc

Temperature, °C

20

1.9883

ibid

Refractive Index (n_D)

Temperature, °C

20

1.3292

ibid

220 329

304

C₁₂F₁₈

Chemical Name	Hexafluorobutadiene trimers
Empirical Formula	C ₁₂ F ₁₈
Molecular Weight	486.1
Formula Composition	29.6% C, 70.4% F

Preparation Boiling Point, °C

64-66 at 10 mm		ibid
----------------	--	------

Density, g/cc

Temperature, °C		
-----------------	--	--

20	1.8891	ibid
----	--------	------

Refractive Index (n_D)

Temperature, °C		
-----------------	--	--

20	1.3470	ibid
----	--------	------

220 330

305

Chemical Name Bis(undecafluorocyclohexane)ether

Empirical Formula C₁₂F₂₂O

Structural Formula

Molecular Weight 578.1

Formula Composition 24.9% C, 72.3% F, 2.8% O

Preparation

MDDC-600 (47)

Boiling Point, °C

175-176

A-3468 (118)

306

 $C_{12}F_2H_8$

Chemical Name 4,4-Difluorodiphenyl

Empirical Formula $C_{12}F_2H_8$

Structural Formula

Molecular Weight 190.1

Formula Composition 75.8% C, 20.0% F, 4.2% H

Melting Point, °C

88.5

A-3786 (92)

220 332

307

 $C_{13}F_{22}$

Chemical Name Docosafluorododecahydrofluorene

Empirical Formula $C_{13}F_{22}$

Structural Formula

Molecular Weight 574.0

Formula Composition 27.2% C, 72.8% F

Melting Point, °C

<-40

Ind. Eng. Chem., 39, 367 (1947)Boiling Point, °C

190

ibid

Density, g/cc

Temperature, °C

20

1.9819

ibid

Refractive Index (n_D)

Temperature, °C

20

1.3264

ibid

220 333

308

 $C_{13}H_{11}F$

Chemical Name Diphenylfluoromethane

Empirical Formula $C_{13}H_{11}F$

Structural Formula

Molecular Weight 186.1

Formula Composition 83.8% C, 10.2% F, 6.0% H

Density, g/cc

Temperature, °C

20

1.1614

BR-645 (12)

Molecular Volume, cc

Temperature, °C

20

160.2

BR-645 (12)

220 334

309

C₁₄F₂₄

Chemical Name

Tetracosafuorotetradecahydroanthracene

Empirical Formula

C₁₄F₂₄

Structural Formula

Molecular Weight

624.0

Formula Composition

26.9% C, 73.1% F

Melting Point, °C

76-81

Ind. Eng. Chem., 39, 367 (1947)

Boiling Point, °C

211-213

ibid

220 335

310

C₁₄F₂₄

Chemical Name Tetracosafuorotetradecahydrophenanthrene

Empirical Formula C₁₄F₂₄

Structural Formula

Molecular Weight 624.0

Formula Composition 26.9% C, 73.1% F

Melting Point, °C

<-40

Ind., Eng. Chem., 39, 367 (1947)

Boiling Point, °C

205-206

ibid

Density, g/cc

Temperature, °C

20

2.0197

ibid

Refractive Index (n_D)

Temperature, °C

20

1.3315

ibid

220 336

311

C₁₆F₃₄

Chemical Name Tetratriacontafluorohexadecane
 Empirical Formula C₁₆F₃₄

Molecular Weight 838.2
 Formula Composition 22.9% C, 77.1% F

Preparation

1. Cetane when fluorinated yields C₁₆F₃₄, 40% crude yield, 29% purified yield. Preparation given in detail. A-3468 (86)
2. Cetane $\xrightarrow{\text{CoF}_3}$ white crystalline solid melting slightly above 100°C. When distilled in a Claissen flask, majority distilled in the range 235°-250°C.

Melting Point, °C

114
 114-115

A-312 (3)
 A-3649 (428)

Boiling Point, °C

238-240
 240

A-3649 (428)
 A-312 (3)

Analysis

F⁻ determined by Na fusion with titration of fluoride with thorium nitrate, Na alizarin sulfonate as indicator. A-311 (2)

220 337

312

 $C_{16}F_{26}$

Chemical Name Hexacosafuorohexadecahydrofluoranthene

Empirical Formula $C_{16}F_{26}$

Structural Formula

Molecular Weight 686.2

Formula Composition 28.0% C, 72.0% F

Melting Point, °C

-36 to -30

Ind. Eng. Chem., 39, 367 (1947)Boiling Point, °C

235-239

ibid

Density, g/cc

Temperature, °C

20

2.0598

ibid

Refractive Index (n_D)

Temperature, °C

20

1.3460

ibid

220 338

313

Chemical Name Octatriacontafluorooctadecane

Empirical Formula C₁₈F₃₈

Structural Formula

Molecular Weight 938.2

Formula Composition 23.0% C, 77.0% F

Specific Refraction

Temperature, °C

20

0.0962

BR-645 (3)

Molecular Refraction (MR_D)

90.25

BR-645 (3)

220 339

Chemical Name	Docosafluoro-7-(heptafluoroisopropyl)-1-(trifluoromethyl)tetradecahydrophenanthrene
---------------	---

Empirical Formula $C_{18}F_{32}$

Molecular Weight	824.2
------------------	-------

Formula Composition 26.2% C, 73.8% F

Boiling Point, °C

ca 135 at 10 mm

Ind. Eng. Chem., 39, 367 (1947)

Density, g/cc

Temperature, °C

30

2.05

ibid

Refractive Index (n_D)

Temperature, °C

25

1.343

ibid

Viscosity, mp

Temperature, °C

99.5

ca 60

ibid

315

 $C_{18}F_{30}$

Chemical Name Triacontafluorooctadecahydrochrysene
 Empirical Formula $C_{18}F_{30}$

Structural Formula

Molecular Weight 786.2
 Formula Composition 27.5% C, 72.5% F

Boiling Point, °C

ca 135 at 10 mm

Ind. Eng. Chem., 39, 367 (1947)Density, g/cc

Temperature, °C

25

2.06

ibid

Refractive Index (n_D)

Temperature, °C

25

1.344

ibid

Viscosity, mp

Temperature, °C

99.5

ca 60

ibid

220 341

316

BIBLIOGRAPHY

- A-199 Grosse, A. V., "Refractometric analysis of fluorocarbons and fluoro-hydrocarbons", Columbia University, July 1942.
- A-208 Urey, H. C., "Progress reports on chemical problems", Columbia University, July 1942.
- A-211 Gross, A. V., "Stability of fluorocarbons against UF_6 ", Columbia University, July 1942.
- A-311 Gross, A. V., "Report on methods for analyzing fluorocarbons", Columbia University, September 1942.
- A-312 Gross, A. V., "Chemical and physical properties of fluorocarbons", Columbia University, September 1942.
- A-503 (b) McBee, E. T., "Monthly progress report on fluorocarbons", Purdue University, January 1943.
- A-558 McBee, E. T., "Monthly progress report on fluorocarbon research", Purdue University, March 1943.
- A-585 Haendler, H. M., "Fluorocarbons", Columbia University, April 1943.
- A-709 Henne, A. L., "Informal monthly report on fluorocarbons", Ohio State University, May 1943.
- A-730 Calcott, W. S., "Preparation of C_7F_{16} , C_6F_{14} and fluoro-lubricants", E. I. du Pont, Jackson Laboratory, May 1943.
- A-768 McBee, E. T., "Final report on fluorocarbons", Purdue University, July 1943.
- A-770 Henne, A. L., "Final report on preparation and purification of fluorocarbons", Ohio State University, June 1943.
- A-879 McBee, E. T., "Monthly progress report on fluorocarbon research", Purdue University, May 1943.
- A-1404 Katz, J. J., "Survey of the inorganic fluorides", University of Chicago, November 1943.
- A-1506 McBee, E. T., "Monthly technical report on fluorocarbon research", Purdue University, April 1944.
- A-1507 McBee, E. T., "Monthly technical report on research", Purdue University, May 1944.
- A-1508 McBee, E. T., "Monthly technical report on research", Purdue University, June 1944.
- A-1509 McBee, E. T., "Monthly technical report on research", Purdue University, July 1944.

317

- A-1510 — McBee, E. T., "Monthly technical report on research", Purdue University, August 1944.
- A-1525 Murray, R. L., "Technical report on fluorocarbon research", Hooker Electrochemical Company, November 1943.
- A-1575 Litant, I., "Cryoscopic determination of molecular weights of fluorocarbons using unsymdifluorotetrachloroethane as solvent", Johns Hopkins University, October 1945.
- A-1730 — Barnes, R. B., "Analysis of materials concerned in the production of fluorocarbons", American Cyanamid Company, December 1943.
- A-1748 — Gilman, H., "The preparation of 2,2,2-Trifluoroethanol", Iowa State College, no date.
- A-1919 Jessup, R. S., "Heat of reaction of C_8F_{16} ", National Bureau of Standards, no date.
- A-1969 — McBee, E. T., "Technical report on research", Purdue University, August 1944.
- A-1991 — Burford, W. B., "Monthly technical report", Johns Hopkins University, September 1944.
- A-2104 Henne, A. L., "Final technical report", Ohio State University, June 1944.
- A-2550 Downing, F. B., "Fluorolubricant liquid phase", E. I. du Pont, Jackson Laboratory, October 1944.
- A-2552 — Downing, F. B., "The disposal of fluorine, oxyfluoride and hydrogen fluoride", E. I. du Pont, Jackson Laboratory, November 1944.
- A-3468 Burford, W. B., "Fluorocarbons to June 30, 1943", Johns Hopkins University.
- A-3500 Downing, F. B., "Fluorination of n-heptane with CoF_3 ", E. I. du Pont, Jackson Laboratory, January 1944.
- A-3649 Libby, W. F., "Chemistry of the diffusion process", Columbia University, October 1945.
- A-3728 Rosen, R., "Special chemicals report", Kellogg Corporation, September 1945.
- A-3786 Brockway, L. O., "Report on electron diffraction investigation of fluorocarbons", U. S. Naval Research Laboratory, June 1944.
- A-3959 Williams, V. Z., "Infrared analysis of C_7F_{16} and C_8F_{16} ", American Cyanamid Company, July 1945.
- A-3962 — Reid, J. C., "Preparation of thenoyltrifluoroacetone", University of California, October 1946.
- B-97 — Haworth, Prof., "Fluorocarbons", Birmingham University, England, July 1942.

220 343

318

- BR-319 Rudge, A. J., "The chemical and physical properties of the fluorocarbons", Widnes Laboratory, Widnes England, October 1943.
- BR-329 Rudge, A. J., "An attempt to forecast some physical constants for selected fluorocarbons", Widnes Laboratory, Widnes England, November 1943.
- BR-331 No author, "Preparation of benzotrifluoride", no date.
- BR-360 Sarsfield, N. F., "The elementary fluorides and their use as fluorinating agents", Widnes Laboratory, Widnes England, June 1943.
- BR-420 No author, "Notes on the production of fluorocarbons", April 1944.
- BR-497 Grove, D. M., "The ultra-violet absorption spectra of some fluorinated hydrocarbons", Widnes Laboratory, Widnes England, October 1944.
- BR-527 Sarsfield, N. F., "The refining of fluorocarbons", Widnes Laboratory, Widnes England, March 1944.
- BR-645 Sarsfield, N. F., "Physical properties and composition of fluorocarbons", Widnes Laboratory, Widnes England, September 1945.
- K-66 Underwood, N., "Ultrasonic velocity in some liquid fluorocarbons", Carbide and Carbon Chemicals Corporation, K-25, October 1947.
- LRG-19 No author, "Progress report", April 1943.
- LRG-21 No author, "Progress report", June 1943.
- LRG-49 No author, "Progress report", October 1945.
- LRG-50 No author, "Progress report", November 1945.
- LRG-64 Simon, F., "British Data Book", 1943.
- M-215 Elley, H. W., "Meeting at du Pont to discuss specifications on fluorocarbons and fluorolubes", August 1943.
- M-222 Rosen, R., "Meeting at du Pont to discuss specifications on fluorocarbons and fluorolubes", July 1943.
- M-255 Downing, F. B., "Preparation of $C_7F_{15}Cl$ from chloro-fluoro-heptanes", E. I. du Pont, Jackson Laboratory, September 1943.
- M-530 Weber, C. E., "The vapor pressure, the critical temperature and the critical density of $n-C_4F_{10}$ ", Johns Hopkins University, no date.
- M-2149 Kharasch, M. S., "The toxicity of compounds containing fluorine", University of Chicago, November 1943.
- M-2534 Libby, W. F., "Fluorocarbons", Carbide and Carbon Chemicals Corporation, SAM Laboratories, August 1945.
- M-2544 Libby, W. F., "Fluorocarbons", Carbide and Carbon Chemicals Corporation, SAM Laboratories, September 1945.

- 319
- M-2567 Libby, W. F., "Fluorocarbons", Carbide and Carbon Chemicals Corporation, SAM Laboratories, October 1945.
- M-3113 Miller, W. T., "The use of perfluoro- and chloro perfluoro-olefins in the synthesis of fluorocarbon materials", Columbia University, SAM Laboratories, 1946.
- M-3811 McBee, E. T., "Monthly progress report on fluorocarbons", Purdue University, January 1943.
- M-3812 McBee, E. T., "Monthly progress report on fluorocarbons", Purdue University, December 1942.
- M-3814 Henne, A. L., "Informal monthly report on fluorocarbons", Ohio State University, April 1943.
- M-3823 Bigelow, L. A., "Progress report", Duke University, December 1942.
- MDDC-142 Murray, R. L., "The preparation of polyperfluorovinylchloride", no date.
- MDDC-162 McBee, E. T., "Identification and reactions of polyhalohydrocarbons and halocarbons", Purdue University, no date.
- MDDC-168 McBee, E. T., "The decomposition and analysis of organic compounds containing fluorine and other halogens", Purdue University, no date.
- MDDC-190 Murray, R. L., "The preparation of sodium trifluoroacetate and ethyl trifluoroacetate", Hooker Electrochemical Company, no date.
- MDDC-208 Safety and Accident Prevention Branch, Manhattan District, "Precautions to be observed in the handling, shipping and storing of fluorine", U. S. Engineer Department, June 1946.
- MDDC-209 Downing, F. B., "The preparation of chlorofluorocarbons", E. I. du Pont, Jackson Laboratory, no date.
- MDDC-213 Weber, C. E., "The vapor pressures and critical constants of C_4F_{10} , C_7F_{16} , C_7F_{14} and C_8F_{16} ", Johns Hopkins University, no date.
- MDDC-278 Downing, F. B., "Fluorination of normal heptane", E. I. du Pont, Jackson Laboratory, August 1946.
- MDDC-300 Parmelee, H. M., "Fluorination of hexafluoroxylene", E. I. du Pont, Jackson Laboratory, August 1946.
- MDDC-319 Cady, G. H., "Early fluorocarbon studies at Columbia University, Columbia University, SAM Laboratories, no date.
- MDDC-575 Grosse, A. V., "The production of fluorocarbons by the reaction of fluorine with silicon carbide", Columbia University, December 1941.
- MDDC-600 Burford, W. B., "Pilot plant synthesis of C_7F_{16} , C_8F_{16} and fluorocarbon oils boiling up to $350^{\circ}C$ ", Johns Hopkins University, no date.
- MDDC-784 Reid, J. C., "Synthesis of ethyl trifluoroacetate", University of California, February 1947.
- N-2037 Reed, F. H., "Informal monthly progress report on aromatic fluorocarbons", March 1943.
- 220 345

320

FIGURE 137

REFRACTIVE INDEX FOR CF₄ AT 25°C AS A FUNCTION OF THE WAVE LENGTH OF LIGHT

321

FIGURE 138

HEAT CAPACITY (C_p) OF SOLID CF_4
AS A FUNCTION OF TEMPERATURE

322

FIGURE 139

HEAT CAPACITY (C_p) OF LIQUID CF_4 AS A FUNCTION OF TEMPERATURE

220 348 878

FIGURE 140

HEAT CAPACITY (C_v) OF GASEOUS CF_4
AS A FUNCTION OF TEMPERATURE

324

220.350

FIGURE 141

DIELECTRIC CONSTANT OF CF₄ AS A FUNCTION OF PRESSURE

325

NOTES:

- a--- Gas cell 10 cm 754 mm Hg
- b--- Gas cell 10 cm 7 mm Hg
- c--- Gas cell 10 cm 320 mm Hg

Perkin-Elmer Infrared Spectrometer

Measurements made at room temperature

FIGURE 142

INFRARED ABSORPTION SPECTRA OF CF_4

220 351

326

FIGURE 143

DENSITY OF CF_2Cl_2
 AS A FUNCTION OF PRESSURE

220 352

327

FIGURE 144

VAPOR PRESSURE OF CF_2Cl_2
AS A FUNCTION OF TEMPERATURE

220 353

328

FIGURE 145

220 354

VISCOSITY OF CF_2Cl_2
AS A FUNCTION OF TEMPERATURE

329

TEMPERATURE-ENTROPY DIAGRAM FOR CF_2Cl_2

FROM KELLEX DATA BOOK

FIGURE 147

ENTHALPY OF CF_2Cl_2
 AS A FUNCTION OF TEMPERATURE

FROM KELLEX DATA BOOK

220 356

331

FIGURE 148

DENSITY OF CFC1_3 AS A FUNCTION OF PRESSURE

FROM KELLEX DATA BOOK

220 357

332

FIGURE 149

VAPOR PRESSURE OF CFC1_3
 AS A FUNCTION OF TEMPERATURE

220 358

333

FIGURE 150

VISCOSITY OF CFCI_3
AS A FUNCTION OF TEMPERATURE

220 359

334

FIGURE 151

TEMPERATURE-ENTROPY DIAGRAM FOR CFC₁₃

098 026

Base:

$H = 0$ for liquid at -40°F
and 0.74 psia

FIGURE 152

ENTHALPY OF CFC1_3 AS A FUNCTION OF TEMPERATURE

336

FIGURE 153

DENSITY OF CF_2ClH AS A
FUNCTION OF PRESSURE

220 352

337

FIGURE 154

VAPOR PRESSURE OF CF_2ClH
 AS A FUNCTION OF TEMPERATURE

220 363

FIGURE 155

220 364

VISCOSITY OF CF_2ClH AS A
FUNCTION OF TEMPERATURE

338

339

FIGURE 156

TEMPERATURE-ENTROPY DIAGRAM FOR CF_2ClH

220 365

340

BASE:

$H=0$ for liquid at -41.44°F
and 760 mm Hg

FIGURE 157

ENTHALPY OF CF_2ClH AS A FUNCTION OF TEMPERATURE

220 366

FIGURE 158

DENSITY OF CFC₁₂H
AS A FUNCTION OF PRESSURE

220 367

341

FIGURE 159

VAPOR PRESSURE OF CFC_{12}H
AS A FUNCTION OF TEMPERATURE

220 368

342

FIGURE 160

VISCOSITY OF CFC_{12}H

AS A FUNCTION OF TEMPERATURE

220 369

343

FIGURE 161

TEMPERATURE-ENTROPY DIAGRAM FOR CFC1₂H

FIGURE 162
ENTHALPY OF CFC_{12}H
AS A FUNCTION OF TEMPERATURE

346

FIGURE 163

DIELECTRIC CONSTANT OF C_2F_6
AS A FUNCTION OF PRESSURE

347

220 373

FIGURE 164

DENSITY OF $\text{C}_2\text{F}_4\text{Cl}_2$ AS A FUNCTION OF PRESSURE

FIGURE 165

VAPOR PRESSURE OF $C_2F_4Cl_2$
AS A FUNCTION OF TEMPERATURE

348

FIGURE 166

VISCOSITY OF $C_2F_4Cl_2$
AS A FUNCTION OF TEMPERATURE

220 375

349

350

FIGURE 167

TEMPERATURE-ENTROPY DIAGRAM FOR $C_2F_4Cl_2$

FROM KELLEX DATA BOOK

220 376

351

BASE:
H = 0 for liquid at -40° F
 and 760 mm Hg

FIGURE 168

220 377

ENTHALPY OF $C_2F_4Cl_2$
 AS A FUNCTION OF TEMPERATURE

352

220 378

FIGURE 169

DENSITY OF $\text{C}_2\text{F}_3\text{Cl}_3$ AS A FUNCTION OF PRESSURE

FIGURE 170

VAPOR PRESSURE OF $C_2F_3Cl_3$
AS A FUNCTION OF TEMPERATURE

220 379
FROM KELLEX DATA BOOK

FIGURE 171

220 380

VISCOSITY OF $\text{C}_2\text{F}_3\text{Cl}_3$
AS A FUNCTION OF TEMPERATURE

220 381

FIGURE 172

TEMPERATURE-ENTROPY DIAGRAM FOR $C_2F_3Cl_3$

FROM KELLEX DATA BOOK

Figure 173 consists of five nomograms for ammonia, arranged in a descending staircase pattern. Each nomogram is a grid with enthalpy (Btu/lb) on the vertical axis and temperature (°F) on the horizontal axis. The nomograms are labeled as follows:

- Top Nomogram:** Saturated Vapor. Enthalpy ranges from 74 to 110 Btu/lb. Temperature ranges from -20 to 200 °F.
- Second Nomogram:** Saturated Vapor. Enthalpy ranges from 116 to 148 Btu/lb. Temperature ranges from 20 to 400 °F.
- Third Nomogram:** Saturated Vapor. Enthalpy ranges from 152 to 184 Btu/lb. Temperature ranges from 40 to 500 °F.
- Fourth Nomogram:** Saturated Vapor. Enthalpy ranges from 188 to 220 Btu/lb. Temperature ranges from 60 to 600 °F.
- Bottom Nomogram:** Saturated Liquid. Enthalpy ranges from 0 to 4 Btu/lb. Temperature ranges from -40 to 20 °F.

The base condition is $H=0$ for liquid at -40°C .

220 382

FIGURE 173

FROM KELLEX DATA BOOK

357

FIGURE 174

VOLATILITY OF $(\text{CH}_3\text{O})_2\text{POF}$
AS A FUNCTION OF TEMPERATURE

FROM M-2149

220 383

358

FIGURE 175
 ORTHOBARIC DENSITY OF C_4F_{10}
 AS A FUNCTION OF TEMPERATURE

220 384

359

FIGURE 176
VAPOR PRESSURE OF C_4F_{10}
AS A FUNCTION OF TEMPERATURE

220 385

360

FIGURURE 177

VOLATILITY OF $(C_2H_5O)_2POF$
AS A FUNCTION OF TEMPERATURE

220 396

361

FIGURE 179

VOLATILITY OF $(C_3H_7O)_2POF$
AS A FUNCTION OF TEMPERATURE

362

NOTE:
 a.....Liquid cell 0.028 mm
 b.....Liquid cell 0.01 mm
 c.....Gas cell 0.5 cm 7 mm Hg
 Perkin-Elmer Infrared Spectrometer

FIGURE 180

INFRARED ABSORPTION SPECTRA OF $C_5F_9(C_2F_5)$

note - there is
 no pg 390
 220 389

FIGURE 181

DENSITY OF $C_6H_5CF_3$
AS A FUNCTION OF TEMPERATURE
(Johns Hopkins Sample)

363

220-390
FROM THIS LABORATORY

FIGURE 182
REFRACTIVE INDEX OF $C_6H_5CF_3$
AS A FUNCTION OF TEMPERATURE
(Johns Hopkins Sample)

220-391

FROM THIS LABORATORY

364

FIGURE 183

VAPOR PRESSURE OF $C_6H_5CF_3$
AS A FUNCTION OF TEMPERATURE
(Johns Hopkins Sample)

220-392

365

FROM THIS LABORATORY

366

FIGURE 184

VISCOSITY OF $C_6H_5CF_3$
AS A FUNCTION OF TEMPERATURE
(Johns Hopkins Sample)

FROM THIS LABORATORY

220-393

367

FIGURE 185

SURFACE TENSION OF $C_6H_5CF_3$ AS A FUNCTION OF TEMPERATURE
(Johns Hopkins Sample)

FROM THIS LABORATORY

220-394

FIGURE 186
SURFACE TENSION OF $C_6H_5CF_3$
AS A FUNCTION OF DENSITY
(Johns Hopkins Sample)

FROM THIS LABORATORY

220 395

369

NOTES:

- a....Liquid cell 0.013 mm
- b....Gas cell 10 cm 2 mm Hg
- c....Liquid cell 0.256 mm
- d....Liquid cell 3.91 mm

Perkin-Elmer Infrared
Spectrometer

Measurements made at room
temperature

FIGURE 187

INFRARED ABSORPTION SPECTRA OF $C_6H_5CF_3$

FROM THIS LABORATORY

220 396

FIGURE 188

DENSITY OF $C_6F_9Cl(CF_3)_2$
AS A FUNCTION OF TEMPERATURE

FIGURE 189

REFRACTIVE INDEX OF $C_6F_9Cl(CF_3)_2$
AS A FUNCTION OF TEMPERATURE

220 398

FROM THIS LABORATORY

DECLASSIFIED

372

373

FIGURE 191

VISCOSITY OF $C_6F_9Cl(CF_3)_2$
AS A FUNCTION OF TEMPERATURE

220 400

FROM THIS LABORATORY

374

FIGURE 192 .

SURFACE TENSION OF $C_6F_9Cl(CF_3)_2$ AS A FUNCTION OF TEMPERATURE

FROM THIS LABORATORY

220 401

FIGURE 193

SURFACE TENSION OF $\text{C}_6\text{F}_9\text{Cl}(\text{CF}_3)_2$
AS A FUNCTION OF DENSITY

220 402

FROM THIS LABORATORY

376

FIGURE 194

ULTRASONIC VELOCITY IN $C_6F_9Cl(CF_3)_2$ AS A FUNCTION OF TEMPERATURE

377

NOTES:

- a....Liquid cell 0.013 mm
- b....Gas cell 10 cm 10 mm Hg
- c....Gas cell 10 cm 27 mm Hg
- d....Liquid cell 0.256 mm
- e....Liquid cell 0.136 mm
- f....Liquid cell 3.91 mm

Perkin-Elmer Infrared Spectrometer

Measurements made at room temperature

FIGURE 195

INFRARED ABSORPTION SPECTRA OF $C_8F_{16}Cl$

FROM THIS LABORATORY

4471 222

378

FIGURE 196

DENSITY OF $C_6F_9(CF_3)_3$
AS A FUNCTION OF TEMPERATURE

379

FIGURE 197

VISCOSITY OF $C_6F_9(CF_3)_3$
AS A FUNCTION OF TEMPERATURE

220 476