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Spectroscopic Library for Alternative Refrigerant Analysis

Thomas J. Bruno

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List of Abbreviations and Symbols

CAS	Chemical Abstracts Service
LEL	Lower Explosive Limit
NA	Not available
NE	Not established
PEL	Permissible Exposure Level (OSHA)
TLV	Threshold Limit Value (ACGIH, see Appendix 2)
UEL	Upper Explosive Limit
*	Indicates calculated values of critical parameters

SPECTROSCOPIC LIBRARY FOR ALTERNATIVE REFRIGERANT ANALYSIS

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Abstract

This Special Publication contains infrared and mass spectra for a wide range of chloro–fluoro–bromo ethanes and ethylenes that are relevant to research on alternative refrigerants. Alternative refrigerants are working fluids that are thought not to contribute significantly to atmospheric ozone depletion. In addition to the spectroscopic data, some physical property and safety information is included for each fluid as well. Not all of the compounds covered in this publication can be used as refrigerants. Indeed, some of them are, in fact, solids under ambient conditions, and others are fully halogenated, thus making them unfavorable from an ozone depletion standpoint. The study of all of these materials is important, however, since many will be found as impurities or reaction/decomposition products of refrigerant fluids. This publication provides a single source for some particularly useful analytical information needed in the identification of these compounds.

Key words: alternative refrigerants; chemical analysis; infrared spectrophotometry; mass spectrometry; safety.

Introduction

In recent years, ozone depletion has become the topic of a great deal of intensive scientific research. One aspect of this research is the development of safe substitutes for fully halogenated chlorofluorcarbon fluids which have been used as refrigerants and propellants. These new materials are now called alternative refrigerants. To properly evaluate the potential of any new working fluid for a refrigeration cycle or propellant application, a complete set of thermophysical property data is required. This will allow the relevant engineering properties of these materials to be mathematically modeled or correlated using some form of an equation of state. The models will then provide a predictive capability over an extensive range of conditions.

In order to provide a large enough database for correlation, the measurement of the relevant thermophysical properties often extends into relatively severe areas of temperature and pressure. This is necessary despite the fact that a working fluid may not be subject to such severe conditions in a typical engineering application. High temperatures and pressures are cause for concern in experimental thermophysics, since there is a significant potential for chemical reactions and decomposition of the fluids being studied. It has been recognized in recent years that the possibility of chemical reactivity must be addressed early in the design of a measurement program, and a sampling and analysis protocol must be built into the program. A detailed description of the NIST protocol for measurements on reactive fluids is available elsewhere [1,2], and will not be repeated here.

Note: Certain commercial equipment, instruments, or materials are identified in this Special Publication in order to provide an adequate description. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

Aside from the temperature and pressure of an experiment, the chemical nature of the fluids themselves must be considered. The fluids that are not fully halogenated appear to be moderately reactive toward many metals. This includes many common component construction materials such as aluminum. In the presence of many finely divided or powdered metals, some of the fluids react vigorously, even violently. In the presence of water, some tend to slowly hydrolyze. Several of the ethylene based fluids react violently in the presence of air. The reaction products of these fluids are potentially dangerous. At elevated temperatures hydrogen fluoride, hydrogen chloride, phosgene, and carbonyl halides, as well as carbon monoxide and carbon dioxide, can form upon the disproportionation of many alternative refrigerant fluids. The temperature range at which reactions begin can be surprisingly low, often between 140 and 160 °C. In addition to thermal decomposition and reactions with metals and oxidants, alternative refrigerant fluids are known to be somewhat aggressive toward elastomeric materials, much more so than the older refrigerants soon to be replaced. Since elastomerics are used extensively in refrigeration and air conditioning process components, the application of extensive chemical analysis programs to alternative refrigerant work is unavoidable.

This collection of infrared and mass spectra has been assembled to assist the experimenter working on alternative refrigerants in the identification of contaminants and reaction products. The compounds are listed by the appropriate American Society of Heating, Refrigerating and Air–Conditioning Engineers (ASHRAE) number and systematic chemical name. The synonyms listed are common or generic names, trade names, or systematic chemical names which may be technically incorrect but which are often encountered either in the older scientific literature or manufacturer/trade literature. A guide to the refrigerant numbering system is provided in Appendix 3. Other physical properties which are relevant to chemical analysis have been included where possible. The sources of these data are listed in Appendix 2. Where they are available, experimental values for the critical parameters are given. When measured critical properties are not available, they have been calculated using the group contribution method of Lydersen, which is described in Appendix 1. The calculated values are denoted by an asterisk. The specific gravity values cited include the temperature of the fluid relative to the temperature of water. When only one temperature is cited, the value is a density value, rather than specific gravity. In some instances, when ambiguity is possible, the state of matter is included. The refractive index values include the temperature and state of matter of the fluid when appropriate. The values for vapor density (at ambient temperature and pressure, unless otherwise indicated) are, with respect to air, assigned a value of 1 by definition. In rare instances, the vapor density is provided in g/mL. The vapor pressures of the fluids have not been included because there is often very significant disagreement among the values cited in the literature. The normal boiling point of each fluid is included, however.

The mass spectra were recorded using a mass selective detector interfaced to a capillary column gas chromatograph. Retention indices and chromatographic parameters have not been included, since separation methods are usually developed and optimized individually for each application. The mass spectrometer operated in electron impact mode, and a quadrupole sector provided mass filtration. Calibration and tuning was done using perfluorotributylamine. The spectra are presented as normalized histograms versus mass/charge, and are also tabulated as mass/charge versus ion current (in arbitrary units). For the sake of clarity, the common contaminant peaks, such as m/e=32 for oxygen and m/e=28 for nitrogen, have been deleted from both the histograms and the tabulations. The infrared spectra were obtained using a ratio recording energy dispersive spectrophotometer. Sodium chloride optics were used in all sample cells. Neat samples (without solvent) were measured in either a liquid or gas cell, depending upon the vapor pressure of the fluid.

The toxicology of each fluid was searched in a variety of sources, all of which are summarized in Appendix 2. When the toxicology is listed as being unknown, or not known in detail, it is ABSOLUTELY ESSENTIAL that the user apply precautions appropriate for a highly hazardous substance [3]. In no case should the lack of detailed information on a fluid be considered reason to treat the fluid with anything but extreme caution. Since SI units are used throughout the body of the text of this Special Publication, a conversion table is provided in Appendix 4 to allow the user to easily convert to the appropriate inch–pound units. Definitions of terms used in this Special Publication are provided in the Glossary.

The financial support of the U.S. Department of Energy, Office of Buildings and Community Systems, is gratefully acknowledged. The assistance of Stephanie L. Outcalt, Laurell R. Phillips, Wesley Breshears, and Douglas Farmer (all of the National Institute of Standards and Technology) in the preparation of this publication is also gratefully acknowledged. The author would like to acknowledge the assistance of the Mountain Administrative Support Center Library, especially librarians Jean M. Bankhead and Jane Watterson.

References

[1] Bruno, T. J., Hume, G. L., J. Res. Natl. Bur. Stand., (U.S.), 90(3), 255, 1985.

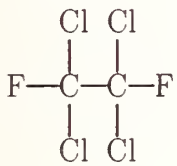
[2] Bruno, T. J., Straty, G. C., J. Res. Natl. Bur. Stand., (U.S.), 91(3), 135, 1986.

[3] Bruno, T. J., Strategy for Chemical Analysis of Alternative Refrigerants, Tech. Note 1340, Natl. Inst. Stand. Tech., (U.S.), May 1990.

112 1,2-difluoro-1,1,2,2-tetrachloroethane

synonyms: 1,2–difluoro–1,1,2,2–tetrachloroethane.

structure:



C. A. S. Registry Number: 76–12–0
Relative Molecular Mass: 203.83

Normal Boiling Point: 92.8 °C

Melting Point: 23.8 °C

Density/Specific Gravity: 1.634 (30/4)

Critical Temperature: 278 °C

Refractive Index: 1.4130

Critical Pressure: 4.83 MPa*

Critical Density: 0.754 g/mL*

****

Vapor Density: >1

PEL: NE

TLV: NE

Flash Point: NA

UEL: NA

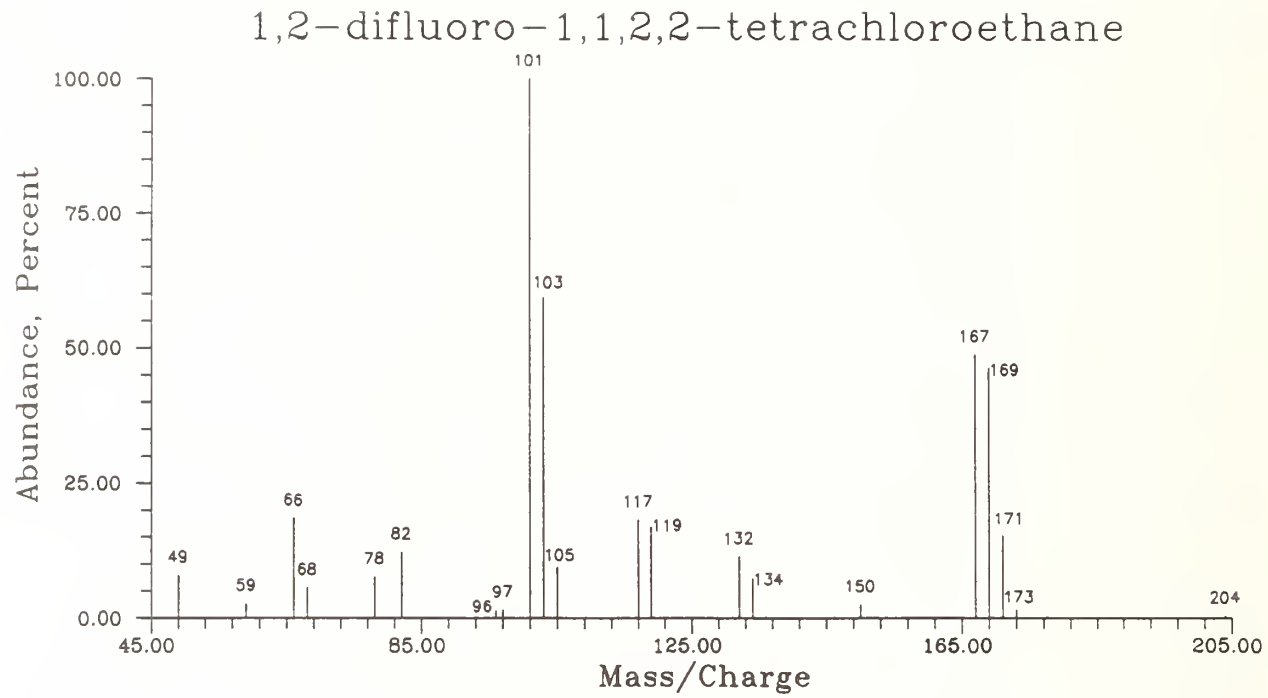
LEL: NA

Toxicology: May cause cardiac arrhythmia, pulmonary edema, conjunctivitis.

Reactivities and Chemical Incompatibilities: Thermal decomposition may produce HCl and HF; avoid contact with active metals.

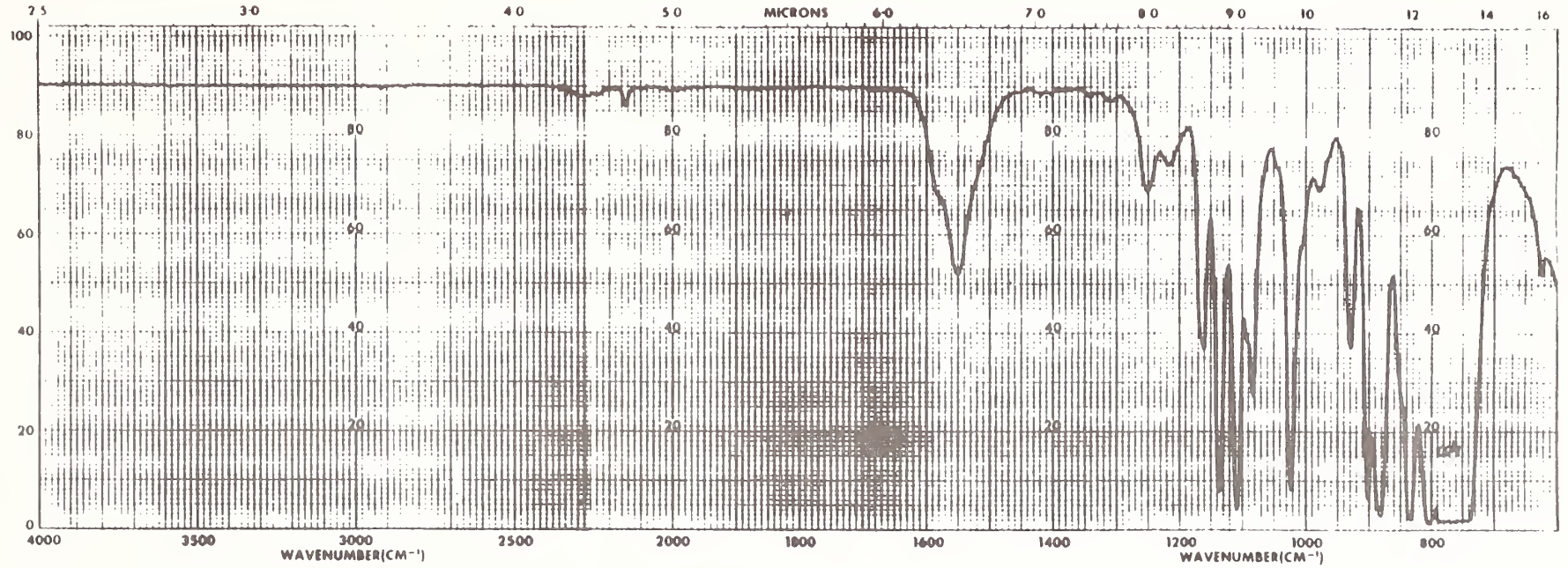
Solubilities: Somewhat soluble in alcohols, ether, chloroform, carbon tetrachloride; H_2O: 0.01 percent at 25 °C.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
35.00	208449	68.00	51952	101.00	923935	134.00	67607
37.00	67832	78.00	70718	103.00	547993	150.00	23200
40.00	26573	82.00	112418	105.00	87869	167.00	449404
47.00	225030	84.00	75951	117.00	168051	169.00	427661
49.00	72700	94.00	18190	119.00	155609	171.00	141961
59.00	24948	96.00	12636	121.00	51755	173.00	14610
66.00	170477	97.00	13451	132.00	105264	204.00	3779

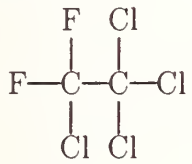
Infrared Spectrum – carbon tetrachloride solution



112a 1,1-difluorotetrachloroethane

synonyms: tetrachloro–1,1–difluoroethane; 2,2–diflorotetrachloroethane.

structure:



C. A. S. Registry Number: 76–11–9
Relative Molecular Mass: 203.83

Normal Boiling Point: 91.5 °C

Melting Point: 40.6 °C

Density/Specific Gravity: 1.649 (20/4)

Critical Temperature: 279.2 °C*

Refractive Index:

Critical Pressure: 4.83 MPa*

Critical Density: 0.754 g/mL*

****

Vapor Density: >1

PEL: NE

TLV: 500 ppm

Flash Point: NA

UEL: NA

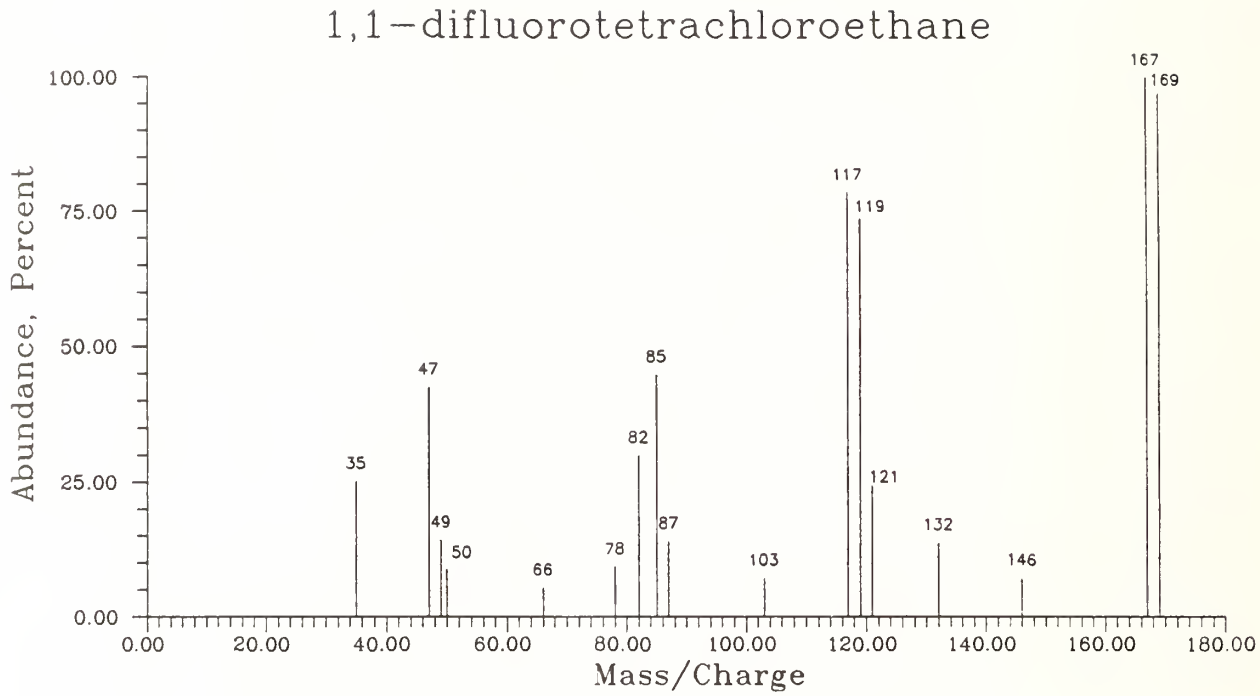
LEL: NA

Toxicology: Detailed toxicology not available; may be mildly irritating to eyes and skin; may be narcotic.

Reactivities and Chemical Incompatibilities: Thermal decomposition can produce HCl and HF; avoid contact with active metals and powdered metals such as Al, Zn, Be.

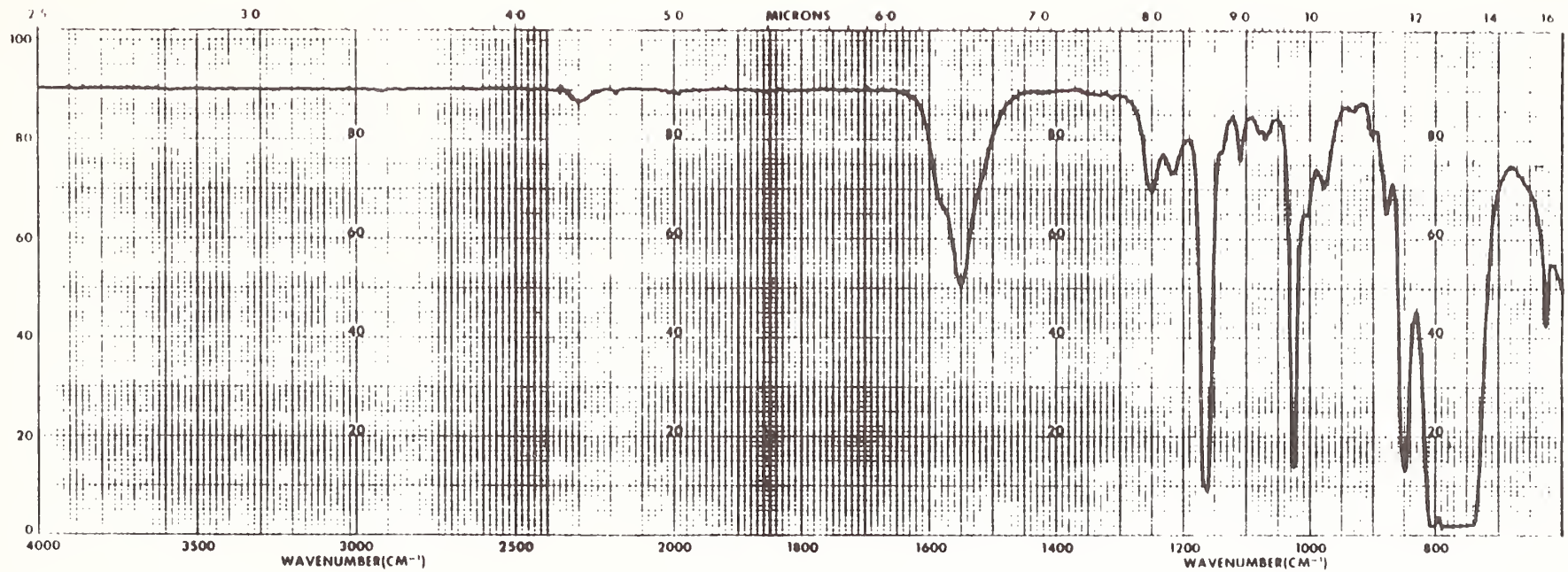
Solubilities: Somewhat soluble in alcohols, ether, chloroform and carbon tetrachloride; negligible solubility in water.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
35.00	105264	50.00	36829	87.00	58572	121.00	101804
37.00	34524	59.00	9798	103.00	29795	132.00	57646
40.00	31814	66.00	22210	113.00	10607	146.00	29700
43.00	12644	78.00	38730	117.00	330929	167.00	421760
47.00	178274	82.00	125384	119.00	310191	169.00	409620
49.00	59407	85.00	188345				

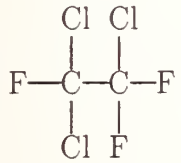
Infrared Spectrum — carbon tetrachloride solution



113 1,1,2-trichlorotrifluoroethane

synonyms: 1,1,2–trichloro–1,2,2–trifluoroethane; Ucon 113; Genetron 113; TTE; trichlorotrifluoroethane; 1,2,2–trifluorotrichloroethane; 1,2,2–trifluoro– 1,1,2–trichloroethane.

structure:



C. A. S. Registry Number: 76–13–1
Relative Molecular Mass: 187.38

Normal Boiling Point: 47.6 °C

Melting Point: –35.0 °C

Density/Specific Gravity: 1.553 g/mL (30 °C)

Critical Temperature: 214.1 °C

Refractive Index: 1.3557 (25 °C)

Critical Pressure: 3.42 MPa

Critical Density: 0.576 g/mL

****

Vapor Density: 2.9

PEL: 1000 ppm

TLV: 1000 ppm

Flash Point: nonflammable

UEL: NE

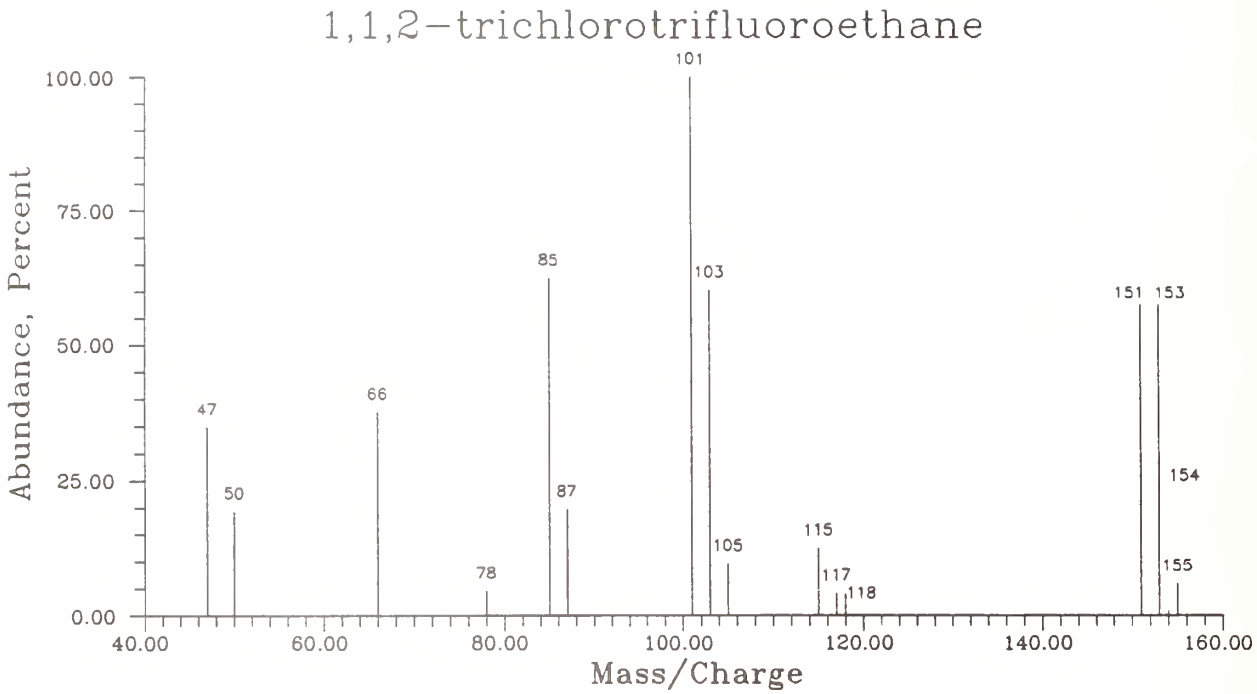
LEL: NE

Toxicology: Relatively low toxicity; anesthetic effect above 10 percent vol/vol air.

Reactivities and Chemical Incompatibilities: Relatively low reactivity; may form CO, CO_2, HF and phosgene upon thermal decomposition; avoid contact with alkali and alkaline earth metals, and powdered metals such as Al, Zn, Be.

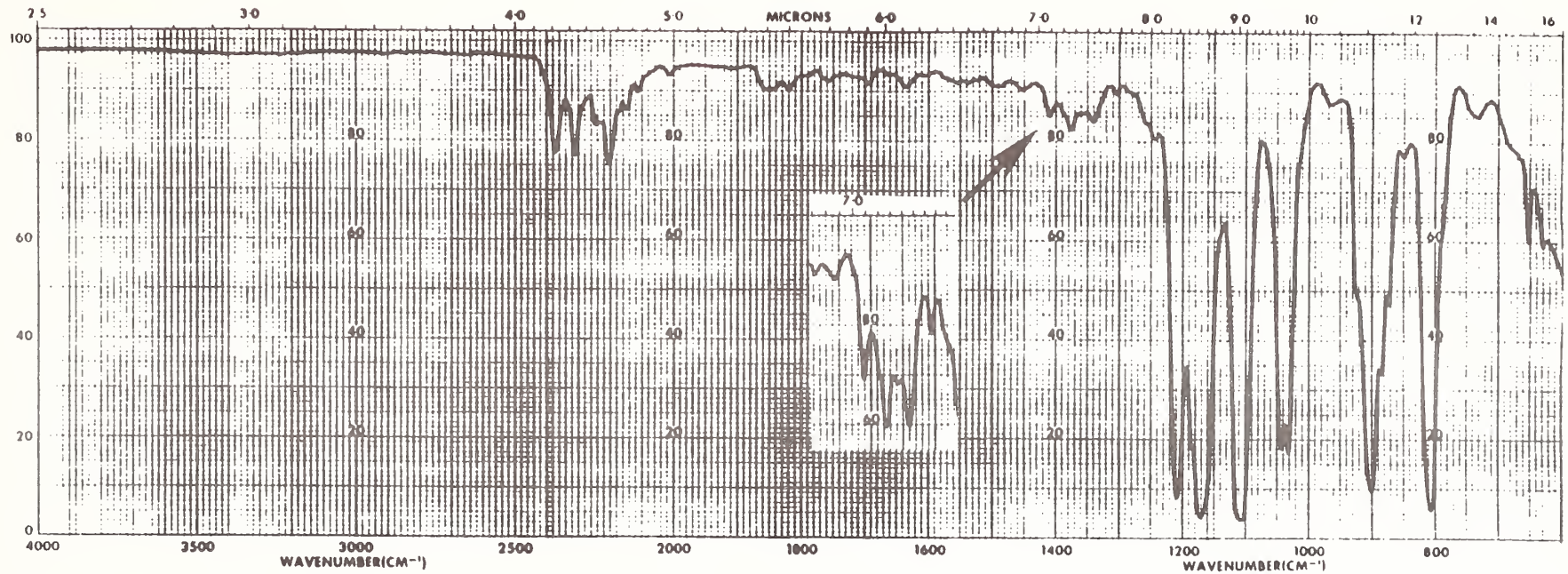
Solubilities: Soluble in alcohols, ether, benzene; H_2O: 30 °C – 0.013 percent, 0 °C – 0.0036 percent by weight.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
50.00	118339	78.00	27733	105.00	58582	134.00	10636
59.00	14712	85.00	382501	116.00	76500	151.00	352973
62.00	16374	87.00	119944	117.00	25402	153.00	224945
66.00	229929	101.00	613640	118.00	24071	154.00	5860
68.00	72188	103.00	368834	132.00	16834	155.00	35869

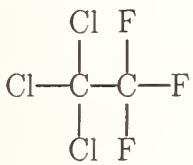
Infrared Spectrum — Liquid Phase (no solvent)



113a 1,1,1-trichloro-2,2,2-trifluoroethane

synonyms: trichlorotrifluoroethane; precision cleaning agent; TF; T–WD602; CFE.

structure:



C. A. S. Registry Number: 354–58–5
Relative Molecular Mass: 187.58

Normal Boiling Point: 45.7 °C

Melting Point: 14.2 °C

Density/Specific Gravity: 1.5792 (20/4)

Critical Temperature: 209.2 °C*

Refractive Index: 1.3610, l, (25 °C)

Critical Pressure: 4.88 MPa*

Critical Density: 0.769 g/mL*

****

Vapor Density: NA

PEL: 1000 ppm

TLV: 1000 ppm

Flash Point: will not flash

UEL: NA

LEL: NA

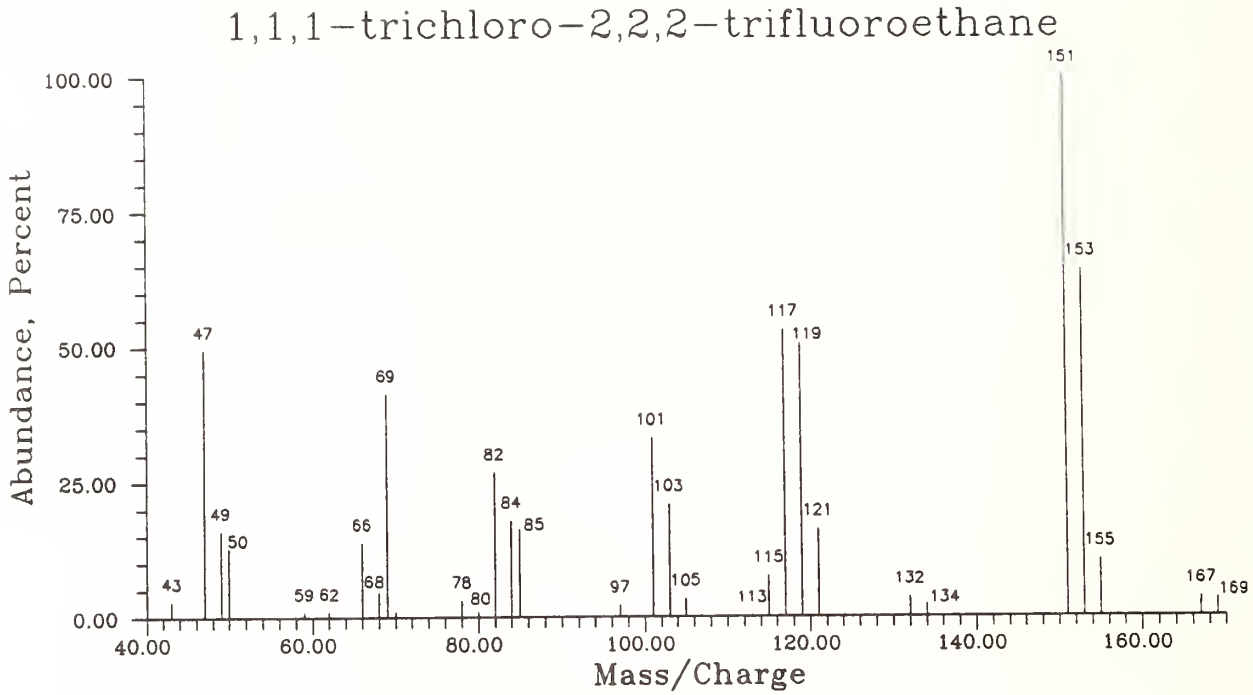
Autoignition temperature 680 °C

Toxicology: Overexposure can cause epinephrine sensitization of the heart; detailed toxicology is not available.

Reactivities and Chemical Incompatibilities: Can produce HF and HCl upon thermal decomposition; avoid contact with active metals.

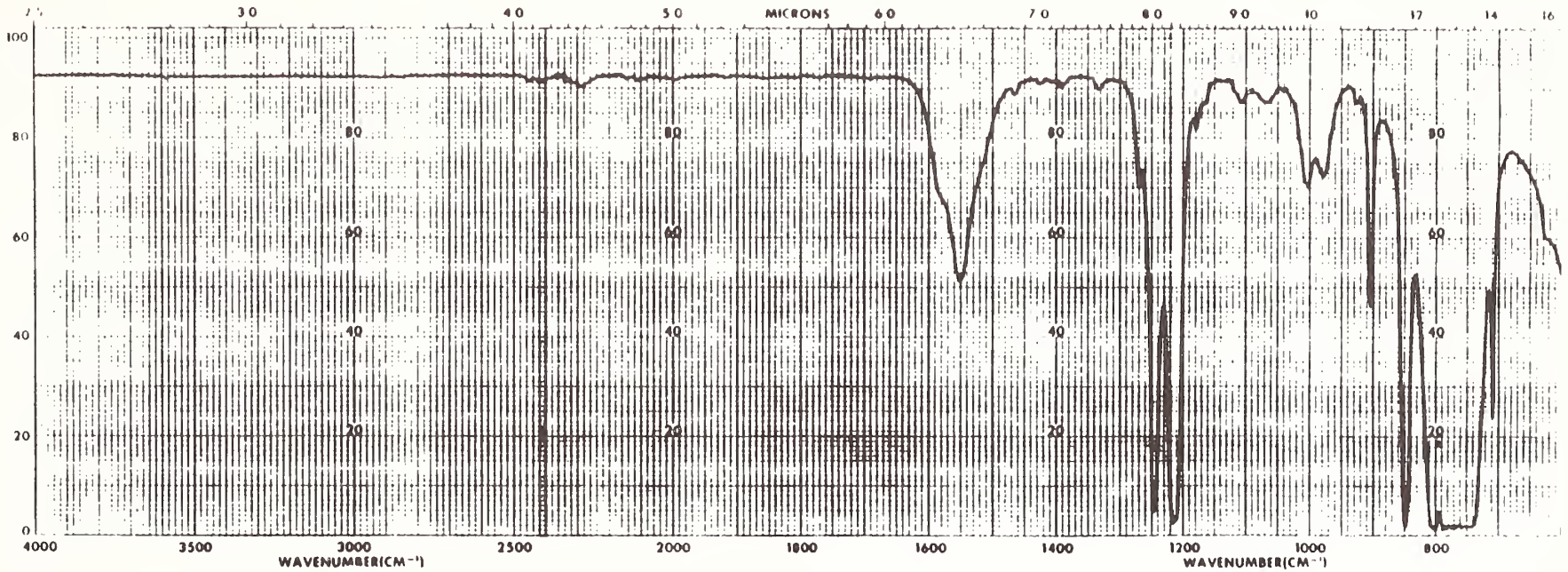
Solubilities: Somewhat soluble in alcohols, ether, chloroform, carbon tetrachloride; negligible solubility in water.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
43.00	33062	69.00	477624	101.00	382613	132.00	41242
47.00	570736	70.00	10712	103.00	239631	134.00	26817
49.00	183496	78.00	35233	105.00	37778	151.00	1156075
50.00	147848	80.00	11636	113.00	1214	153.00	740271
59.00	10753	82.00	308653	116.00	86812	155.00	120312
62.00	11309	84.00	206507	117.00	612060	167.00	40504
66.00	159446	85.00	187528	119.00	583668	169.00	37527
68.00	53140	97.00	23714	121.00	186697		

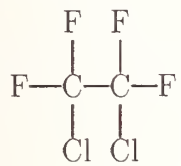
Infrared Spectrum – carbon tetrachloride solution



114 1,2-dichlorotetrafluoroethane

synonyms: dichlorotetrafluoroethane; sym–dichlorotetrafluoroethane; Fluorane 114; Genetron 114; Genetron 316; Ledon 114; halocarbon 114; Frigen 114.

structure:



C. A. S. Registry Number: 76–14–2
Relative Molecular Mass: 170.91

Normal Boiling Point: 3.77 °C

Melting Point: –94 °C

Density/Specific Gravity: 1.456 g/mL (25 °C)

Critical Temperature: 145.7 °C

Refractive Index: 1.294 (25 °C)

Critical Pressure: 3.26 MPa

Critical Density: 0.582 g/mL

****

Vapor Density: 5.93

PEL: 1000 ppm

TLV: 1000 ppm

Flash Point: does not flash

UEL: NA

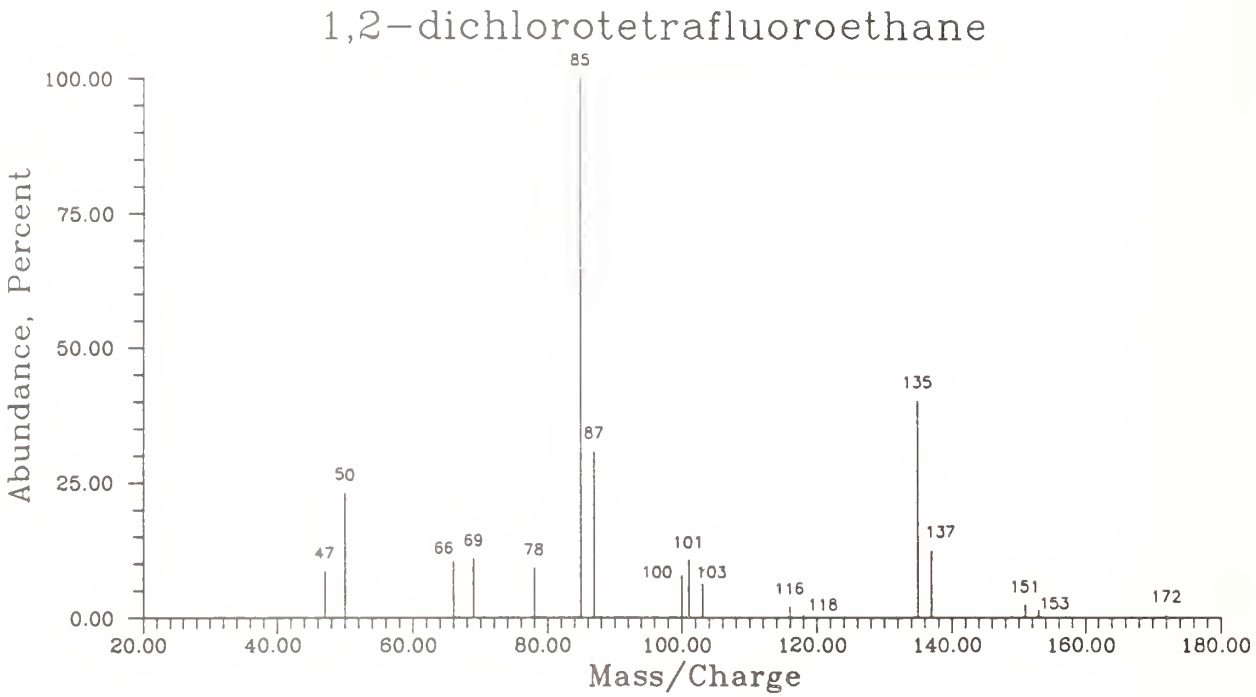
LEL: NA

Toxicology: Moderate concentrations can cause nausea, dizziness, disorientation; narcotic at high concentrations.

Reactivities and Chemical Incompatibilities: May produce HCl, HF, CO, CO_2 upon thermal decomposition; avoid contact with active metals.

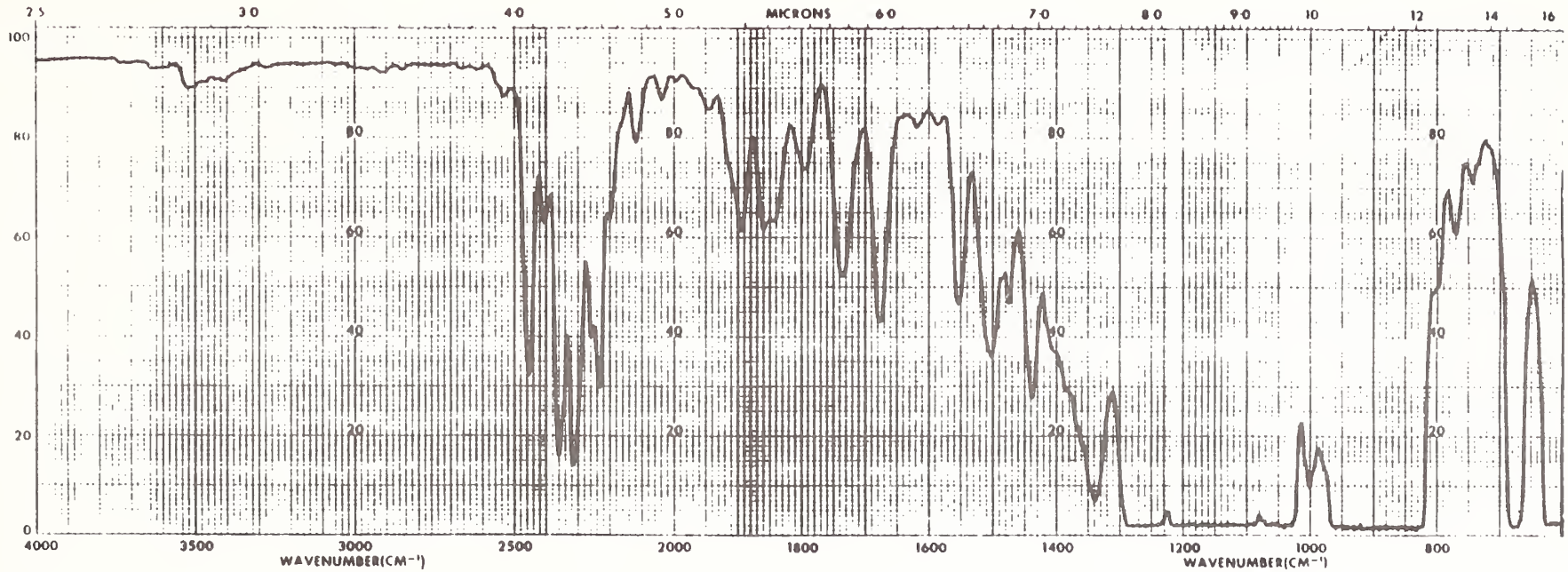
Solubilities: Somewhat soluble in carbon tetrachloride; H_2O: 0.013 percent by weight, 25 °C.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	1592218	51.00	6965	81.00	11410	116.00	51081
35.00	546798	62.00	26121	85.00	2690774	118.00	15438
37.00	179379	66.00	279293	87.00	826667	135.00	1079785
40.00	33831	69.00	292513	97.00	5612	137.00	330475
43.00	43291	70.00	7406	100.00	210429	151.00	63559
47.00	231702	78.00	20617	101.00	285587	153.00	40479
50.00	622180	80.00	7133	103.00	167783	172.00	209

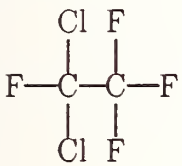
Infrared Spectrum – Gas Phase



114a 1,1-dichlorotetrafluoroethane

synonyms: dichlorotetrafluoroethane; 1,1–dichloro–1,2,2,2–tetrafluoroethane.

structure:



C. A. S. Registry Number: 374–07–2
Relative Molecular Mass: 170.92

Normal Boiling Point: 3.6 °C

Melting Point: –94 °C

Density/Specific Gravity: 1.440 g/mL, l, (30 °C)

Critical Temperature: 145.7 °C*

Refractive Index: 1.3092 (0 °C)

Critical Pressure: 4.92 MPa*

Critical Density: 0.820 g/mL*

****

Vapor Density: >1

PEL: NE

TLV: NE

Flash Point: does not flash

UEL: NA

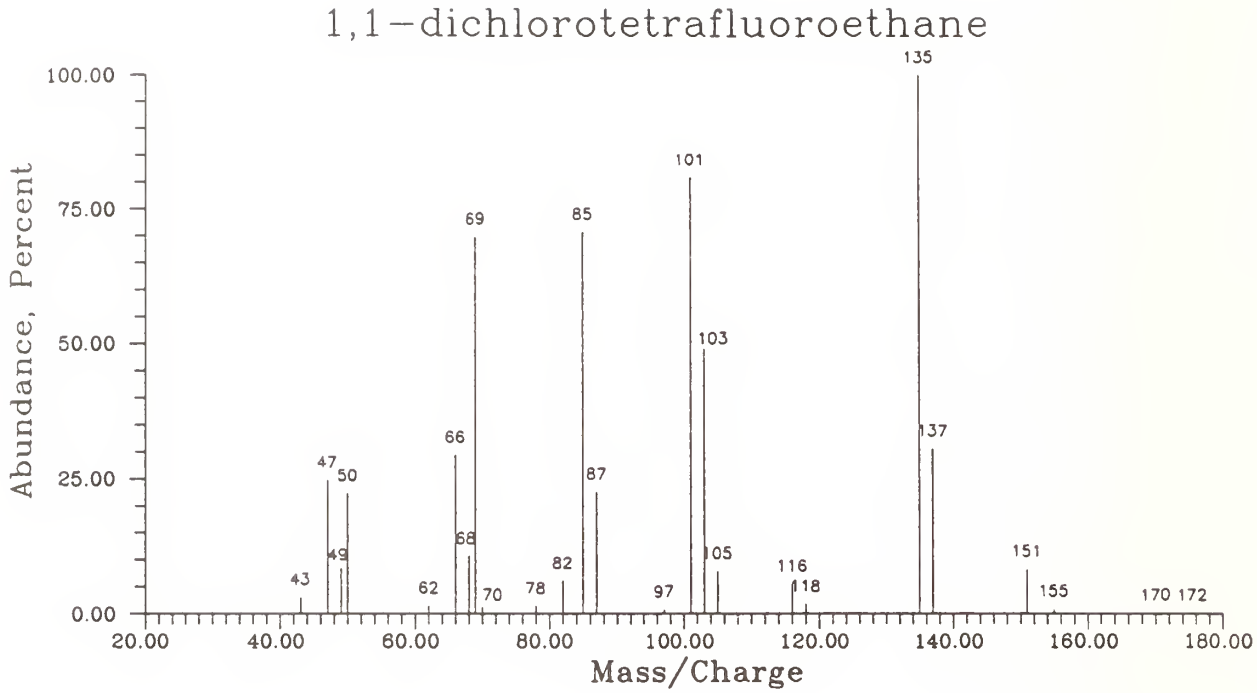
LEL: NA

Toxicology: May cause skin, eye and pulmonary irritation; may have anesthetic properties at high concentrations; narcotic at high concentrations; may aggravate existing heart conditions.

Reactivities and Chemical Incompatibilities: Thermal decomposition can produce HCl, HF, CO, CO_2; avoid contact with active metals; reacts violently with aluminum.

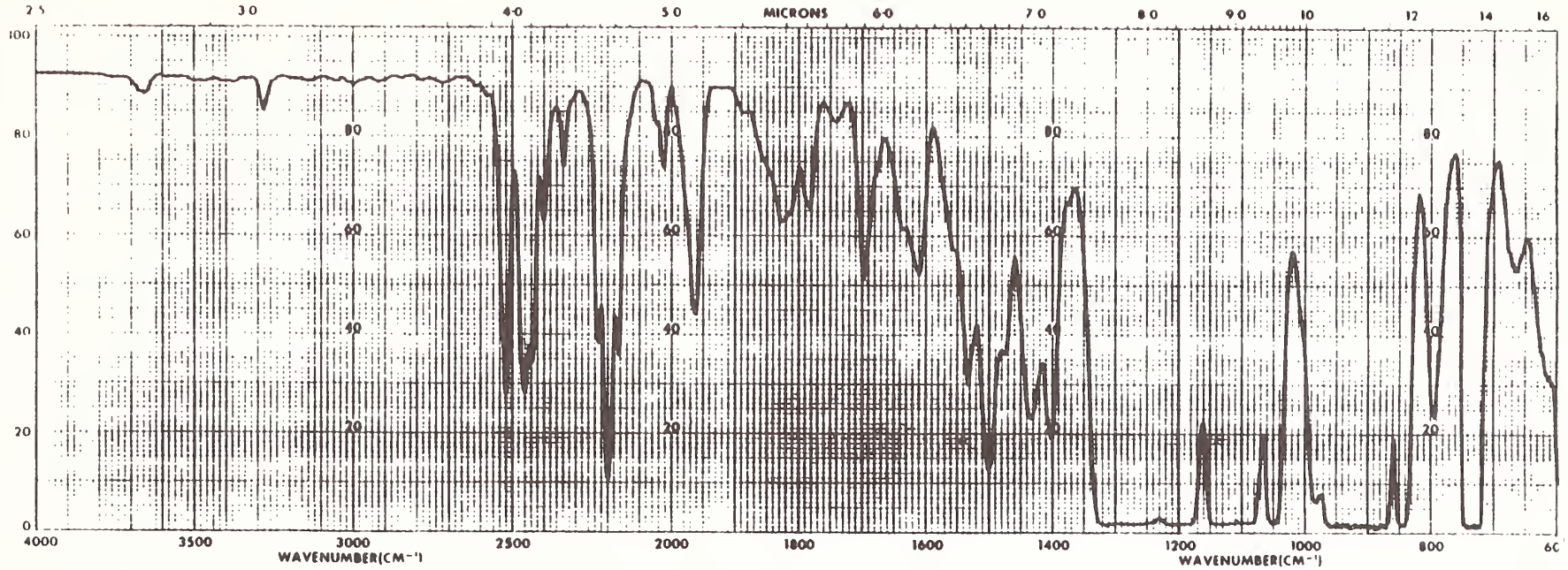
Solubilities: Somewhat soluble in alcohol, benezene, chloroform, ether, carbon tetrachloride.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	1839593	58.00	14908	82.00	106438	118.00	30177
35.00	647040	59.00	16452	85.00	1260452	135.00	1785336
37.00	200755	62.00	23950	87.00	400905	137.00	544151
40.00	29807	66.00	522614	97.00	11749	151.00	145633
43.00	52066	68.00	190189	101.00	1443151	153.00	94913
47.00	438884	69.00	1243685	103.00	873288	155.00	14444
49.00	150233	70.00	21439	105.00	138543	170.00	1364
50.00	3955528	78.00	23253	116.00	96936	172.00	687

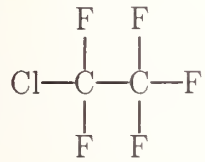
Infrared Spectrum – Gas Phase



115 chloropentafluoroethane

synonyms: monochloropentafluoroethane; Genetron 115.

structure:



C. A. S. Registry Number: 76–15–3
Relative Molecular Mass: 154.47

Normal Boiling Point: –38.7 °C

Melting Point: –106 °C

Density/Specific Gravity: 1.26 g/mL, l, (30 °C)

Critical Temperature: 79.9 °C

Refractive Index: 1.221 (25 °C)

Critical Pressure: 3.12 MPa

Critical Density: 0.596 g/mL

****

Vapor Density: 8.37 (at boiling point)

PEL: NE

TLV: 1000 ppm

Flash Point: nonflammable

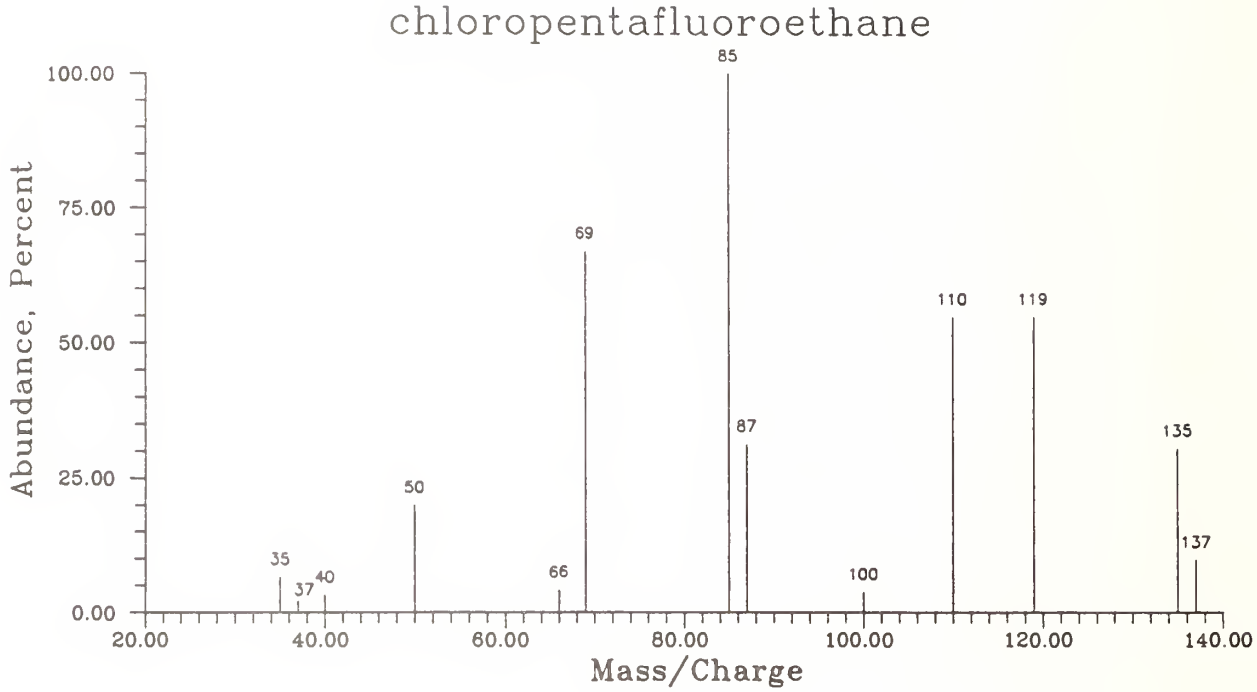
UEL: NA **LEL:** NA

Toxicology: Anesthetic at high concentrations, prolonged exposure results in unconsciousness.

Reactivities and Chemical Incompatibilities: Thermal decomposition can form HCl, HF; avoid contact with active metals and powdered metals such as Al, Zn, Be.

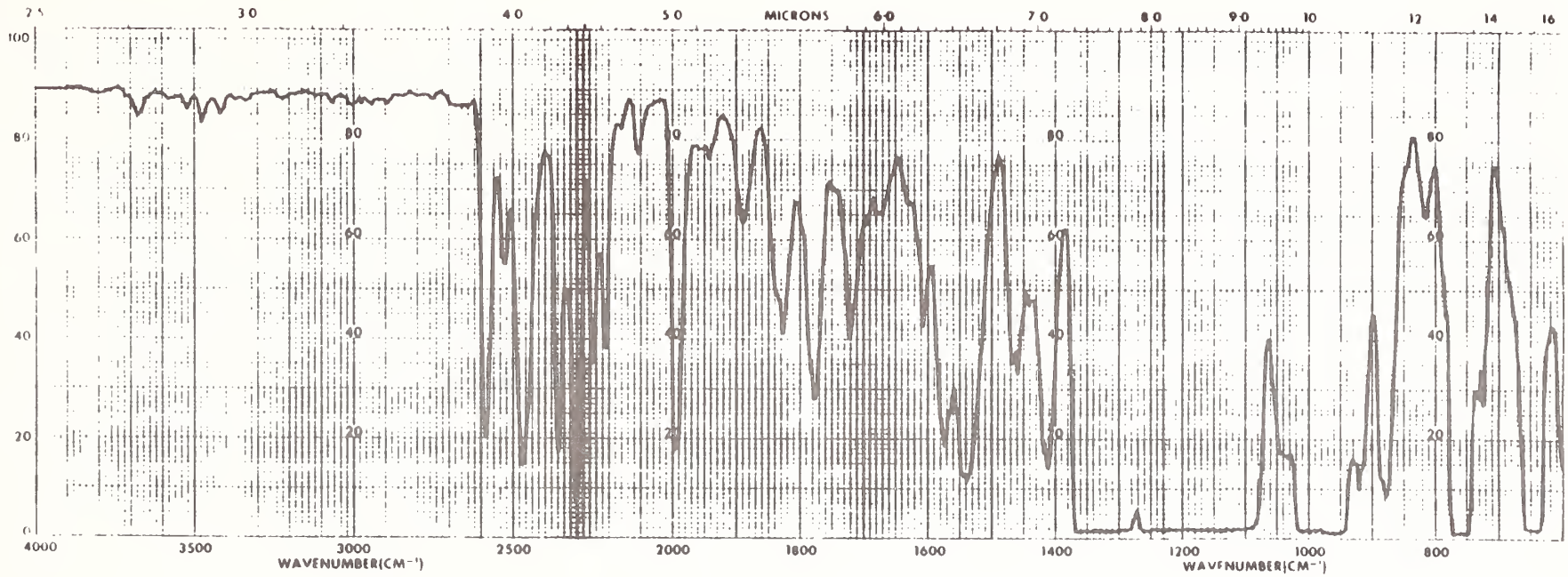
Solubilities: Somewhat soluble in alcohols, ether, and carbon tetrachloride; H_2O: 0.006 percent at 25 °C.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
35.00	99578	47.00	46202	69.00	1024291	119.00	836391
37.00	31821	49.00	11502	85.00	1532034	135.00	464217
40.00	48138	50.00	302875	87.00	475927	137.00	148434
44.00	7486	66.00	62016	100.00	56216		

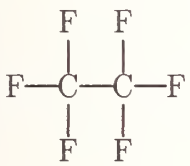
Infrared Spectrum – Gas Phase



116 hexafluoroethane

synonyms: perfluoroethane; UN 2193.

structure:



C. A. S. Registry Number: 76–16–4
Relative Molecular Mass: 138.01

Normal Boiling Point: 78.19 °C

Melting Point: –100.06 °C

Density/Specific Gravity:

Critical Temperature: 19.89 °C

Refractive Index:

Critical Pressure: 3.042 MPa

Critical Density: 0.622 g/mL^3

****

Vapor Density: NA

PEL: N/E

TLV: N/E

Flash Point: does not flash

UEL: N/A

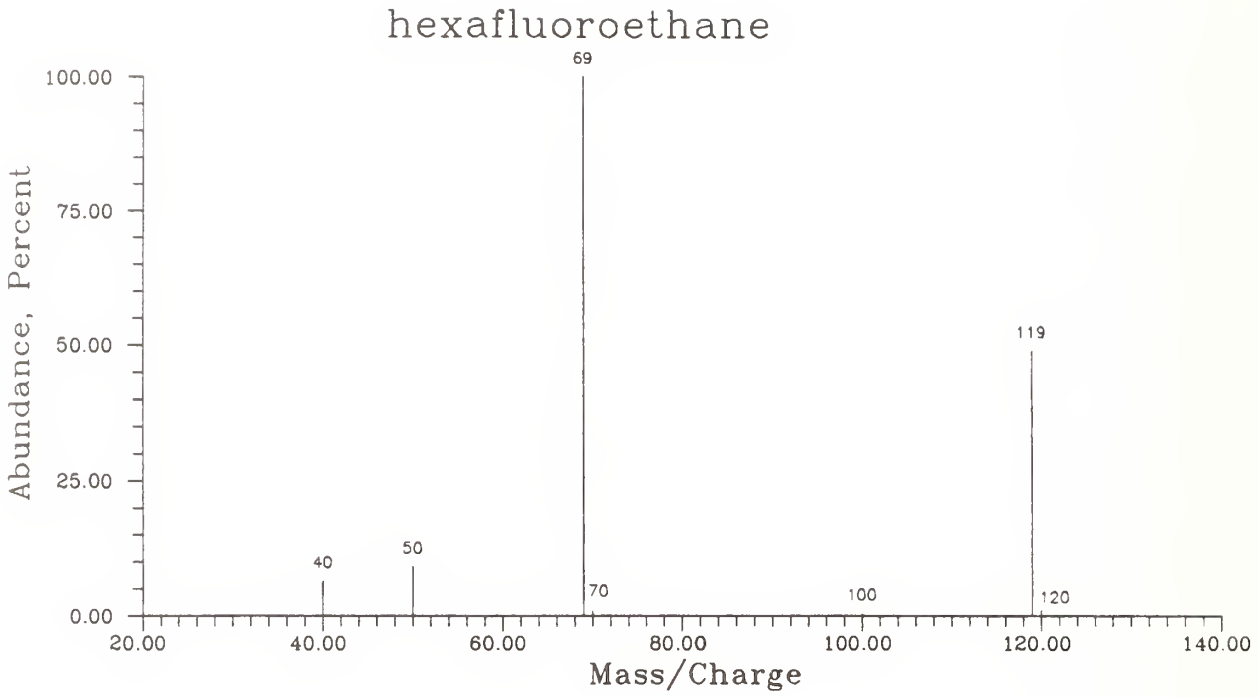
LEL: N/A

Toxicology: Can produce light–headedness, shortness of breath; moderate symptoms of intoxication are observed in rats; simple asphyxiant.

Reactivities and Chemical Incompatibilities: Forms toxic fumes at high temperatures; avoid contact with active metals, alkali or alkaline earth metals, and powdered metals such as Al, Zn, and Be.

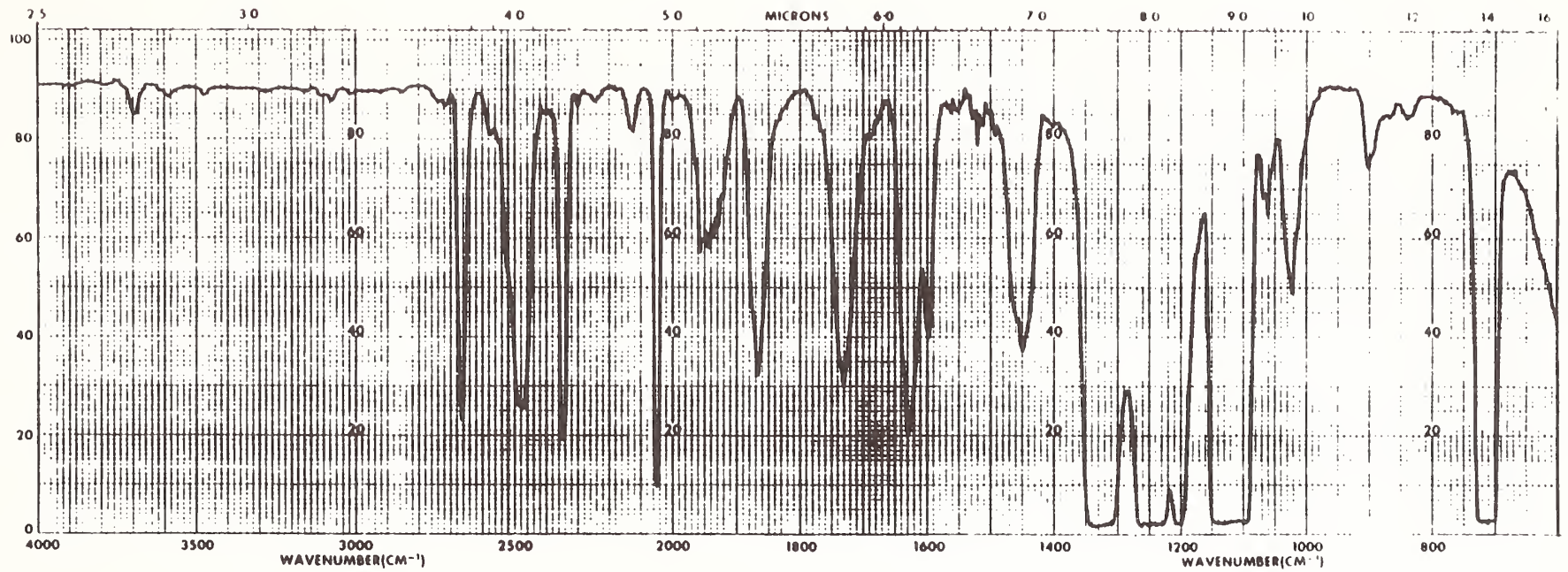
Solubilities: Very low solubility in water; slightly soluble in carbon tetrachloride and some alcohols.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	140890	50.00	81143	70.00	9063	119.00	433906
40.00	57697	69.00	885750	100.00	4450	120.00	9488

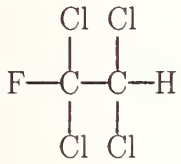
Infrared Spectrum – Gas Phase



121 1,1,2,2-tetrachlorofluoroethane

synonyms: tetrachlorofluoroethane; tetrachloromonofluoroethane; monofluorotetrachloroethane.

structure:



C. A. S. Registry Number: 354–14–3
Relative Molecular Mass: 185.8

Normal Boiling Point: 116.6 °C

Melting Point: –82.6 °C

Density/Specific Gravity: 1.622 (20/4)

Critical Temperature: 321.5 °C*

Refractive Index:

Critical Pressure: 4.45 MPa*

Critical Density: 0.613 g/mL*

****

Vapor Density: >1

PEL: NE

TLV: NE

Flash Point: NA

UEL: NA

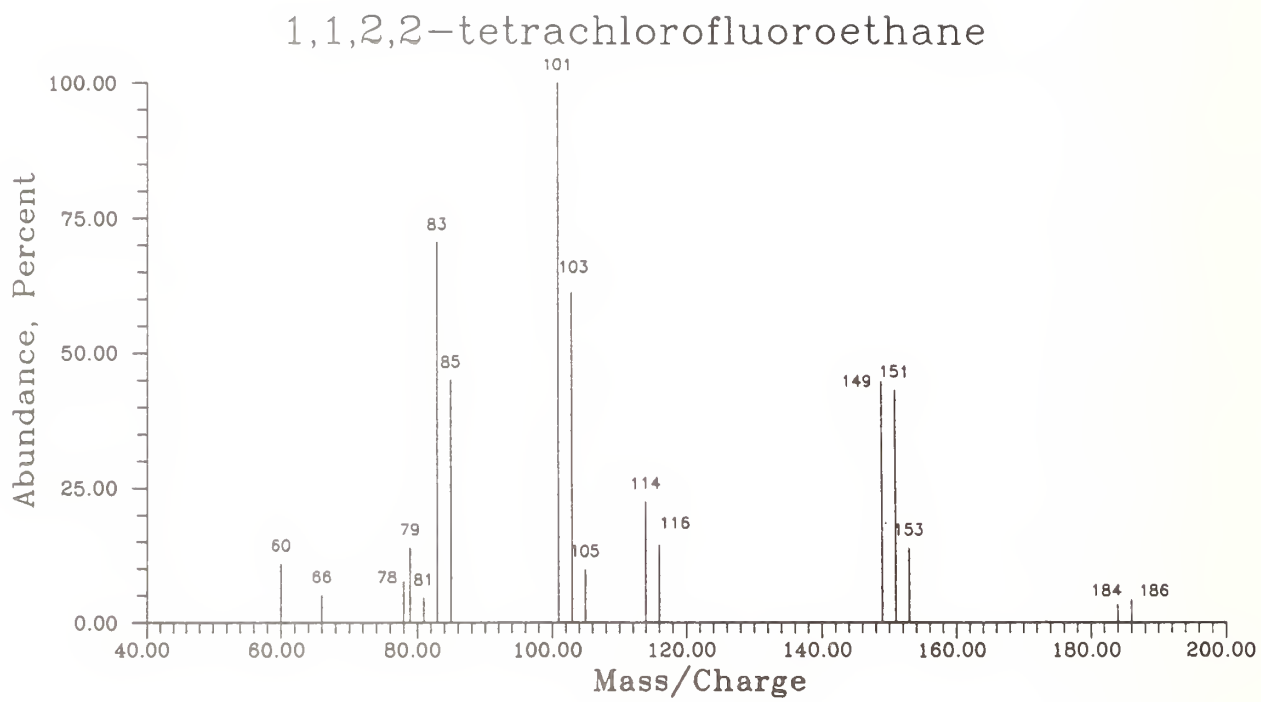
LEL: NA

Toxicology: May be anesthetic at high concentrations; detailed toxicology not available.

Reactivities and Chemical Incompatibilities: May form HCl and HF on thermal decomposition, as well as CO, CO_2; avoid contact with active metals.

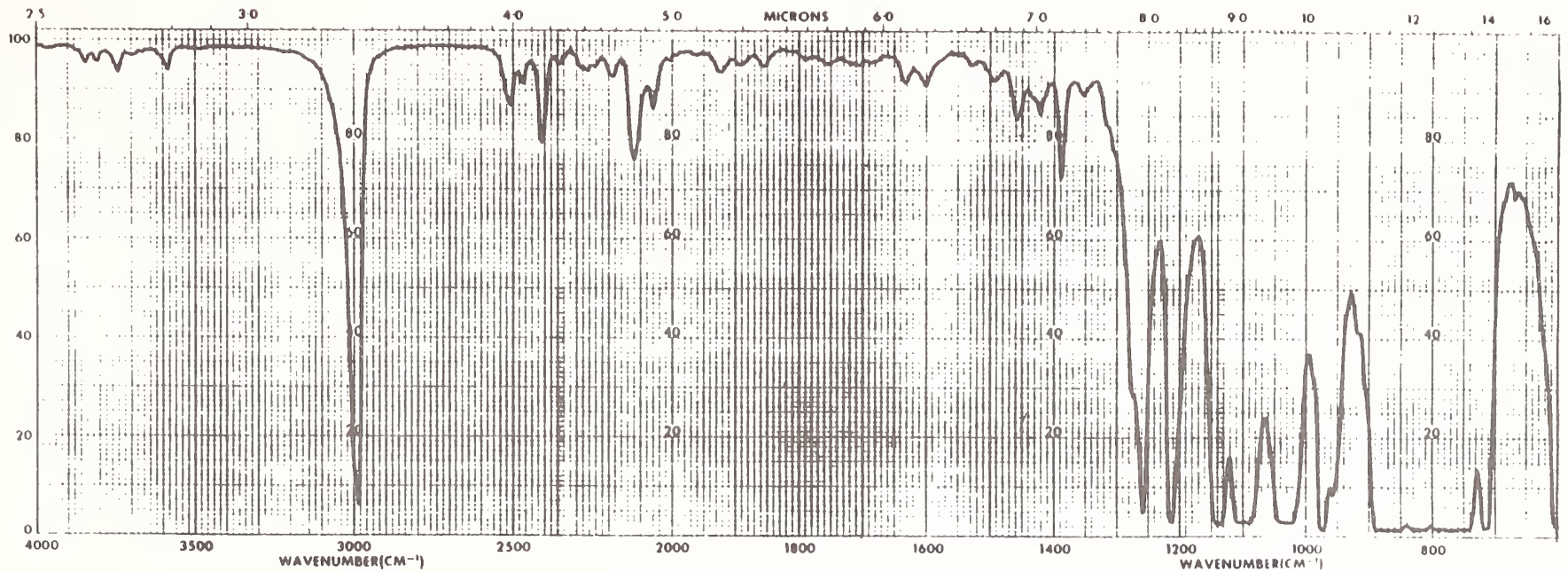
Solubilities: Somewhat soluble in carbon tetrachloride; negligible solubility in water.

Mass Spectrum:

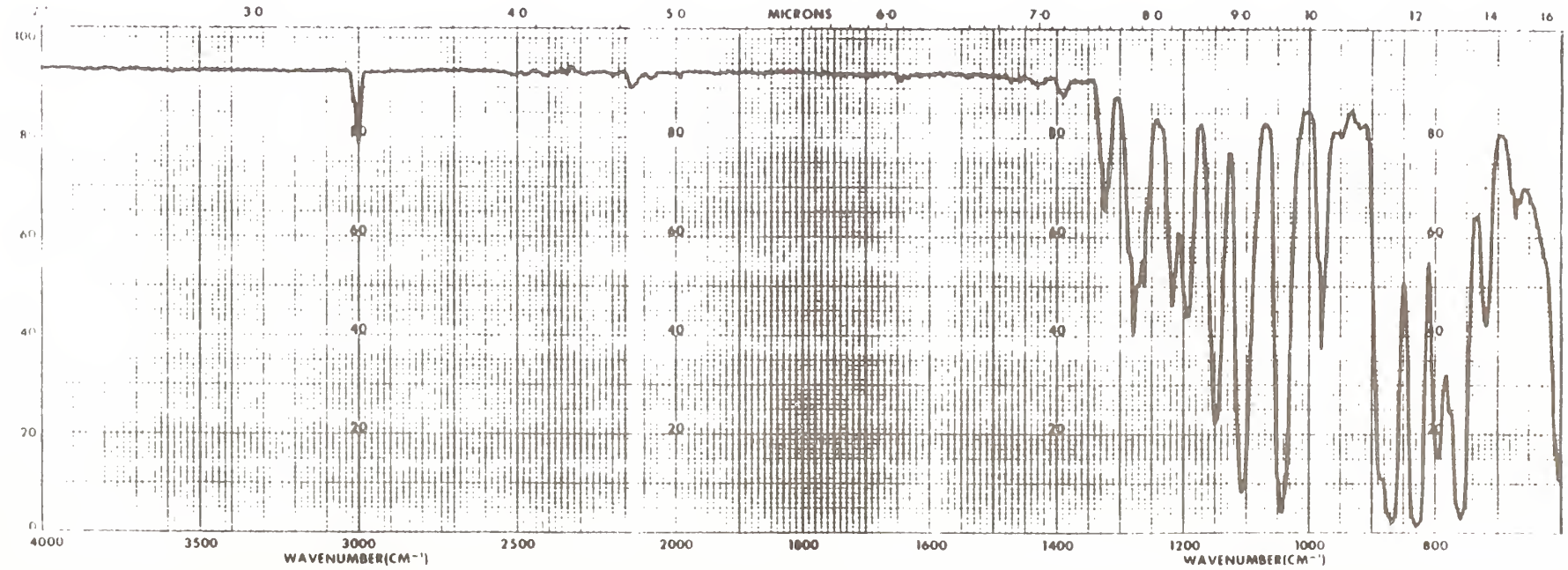


m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
60.00	26145	83.00	168634	105.00	23596	151.00	103044
66.00	121116	85.00	107718	114.00	53413	153.00	32936
78.00	18226	101.00	239289	116.00	34344	184.00	8015
79.00	33096	103.00	146410	149.00	106654	186.00	10159
81.00	10894						

Infrared Spectrum – Liquid Phase (no solvent)



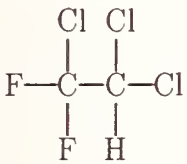
Infrared Spectrum – Gas Phase



122 1,1-difluoro-1,2,2-trichloroethane

synonyms: 1,1–difluoro–1,2,2–trichloroethane.

structure:



C. A. S. Registry Number: 354–21–2
Relative Molecular Mass: 169.5

Normal Boiling Point: 72 °C

Melting Point: NA

Density/Specific Gravity: 1.559 (25/4)

Critical Temperature: 252.8 °C*

Refractive Index:

Critical Pressure: 4.48 MPa*

Critical Density: 0.610* g/mL

****

Vapor Density: NA

PEL: NE

TLV: NE

Flash Point: NA

UEL: NA

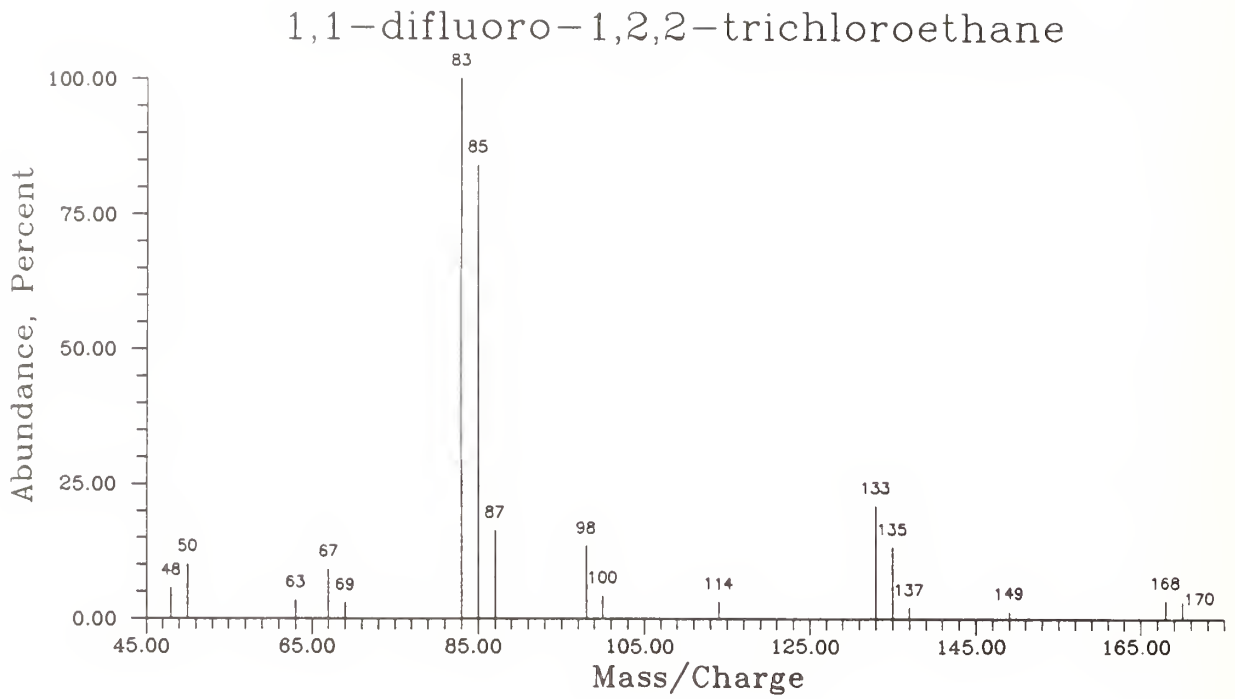
LEL: NA

Toxicology: Possible skin and eye irritant; possible pulmonary irritant; detailed toxicology is not available.

Reactivities and Chemical Incompatibilities: May form HCl, and HF upon thermal decomposition; avoid contact with alkali and alkaline earth metals and powdered metals such as Zn, Al, Be.

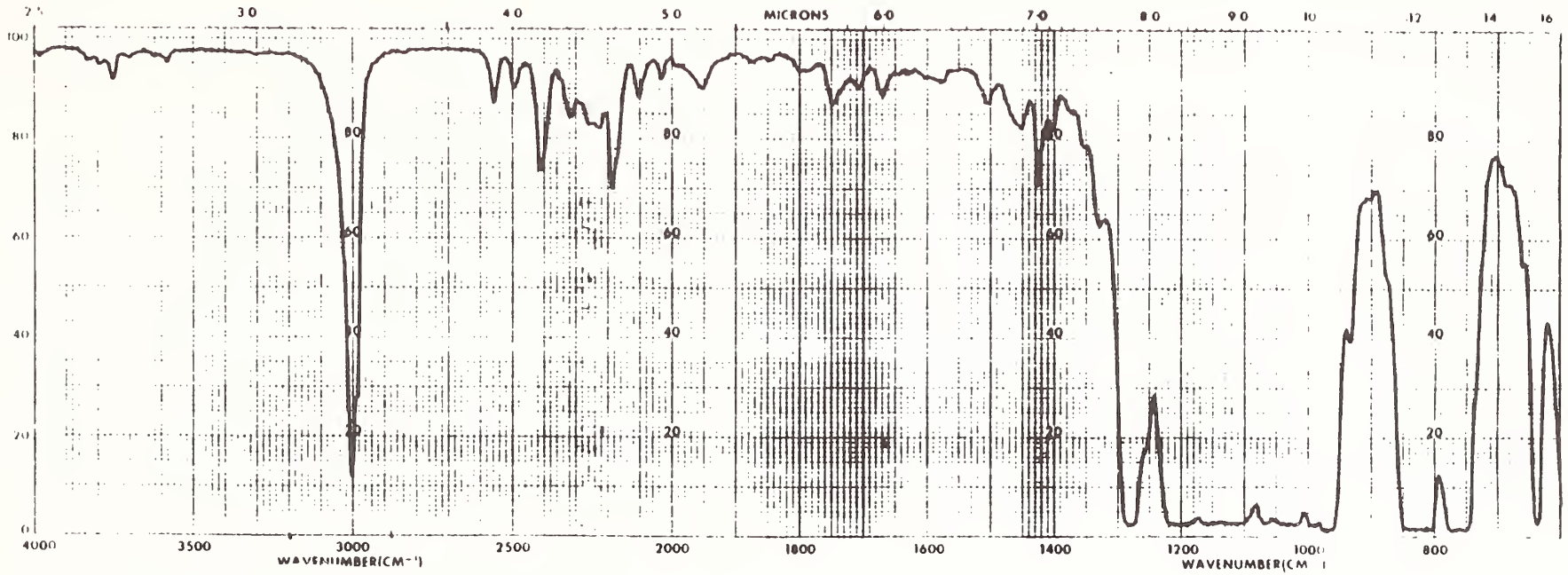
Solubilities: Somewhat soluble in carbon tetrachloride; minimal solubility in water.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
49.00	52367	78.00	26596	97.00	19500	135.00	122450
50.00	92858	79.00	29558	98.00	124261	137.00	18524
60.00	23502	83.00	926053	100.00	39556	149.00	12590
63.00	31549	85.00	777516	114.00	29273	151.00	11894
67.00	84007	86.00	13478	116.00	18785	168.00	31434
69.00	27224	87.00	151057	133.00	193121	170.00	29153

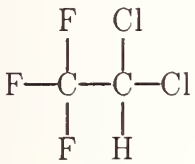
Infrared Spectrum – Liquid Phase (no solvent)



123 2,2-dichloro-1,1,1-trifluoroethane

synonyms: dichlorotrifluoroethane.

structure:



C. A. S. Registry Number: 306–83–2
Relative Molecular Mass: 152.93

Normal Boiling Point: 27.9 °C

Melting Point: –107 °C

Density/Specific Gravity: 1.475 (15/4)

Critical Temperature: 183.8 °C

Refractive Index: 1.329 (25 °C)

Critical Pressure: 3.674 MPa

Critical Density: 0.550 g/mL

****

Vapor Density: 4.1–6.5

PEL: 1000 ppm

TLV: 1000 ppm

Flash Point: does not flash

UEL: NA

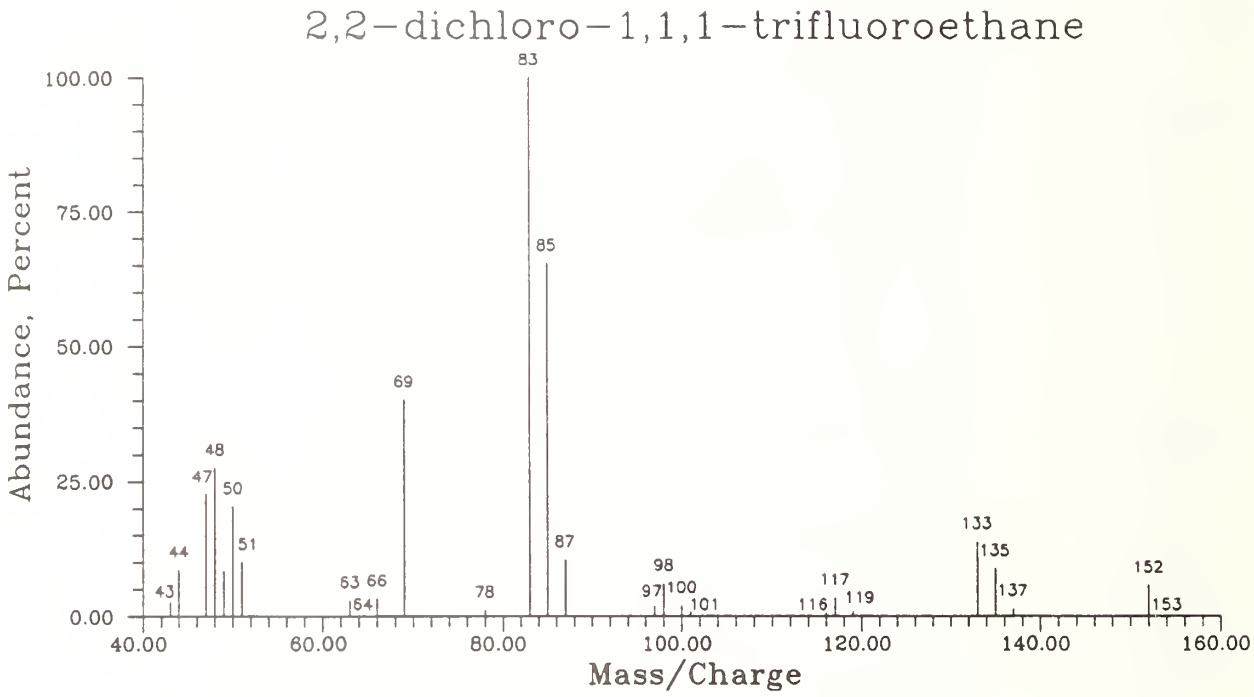
LEL: NA

Toxicology: Mild eye irritant; anesthetic at high concentrations; possible pulmonary irritant; detailed toxicology is not available.

Reactivities and Chemical Incompatibilities: May form HCl, HF, CO, CO_2 upon thermal decomposition; avoid contact with active metals.

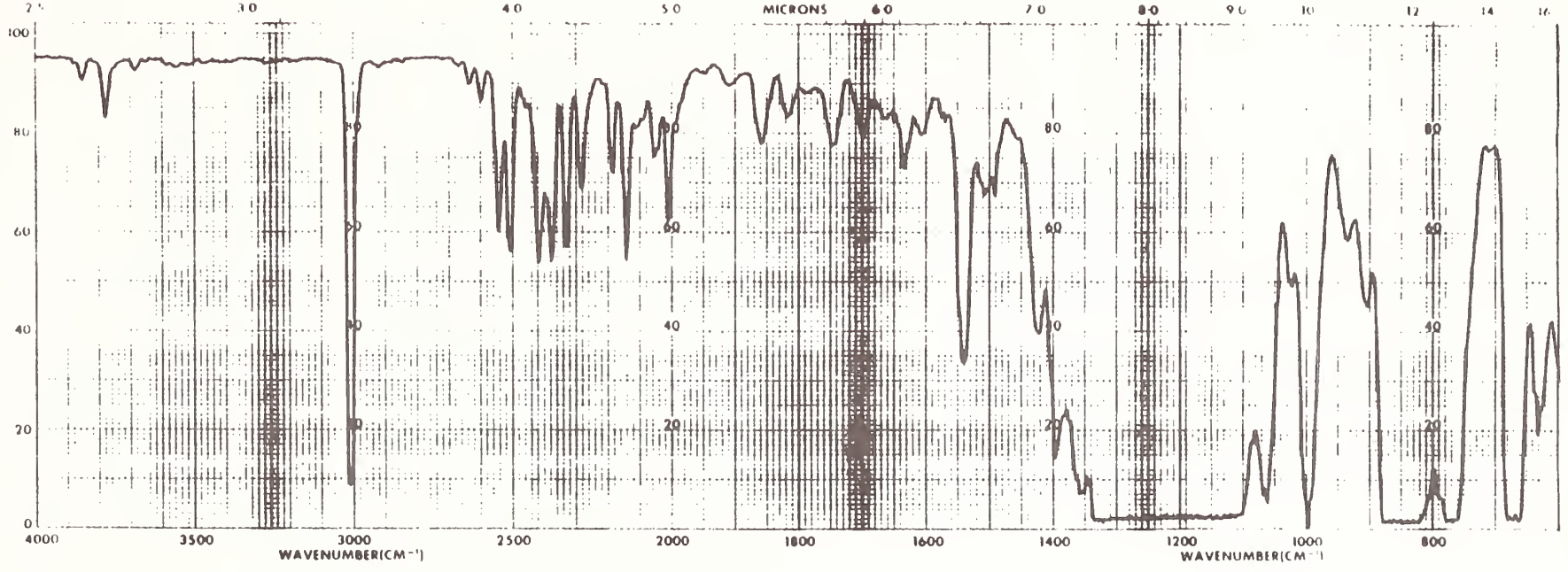
Solubilities: Soluble in alcohols, chloroform ether, carbon tetrachloride; H_2O: 0.39 percent (24 °C).

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	531703	50.00	253033	83.00	1243984	117.00	41291
35.00	445542	51.00	124596	85.00	811732	119.00	12539
37.00	140426	63.00	36789	87.00	129820	133.00	171812
43.00	33113	64.00	1375	97.00	22010	135.00	109458
44.00	107085	66.00	40100	98.00	73925	137.00	16436
47.00	281832	67.00	275713	100.00	23523	152.00	71285
48.00	341514	69.00	497228	101.00	10857	153.00	1293
49.00	103705	78.00	13305	116.00	7868		

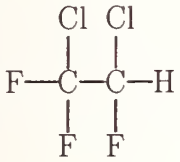
Infrared Spectrum – Gas Phase



123a 1,2-dichlorotrifluoroethane

synonyms: 1,2 dichloro–1,1,2–trifluoroethane.

structure:



C. A. S. Registry Number: 354–23–4
Relative Molecular Mass: 152.93

Normal Boiling Point: 28 °C

Melting Point: –78 °C

Density/Specific Gravity: 1.5 g/mL (0 °C)

Critical Temperature: 185.2 °C*

Refractive Index:

Critical Pressure: 4.47 MPa*

Critical Density: 0.627*

****

Vapor Density: NE

PEL: NE

TLV: NE

Flash Point: NE

UEL: NE

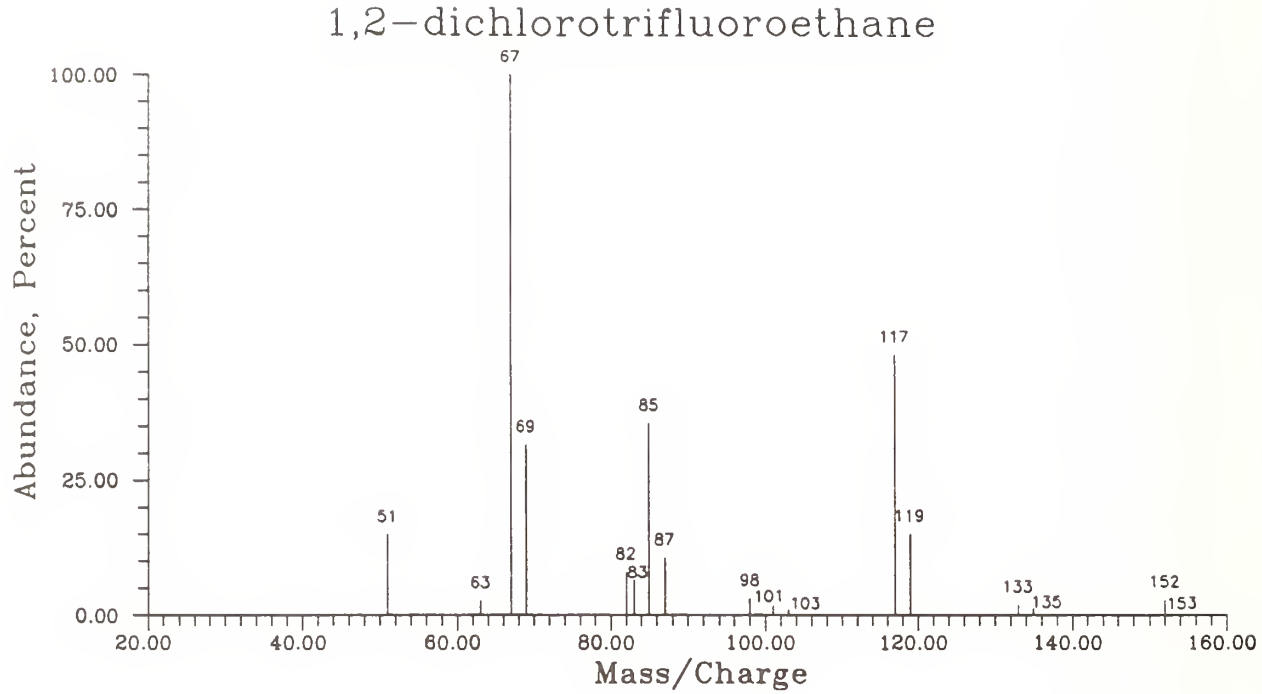
LEL: NE

Toxicology: Possible pulmonary irritant; detailed toxicology is not available.

Reactivities and Chemical Incompatibilities: Thermal decomposition may produce HCl and HF; avoid contact with active metals.

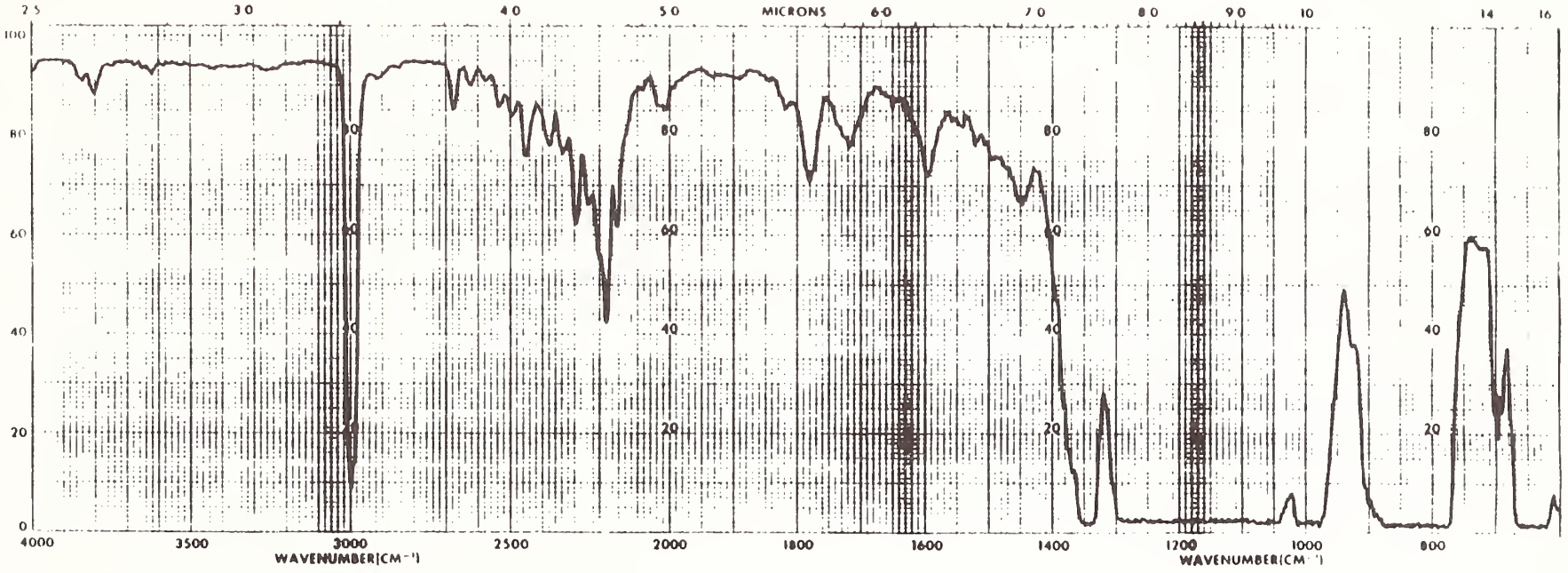
Solubilities: Somewhat soluble in carbon tetrachloride.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	546412	51.00	202665	83.00	88833	117.00	653807
35.00	186693	62.00	17244	85.00	481331	119.00	204167
37.00	59320	63.00	35621	87.00	143040	133.00	25247
40.00	39523	67.00	1362707	98.00	41561	135.00	15896
43.00	22577	69.00	428264	101.00	22795	152.00	38285
50.00	105153	82.00	107958	103.00	13426	153.00	496

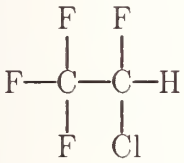
Infrared Spectrum – Gas Phase



124 2-chloro-1,1,1,2-tetrafluoroethane

synonyms: monochloro–1,1,1,2–tetrafluoroethane; monochloro–1,2,2,2–tetrafluoroethane; 1,1,1,2–tetrafluoro–2–chloroethane.

structure:



C. A. S. Registry Number: 2837–89–0
Relative Molecular Mass: 136.48

Normal Boiling Point: –12.1 °C

Melting Point: –199 °C

Density/Specific Gravity: 1.472 g/mL, l, (–12.1 °C)

Critical Temperature: 122.5 °C

Refractive Index:

Critical Pressure: 3.63 MPa

Critical Density: 0.560 g/mL

****

Vapor Density: >1

PEL: NE

TLV: NE

Flash Point: does not flash

UEL: NA

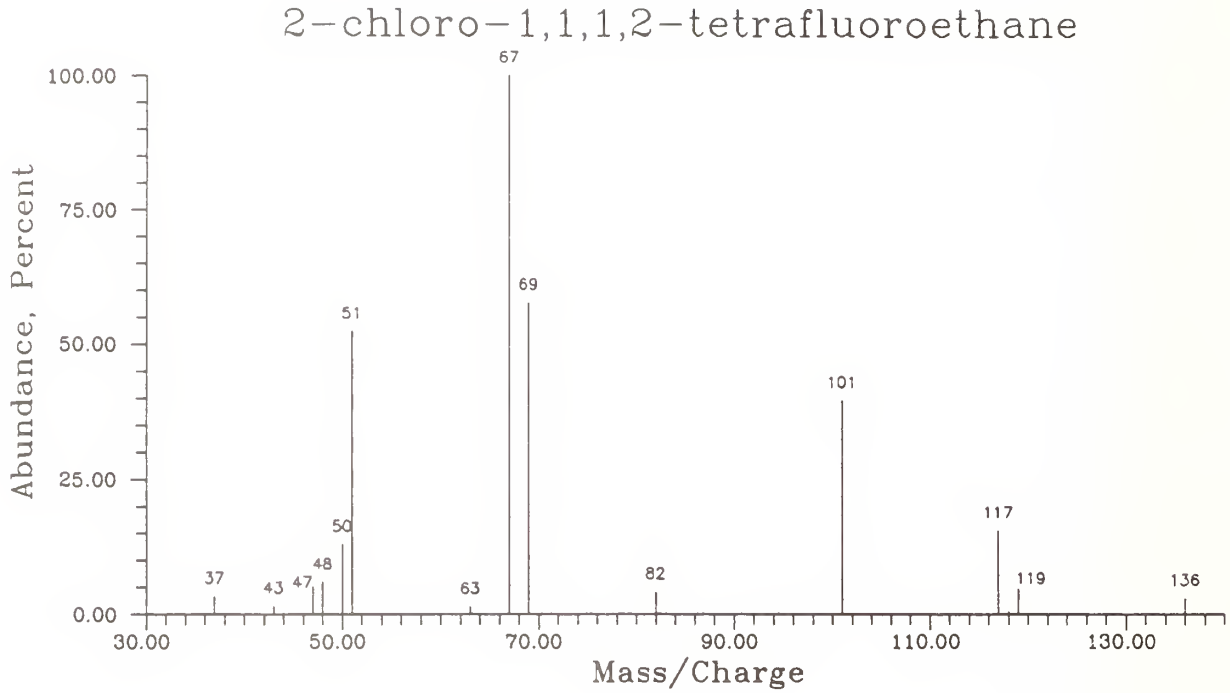
LEL: NA

Toxicology: Low acute toxicity; moderate cardiac sensitizer; mild anesthetic at high concentrations; detailed toxicology is not available.

Reactivities and Chemical Incompatibilities: Thermal decomposition may form HCl, HF, CO, CO_2, phosgene; avoid contact with active metals and powdered metals such as Al, Zn, Be.

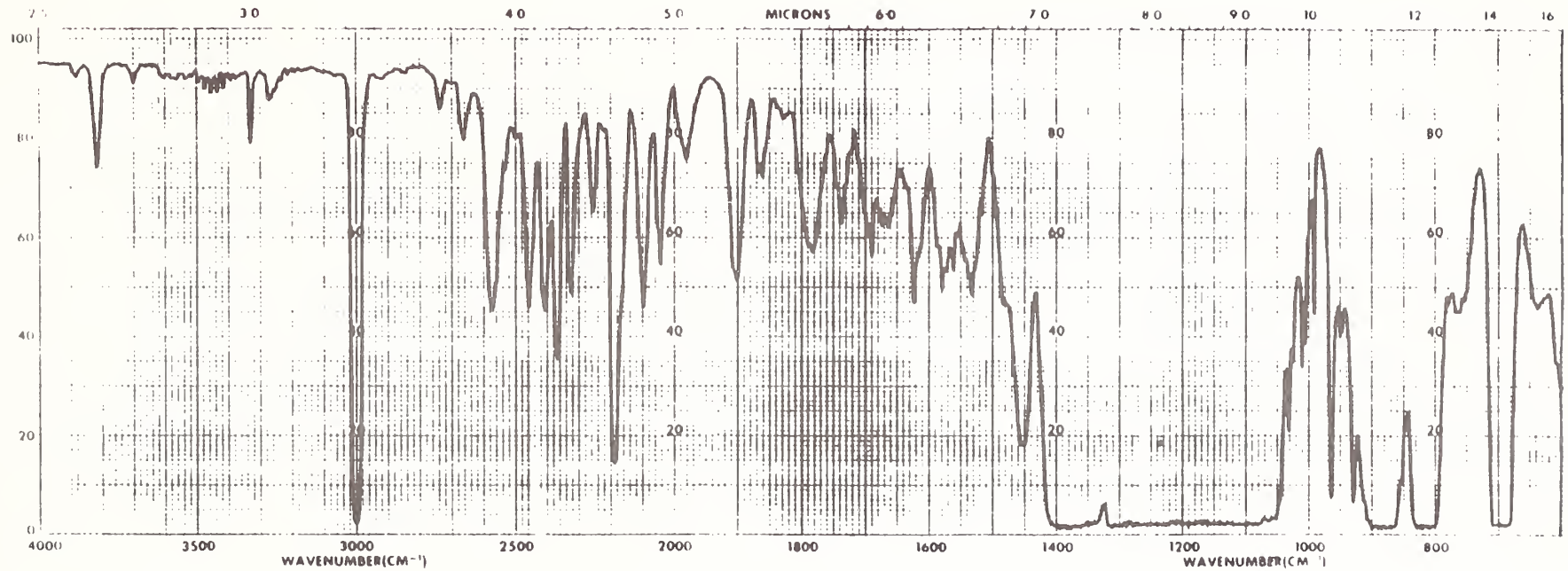
Solubilities: Relatively high solubility in water (17.1 g/L, ambient T & P).

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	1650544	48.00	202006	67.00	3402368	117.00	527536
37.00	111108	50.00	439136	69.00	961344	118.00	18915
43.00	51968	51.00	1780096	82.00	141474	119.00	159344
47.00	173772	63.00	46302	101.00	1344000	136.00	99452

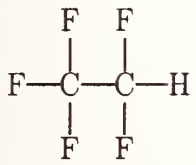
Infrared Spectrum – Gas Phase



125 pentafluoroethane

synonyms:

structure:



C. A. S. Registry Number: 354–33–6
Relative Molecular Mass: 120.02

Normal Boiling Point: –48.5 °C

Melting Point: –103 °C

Density/Specific Gravity: 1.515 g/mL, l (–48.5 °C)

Critical Temperature: 68.3 °C

Refractive Index:

Critical Pressure: 3.631 MPa

Critical Density: 0.572 g/mL

****

Vapor Density: >1

PEL: NA

TLV: NA

Flash Point: NA

UEL: NE

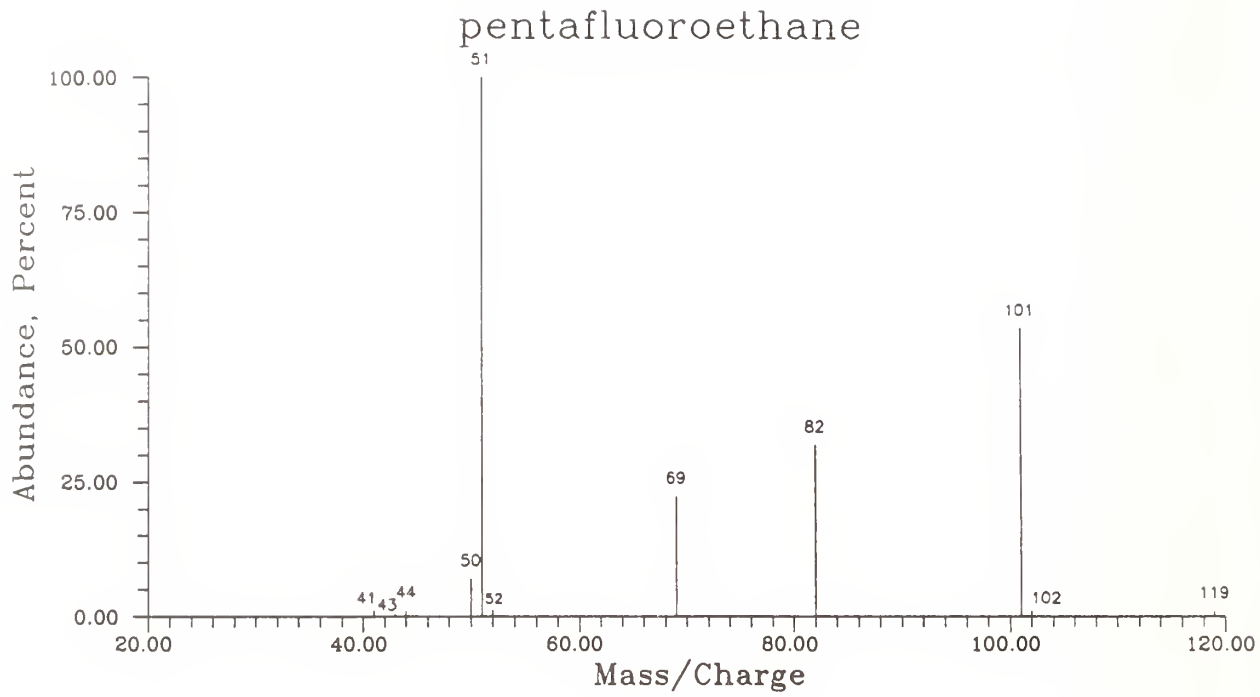
LEL: NE

Toxicology: Can cause headache and nausea, giddiness, and unconsciousness at higher concentrations.

Reactivities and Chemical Incompatibilities: Can form HF, CO, CO_2 upon thermal decomposition; avoid contact with active metals.

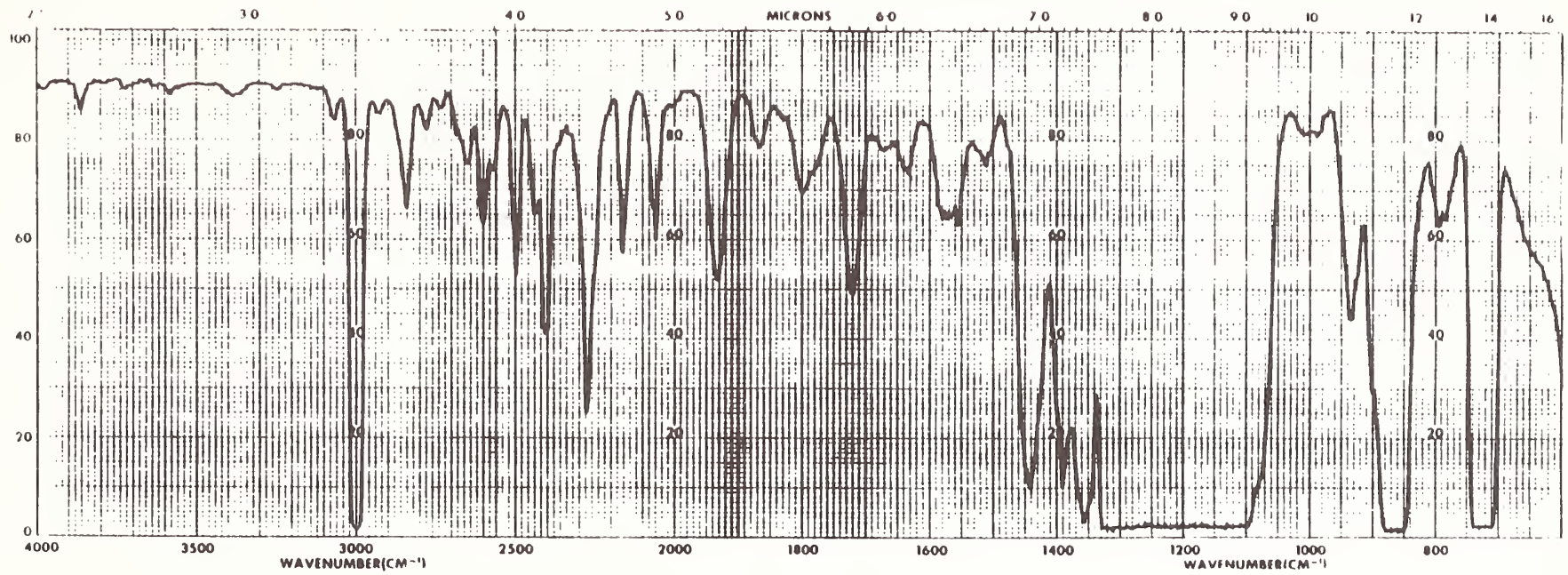
Solubilities: Negligible solubility in H_2O; slightly soluble in carbon tetrachloride.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	521810	44.00	29973	52.00	28854	101.00	1473472
41.00	28605	50.00	192299	69.00	613397	102.00	30722
43.00	13288	51.00	2758549	82.00	8752	119.00	28523

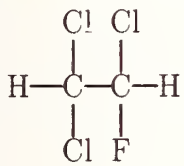
Infrared Spectrum – Gas Phase



131 1,1,2-trichloro-2-fluoroethane

synonyms: 1,1,2–trichlorofluoroethane.

structure:



C. A. S. Registry Number: NA
Relative Molecular Mass: 151.35

Normal Boiling Point: 102.5 °C

Melting Point: NA

Density/Specific Gravity: 1.5497 (17/4)

Critical Temperature: 312.5 °C*

Refractive Index:

Critical Pressure: 5.1 MPa*

Critical Density: 0.591 g/mL*

****

Vapor Density: >1

PEL: NE

TLV: NE

Flash Point: NA

UEL: NA

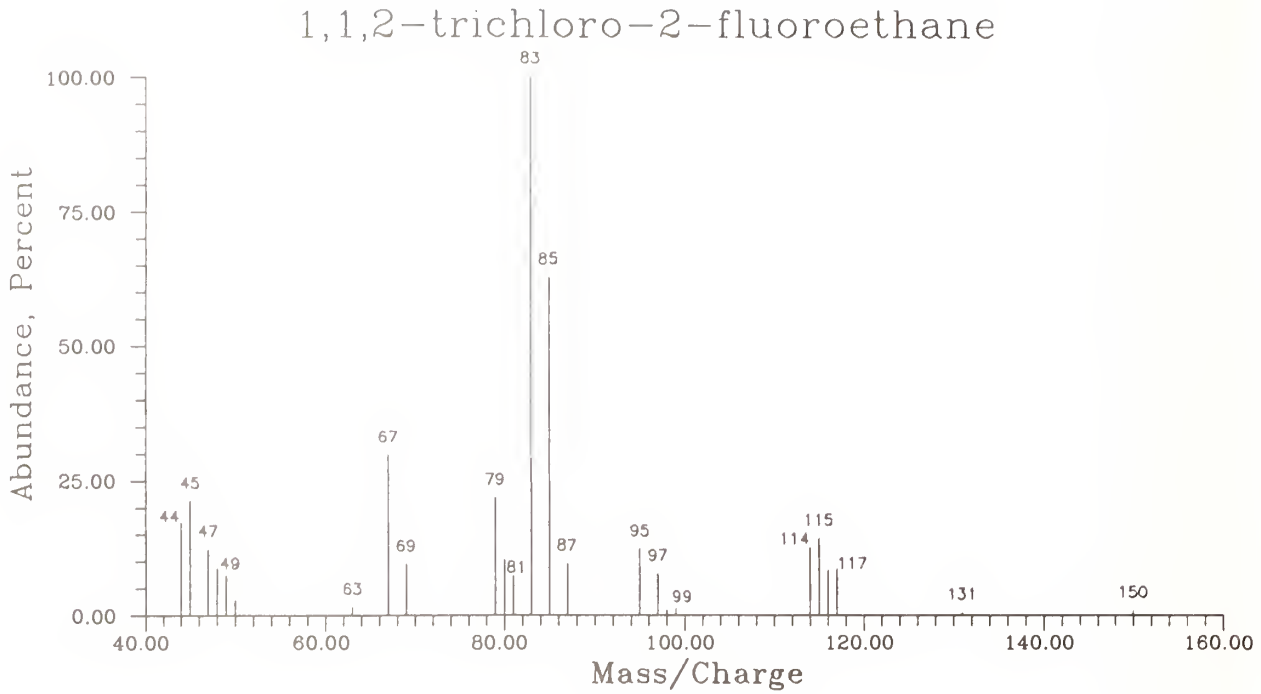
LEL: NA

Toxicology: Detailed toxicology is not available; may cause irritation of skin, eyes, and upper respiratory tract; dizziness, weakness, fatigue, nausea, headache.

Reactivities and Chemical Incompatibilities: Can form HCl, HF, CO, CO_2, and phosgene upon thermal decomposition; avoid contact with alkali and powdered metals.

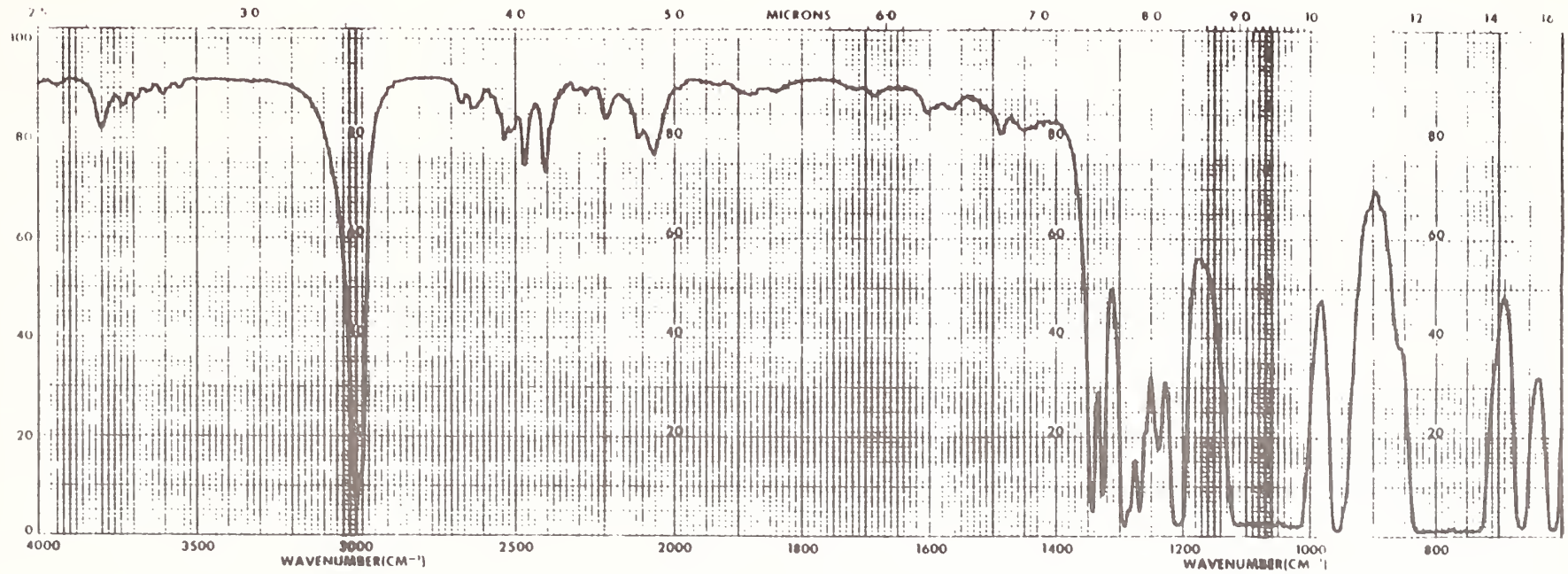
Solubilities: Somewhat soluble in carbon tetrachloride; negligible solubility in water.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	277130	50.00	67590	83.00	2423931	114.00	305018
35.00	584668	63.00	35983	85.00	1518438	115.00	344721
37.00	185605	67.00	719425	87.00	233005	116.00	203456
44.00	419870	69.00	229482	95.00	296705	117.00	208769
45.00	513804	70.00	22070	97.00	186407	118.00	34627
47.00	294875	79.00	528058	98.00	22827	131.00	11946
48.00	211715	80.00	248903	99.00	29754	150.00	117540
49.00	180812	81.00	176685				

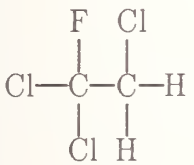
Infrared Spectrum – Liquid Phase (no solvent)



131a 1,1,2-trichloro-1-fluoroethane

synonyms: trichlorofluoroethane.

structure:



C. A. S. Registry Number: 811–95–0
Relative Molecular Mass: 151.39

Normal Boiling Point: 88 °C

Melting Point: –104.7 °C

Density/Specific Gravity: 1.4921 (20 °C)

Critical Temperature: 284.4 °C*

Refractive Index:

Critical Pressure: 5.0 MPa*

Critical Density: 0.582 g/mL*

****

Vapor Density: >1

PEL: NE

TLV: NE

Flash Point: NA

UEL: NA

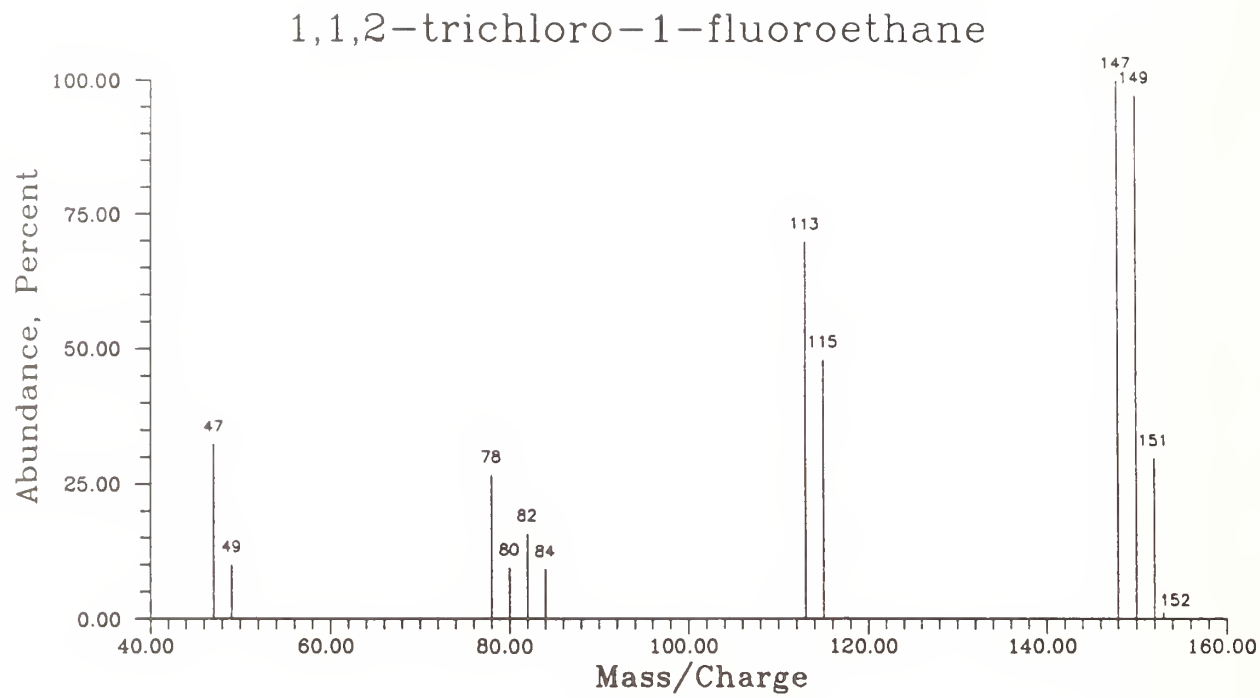
LEL: NA

Toxicology: Detailed toxicology is not available; however, E.I. du Pont de Nemours & Co. reported testicular cancer is produced in rats upon exposure to all concentrations tested.

Reactivities and Chemical Incompatibilities: Thermal decomposition can produce HF, HCl, CO, CO_2; avoid contact with active metals and strong bases.

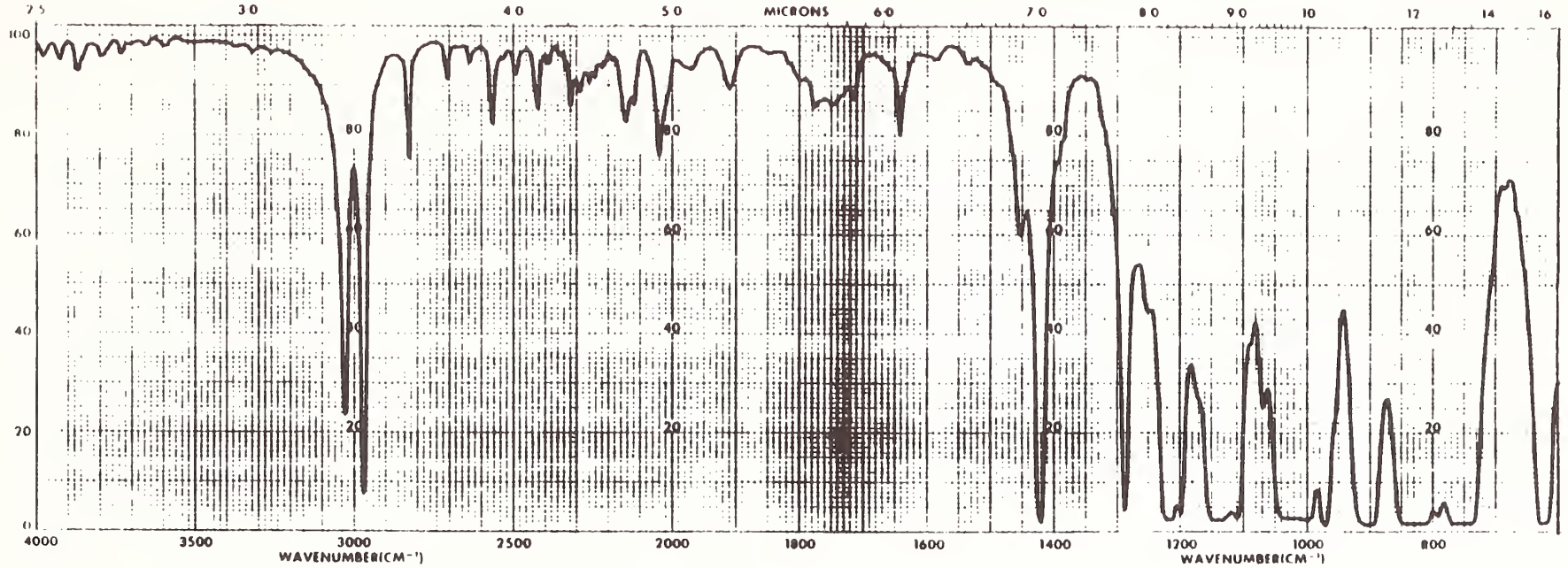
Solubilities: Somewhat soluble in carbon tetrachloride.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	29208	78.00	40352	84.00	13746	149.00	147840
35.00	24608	80.00	14203	113.00	105968	151.00	45104
47.00	48928	82.00	23780	147.00	151936	152.00	1717
49.00	15122						

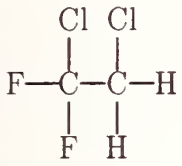
Infrared Spectrum – Liquid Phase (no solvent)



132b 1,2-dichloro-1,1-difluoroethane

synonyms: dichlorodifluoroethane.

structure:



C. A. S. Registry Number: 1649–08–7
Relative Molecular Mass: 134.94

Normal Boiling Point: 46.8 °C

Melting Point: –101.2 °C

Density/Specific Gravity:

Critical Temperature: 220 °C*

Refractive Index: 1.36193 (20)

Critical Pressure: 4.9 MPa*

Critical Density: 0.594*

****

Vapor Density: >1 PEL: NE TLV: NE

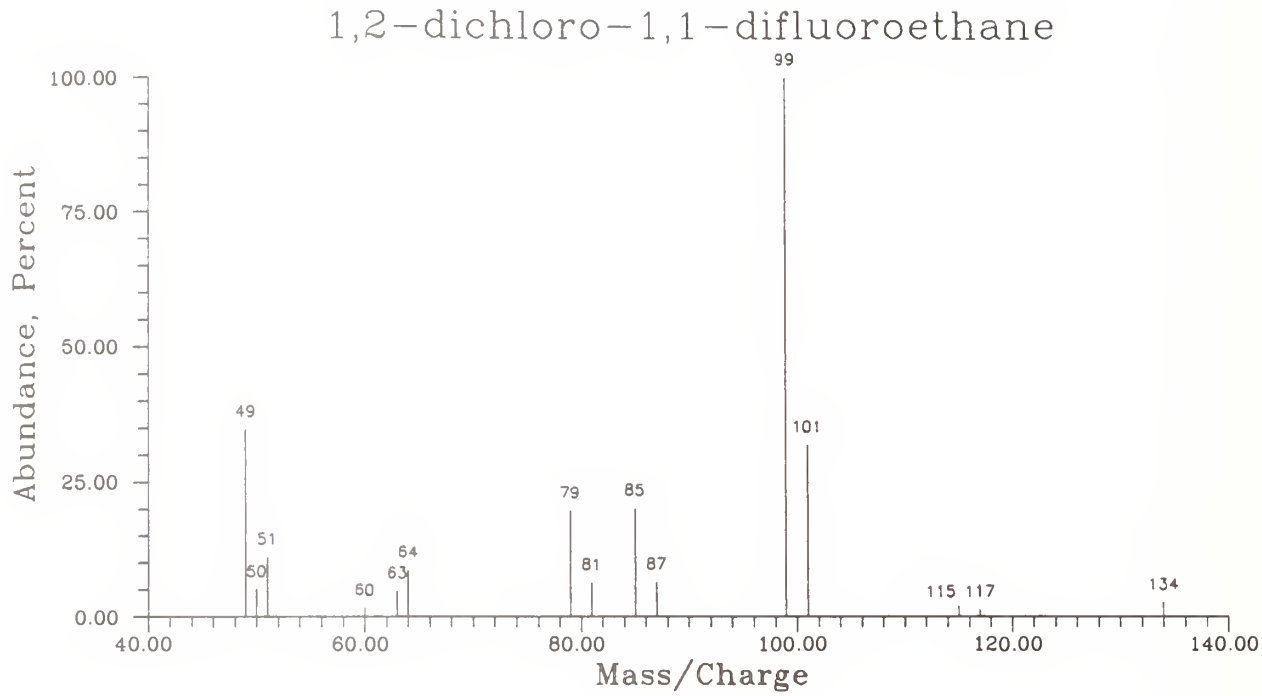
Flash Point: NA UEL: NA LEL: NA

Toxicology: Reproductive effector; possible pulmonary irritant.

Reactivities and Chemical Incompatibilities: May form HCl, HF, CO, CO_2 upon thermal decomposition; avoid contact with active metals.

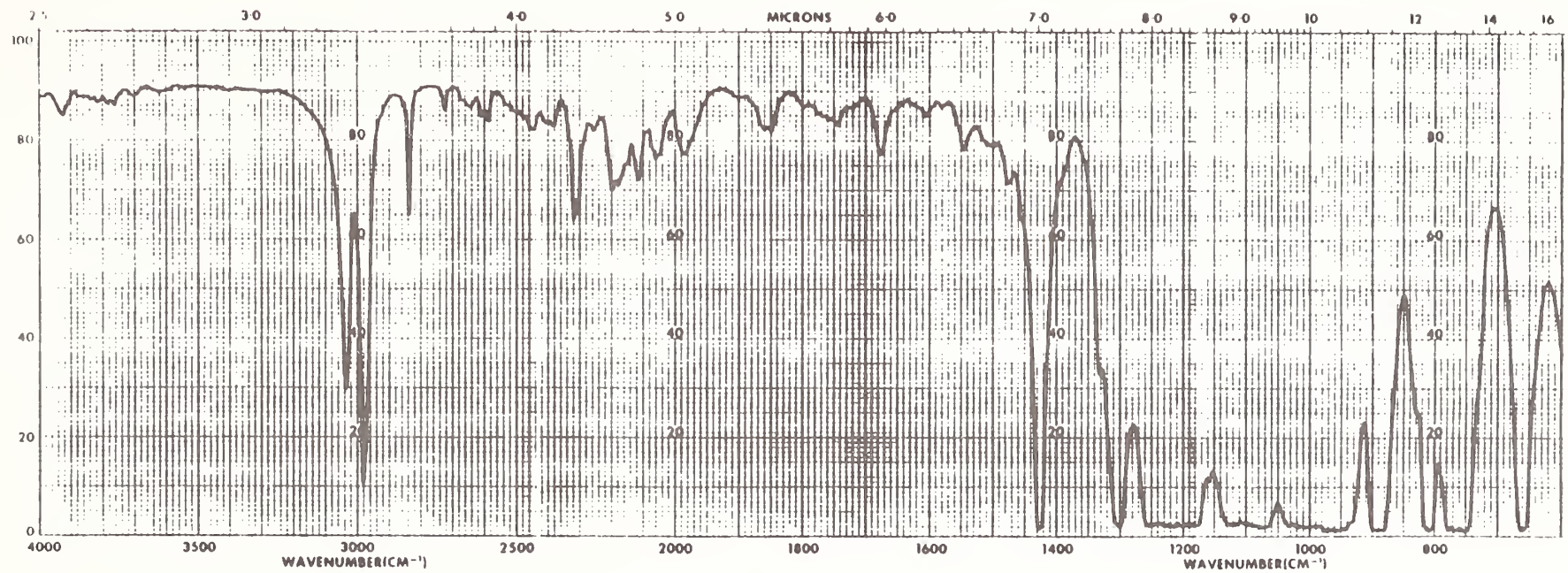
Solubilities: Somewhat soluble in carbon tetrachloride; negligible solubility in water.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	332457	49.00	741609	69.00	14741	99.00	2141678
35.00	220767	50.00	107049	79.00	418215	101.00	678899
44.00	236603	51.00	236227	81.00	133853	115.00	41931
45.00	161386	60.00	33142	85.00	428624	117.00	26799
47.00	105205	63.00	101186	87.00	136165	134.00	65453
48.00	108645	64.00	194129				

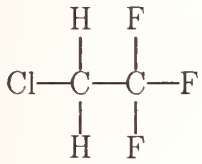
Infrared Spectrum – Liquid Phase (no solvent)



133a 2,2,2-trifluoroethyl chloride

synonyms: 2–chloro–1,1,1–trifluoroethane.

structure:



C. A. S. Registry Number: 75–88–7
Relative Molecular Mass: 118.49

Normal Boiling Point: 6.93 °C

Melting Point: –105.5 °C

Density/Specific Gravity: 1.389 (0/4)

Critical Temperature: 162.5 °C*

Refractive Index: 1.3090

Critical Pressure: 4.94 MPa*

Critical Density: 0.604*

****

Vapor Density: >1

PEL: NE

TLV: NE

Flash Point: NA

UEL: NA

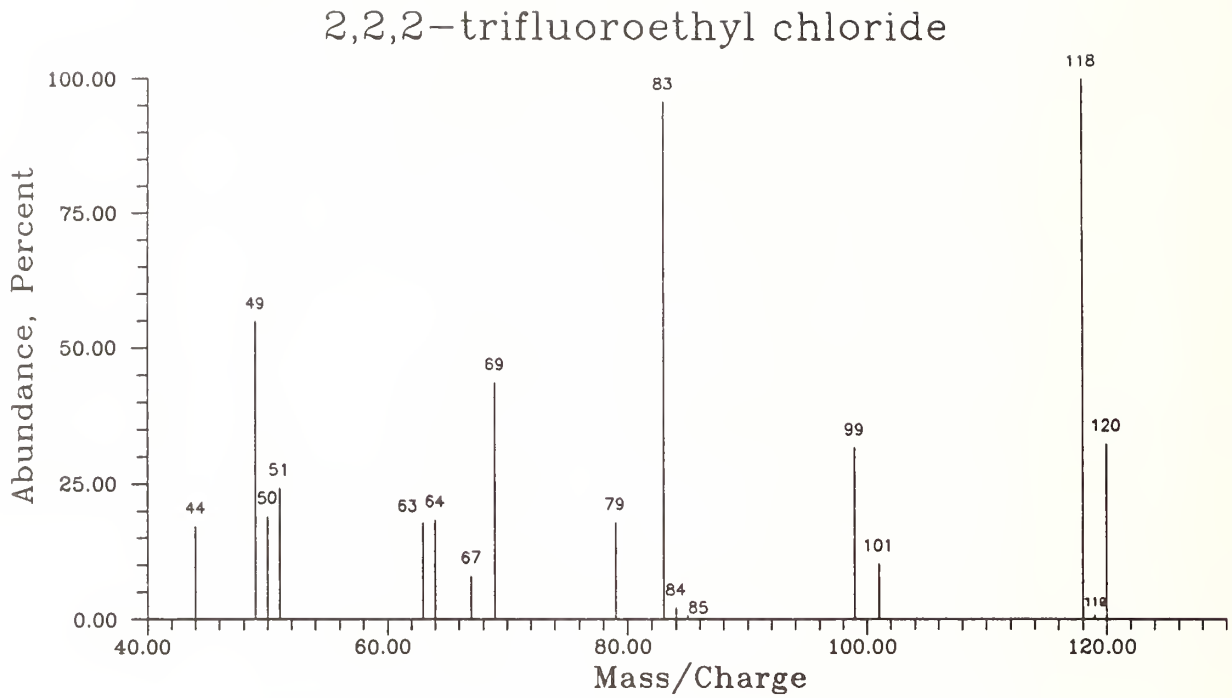
LEL: NA

Toxicology: Detailed toxicology is not available; possible carcinogen.

Reactivities and Chemical Incompatibilities: Thermal decomposition can produce HCl and HF; avoid contact with active metals.

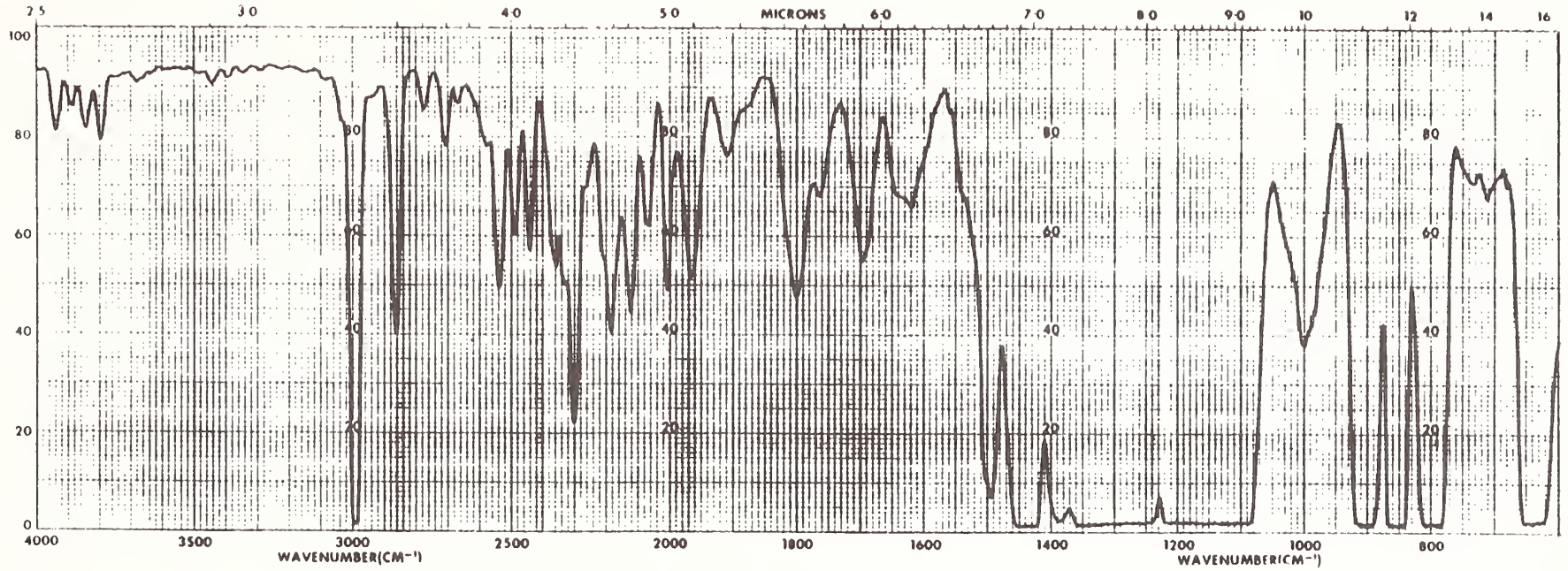
Solubilities: Somewhat soluble in carbon tetrachloride.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	757396	49.00	792577	69.00	630666	99.00	457382
33.00	1260273	50.00	273361	79.00	257417	101.00	147814
35.00	301914	51.00	349262	83.00	1384521	118.00	1448220
44.00	247664	63.00	257015	84.00	29094	119.00	10772
47.00	166560	64.00	265408	85.00	10489	120.00	468152
48.00	188401	67.00	115192				

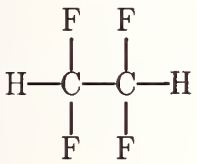
Infrared Spectrum – Gas Phase



134 1,1,2,2-tetrafluoroethane

synonyms: tetrafluoroethane; sym–tetrafluoroethane.

structure:



C. A. S. Registry Number: 359–35–3
Relative Molecular Mass: 102.04

Normal Boiling Point: –23 °C

Melting Point: –89 °C

Density/Specific Gravity:

Critical Temperature: 118.5 °C

Refractive Index:

Critical Pressure: 4.615 MPa*

Critical Density: 0.542 g/mL*

****

Vapor Density: >1

PEL: NE

TLV: NE

Flash Point: <–17 °C

UEL: NA

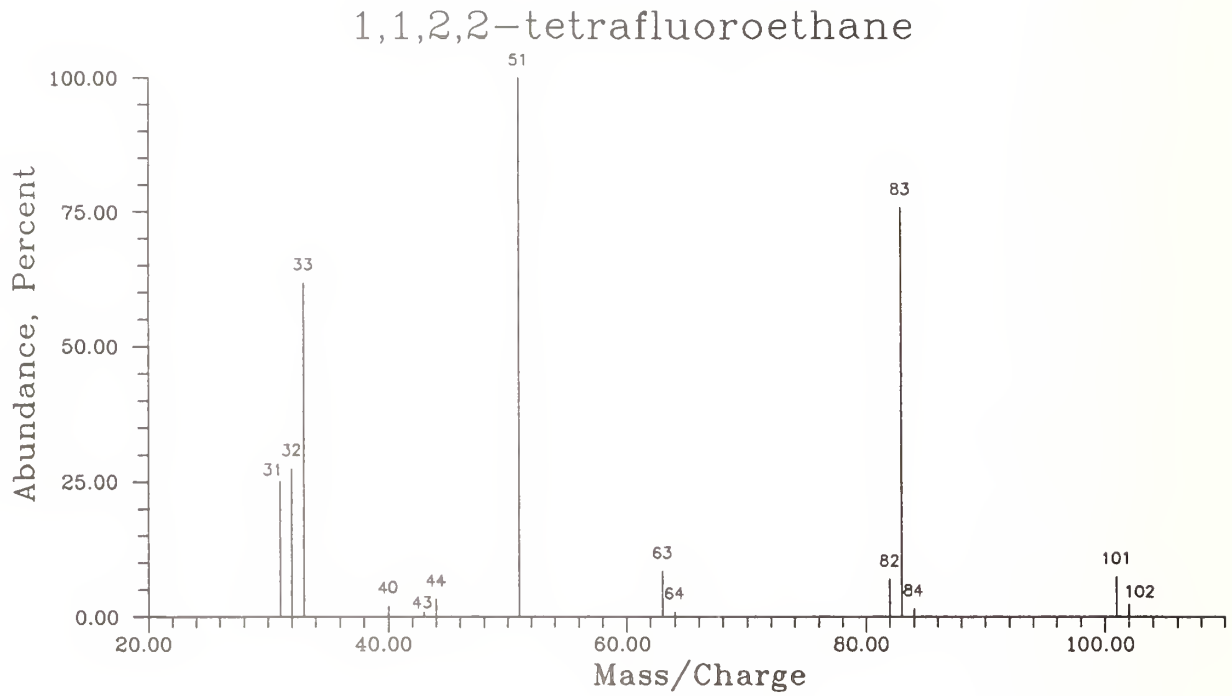
LEL: NA

Toxicology: May aggravate existing heart conditions; detailed toxicology is not available.

Reactivities and Chemical Incompatibilities: May produce HF and F^- upon thermal decomposition.

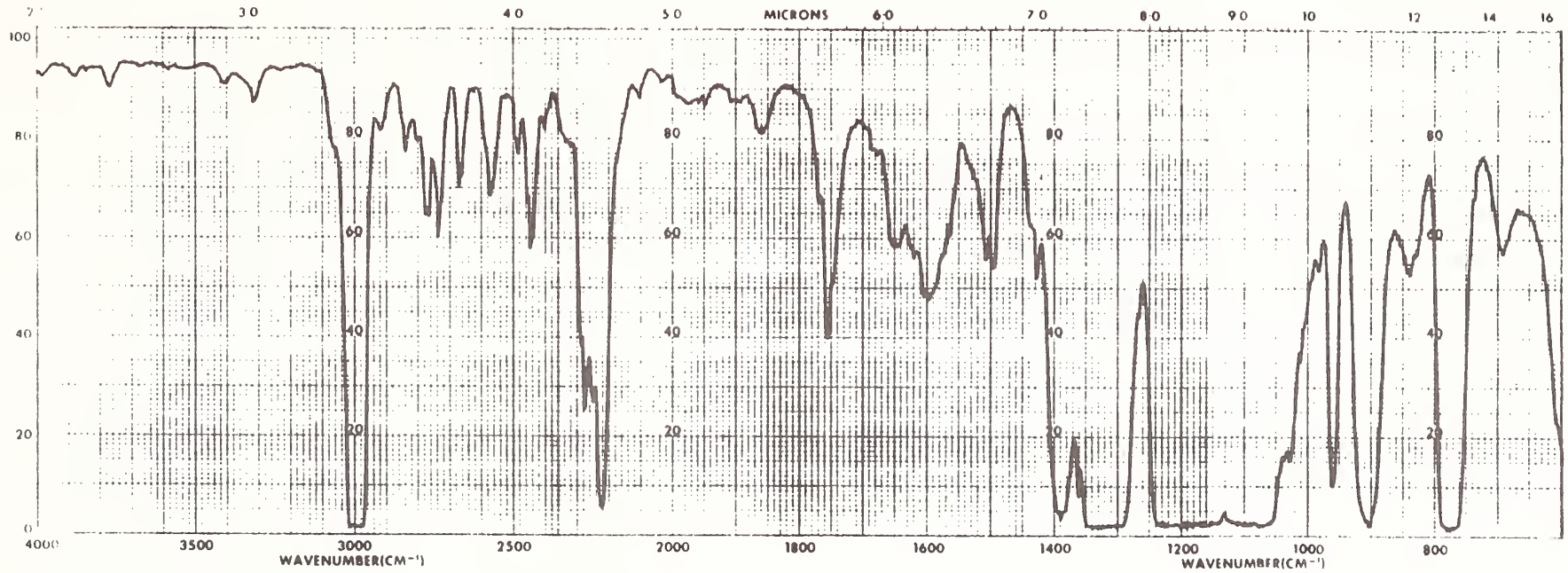
Solubilities: Slightly soluble in carbon tetrachloride; negligible solubility in water.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	789663	43.00	25892	63.00	262266	84.00	48248
32.00	860528	44.00	102894	64.00	27276	101.00	232335
33.00	1938322	45.00	24955	82.00	218148	102.00	73032
40.00	60369	51.00	3143958	83.00	2385287		

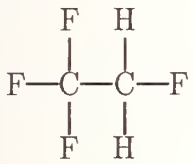
Infrared Spectrum – Gas Phase



134a 1,1,1,2-tetrafluoroethane

synonyms: tetrafluoroethane.

structure:



C. A. S. Registry Number: 811–97–2
Relative Molecular Mass: 102.03

Normal Boiling Point: –26.5 °C

Melting Point: –101 °C

Density/Specific Gravity: 1.21 g/mL, l, (25 °C)

Critical Temperature: 101.06 °C

Refractive Index:

Critical Pressure: 4.06 MPa

Critical Density: 0.515 g/mL

****

Vapor Density: 3.18

PEL: NE

TLV: NE

Flash Point: does not flash

UEL: none

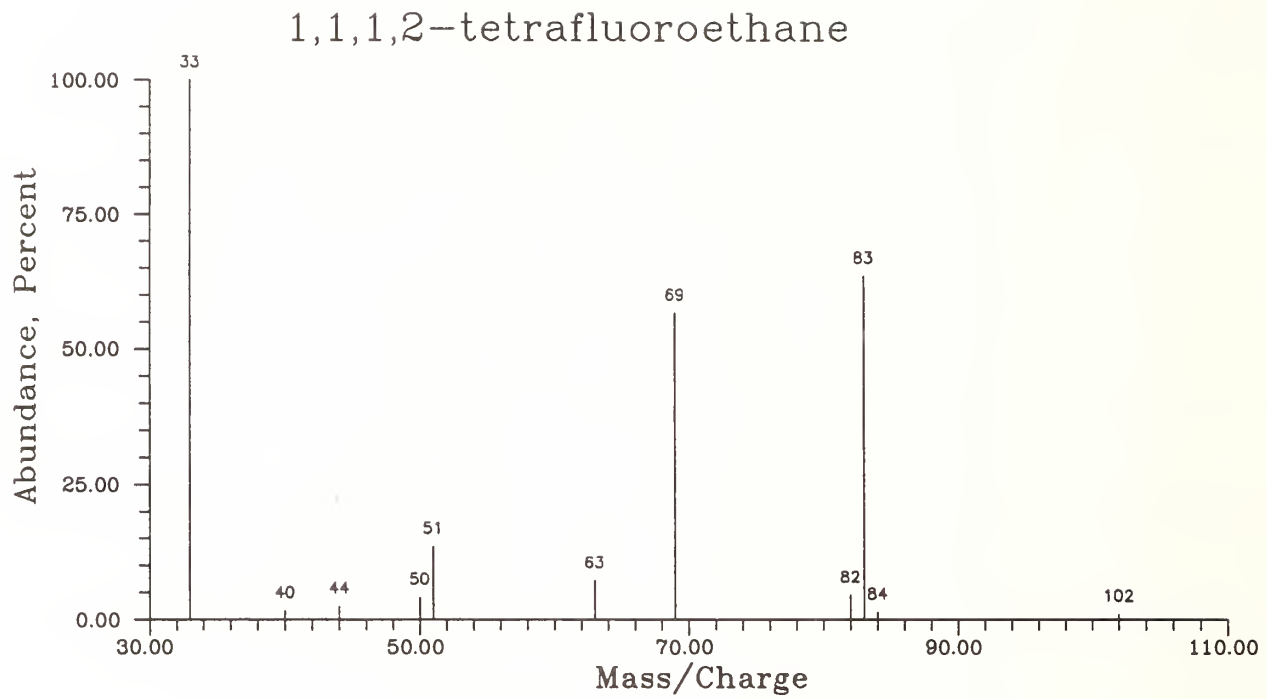
LEL: none

Toxicology: Inhalation of low to moderate concentrations can cause cardiac irregularities; higher concentrations cause pulmonary edema and congestion.

Reactivities and Chemical Incompatibilities: Thermal decomposition can form HF, possibly COF_2; avoid contact with alkali and alkaline earth metals and powdered metals, especially Al, Zn, Be.

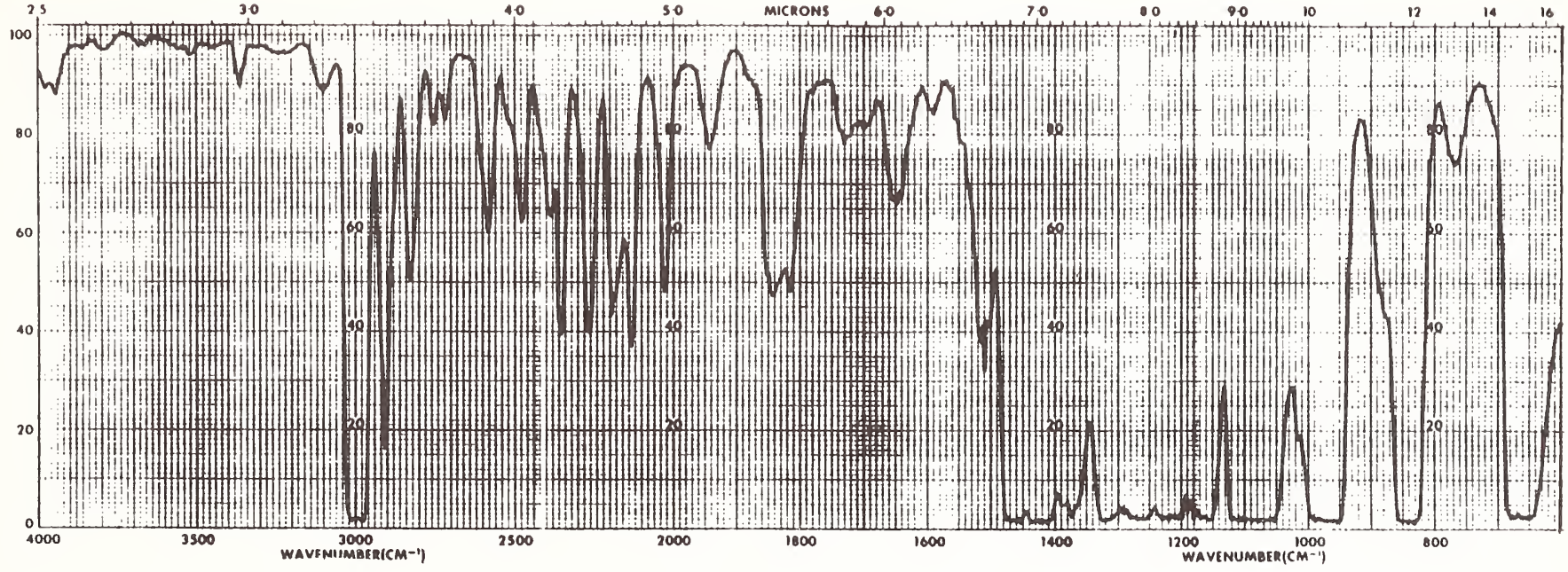
Solubilities: H_2O: 25 °C – 0.15 percent by weight; slightly soluble in ether and carbon tetrachloride.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	462057	40.00	40796	50.00	103527	82.00	113162
32.00	444370	43.00	19631	51.00	340789	83.00	1595574
33.00	2514404	44.00	62144	63.00	179853	84.00	35244
34.00	27386	45.00	11566	69.00	1423314	102.00	24852

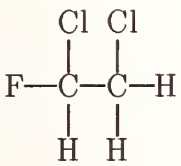
Infrared Spectrum – Gas Phase



141 1,2-dichloro-1-fluoroethane

synonyms: dichlorofluoroethane.

structure:



C. A. S. Registry Number: 25167–88–8
Relative Molecular Mass: 116.95

Normal Boiling Point: 76 °C

Melting Point: –6 °C

Density/Specific Gravity: 1.3814 (20/4)

Critical Temperature: 269.1 °C*

Refractive Index: 1.41132, l (20 °C)

Critical Pressure: 4.40 MPa*

Critical Density: 0.444 g/mL*

****

Vapor Density: > 1

PEL: NE

TLV: NE

Flash Point: NA

UEL: NA

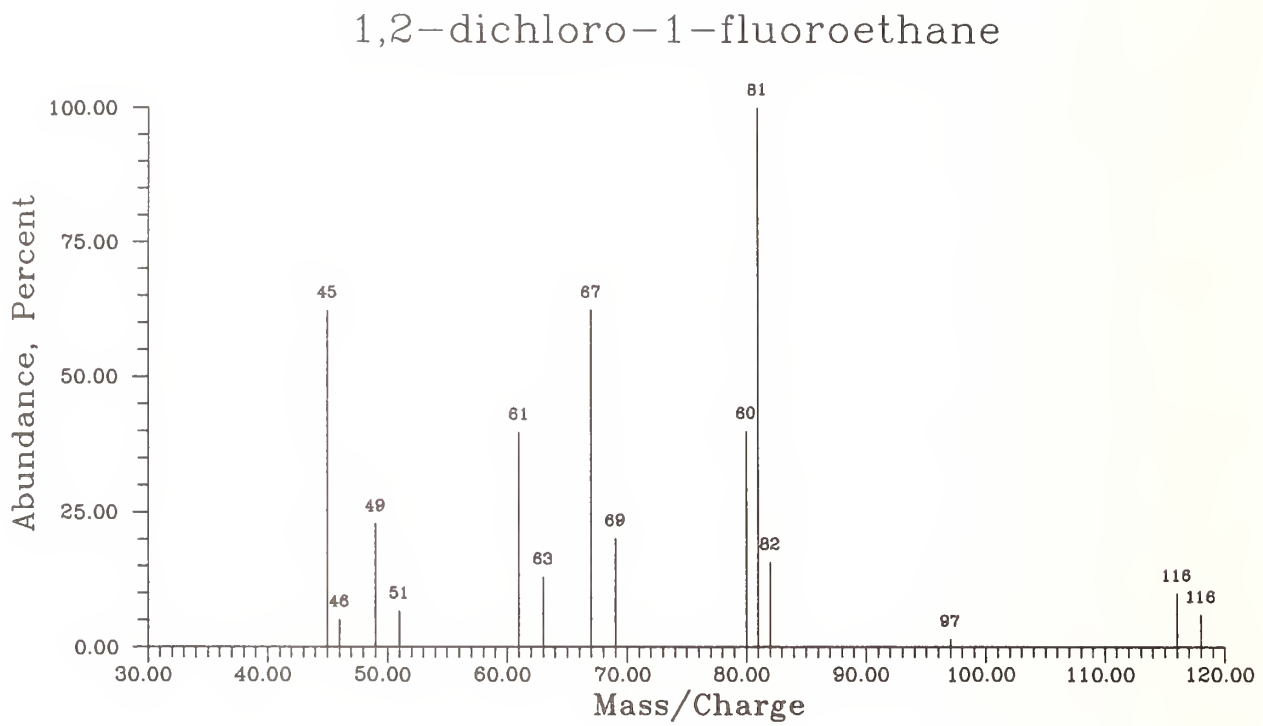
LEL: NA

Toxicology: Detailed toxicology is not available; may cause eye and pulmonary irritation.

Reactivities and Chemical Incompatibilities: Thermal decomposition may produce HF, HCl, CO, CO_2; avoid contact with active metals.

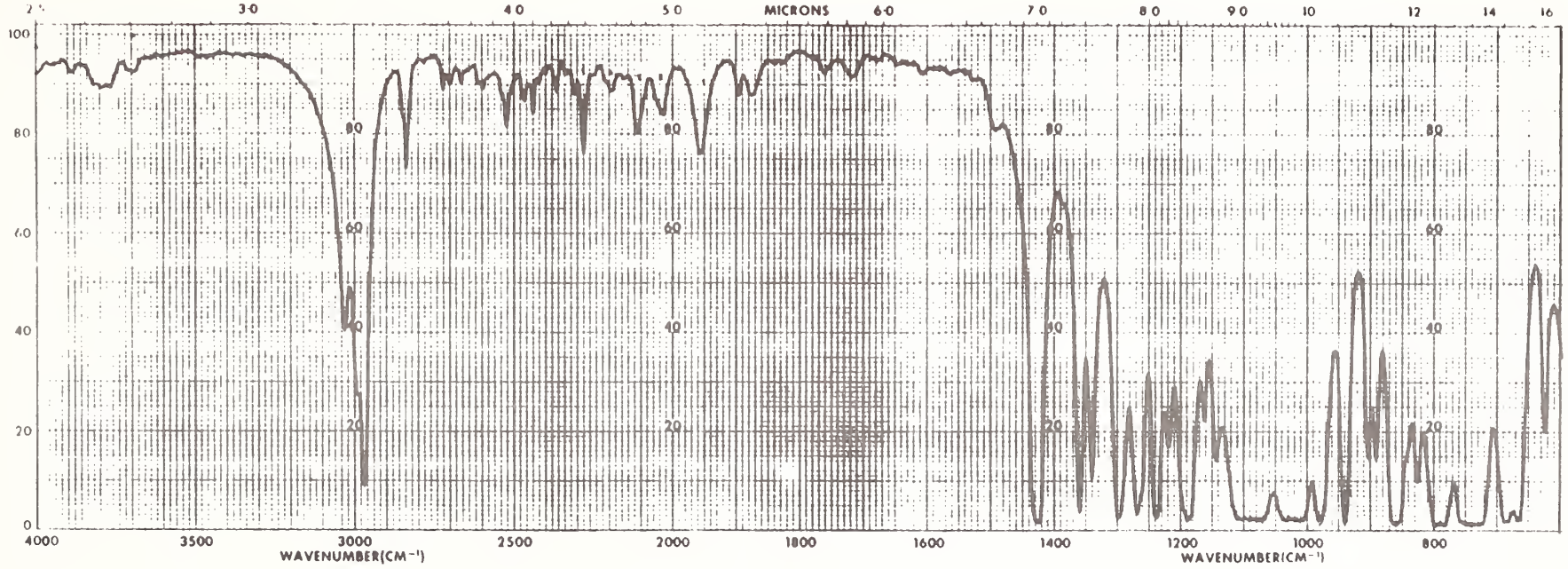
Solubilities: Somewhat soluble in carbon tetrachloride; negligible solubility in water.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
35.00	145275	49.00	183369	67.00	501977	83.00	260501
37.00	49666	51.00	53304	69.00	161052	97.00	11527
44.00	125414	60.00	48264	80.00	321364	116.00	80179
45.00	500620	61.00	319204	81.00	805626	118.00	48422
46.00	95629	63.00	103849	82.00	125865		

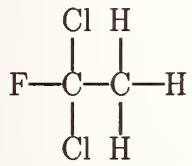
Infrared Spectrum – Liquid Phase (no solvent)



141b 1,1-dichloro-1-fluoroethane

synonyms: fluorodichloroethane; 1–fluoro–1,1–dichloroethane.

structure:



C. A. S. Registry Number: 1717–00–6
Relative Molecular Mass: 116.95

Normal Boiling Point: 32 °C

Melting Point: –103.3 °C

Density/Specific Gravity: 1.25 g/mL (10 °C)

Critical Temperature: 210.3 °C

Refractive Index: 1.3600 (10 °C)

Critical Pressure: 4.64 MPa

Critical Density: 0.43 g/mL

****

Vapor Density: 4.0

PEL: NA

TLV: NA

Flash Point: NA

UEL: 16%

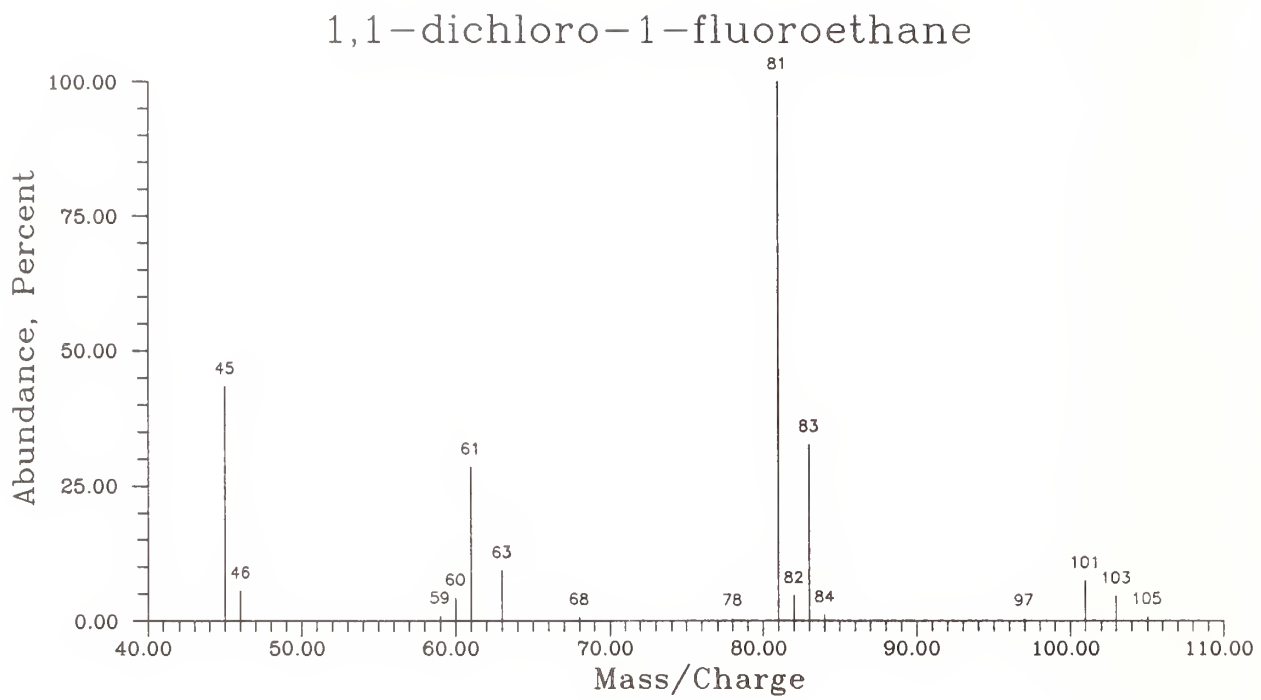
LEL: 7%

Toxicology: Mildly irritating to the eyes; can cause irregular heartbeat; simple asphyxiant; detailed toxicology is not available.

Reactivities and Chemical Incompatibilities: Thermal decomposition can produce HCl, HF, CO, CO_2; avoid contact with active metals.

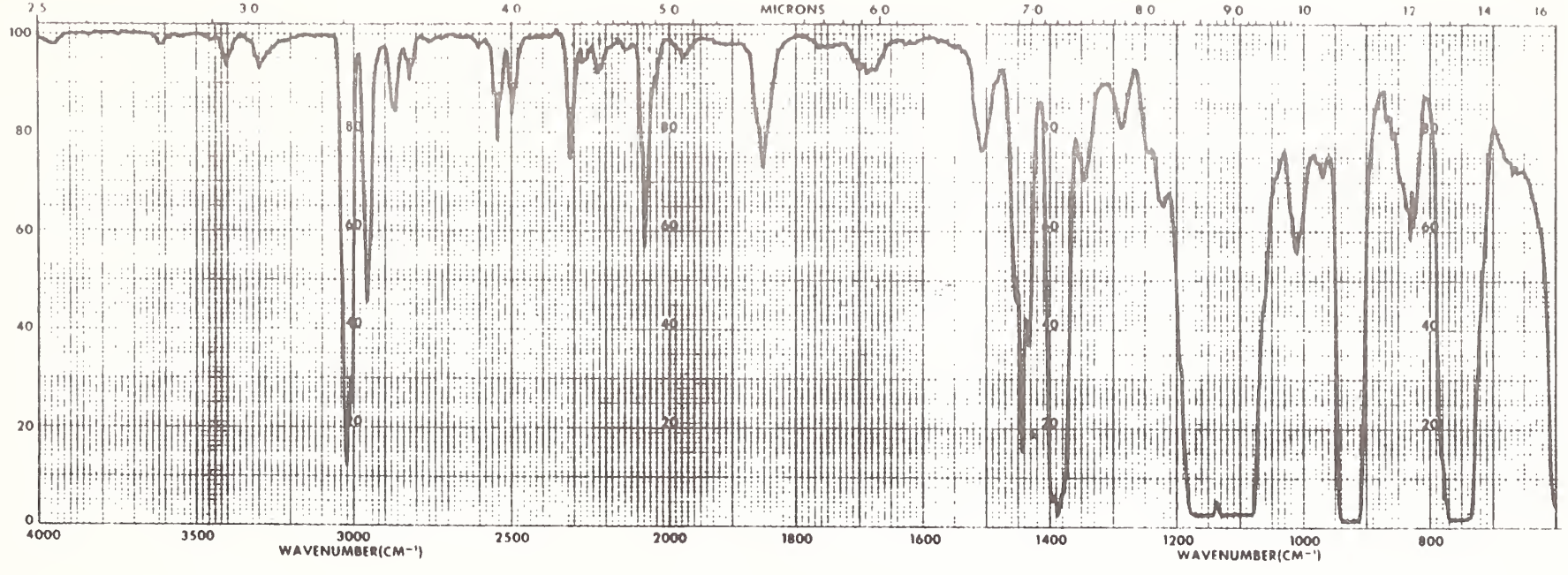
Solubilities: Slightly soluble in H_2O (slight tendency to hydrolyze).

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
35.00	636743	59.00	36381	78.00	15514	84.00	42659
36.00	137182	60.00	167951	79.00	83721	97.00	15520
37.00	205144	61.00	1133645	81.00	3984809	101.00	295805
44.00	498138	63.00	371436	82.00	184096	103.00	181225
45.00	1727198	66.00	76016	83.00	1298004	105.00	29165
46.00	220976	68.00	25228				

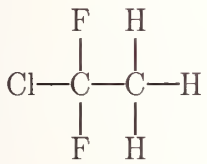
Infrared Spectrum – Gas Phase



142b 1-chloro-1,1-difluoroethane

synonyms: difluoromonochloroethane; α–chloroethylidene fluoride.

structure:



C. A. S. Registry Number: 75–68–3
Relative Molecular Mass: 100.50

Normal Boiling Point: –9.2 °C

Melting Point: –130.8 °C

Density/Specific Gravity: 1.118 g/mL, l, (21 °C)

Critical Temperature: 137.1 °C

Refractive Index:

Critical Pressure: 4.12 MPa

Critical Density: 0.435 g/mL

****

Vapor Density: 3.7

PEL: NA

TLV: NA

Flash Point: flashes with difficulty

UEL: 14.8

LEL: 9

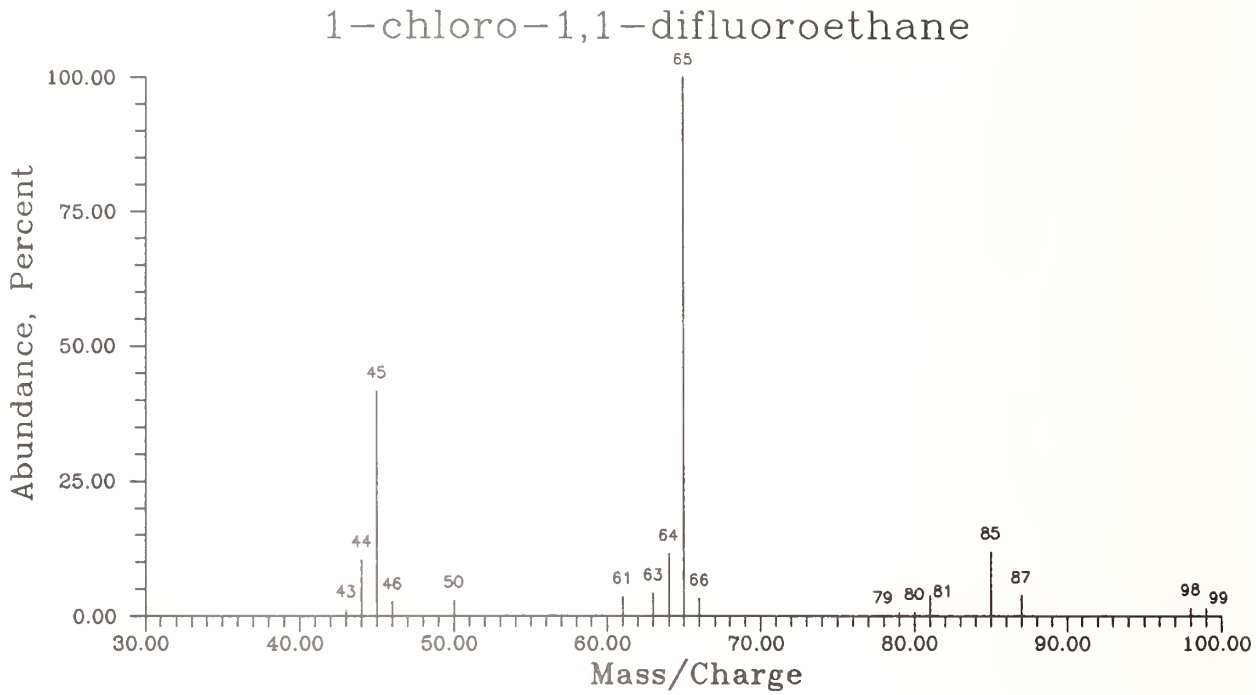
Auto ignition temperature 632 °C

Toxicology: Simple asphyxiant; irritant to lungs; detailed toxicology is not available.

Reactivities and Chemical Incompatibilities: Thermal decomposition may form HCl, HF, CO, CO_2; avoid contact with alkali and alkaline earth metals, powdered metals such as Al, Zn, Be.

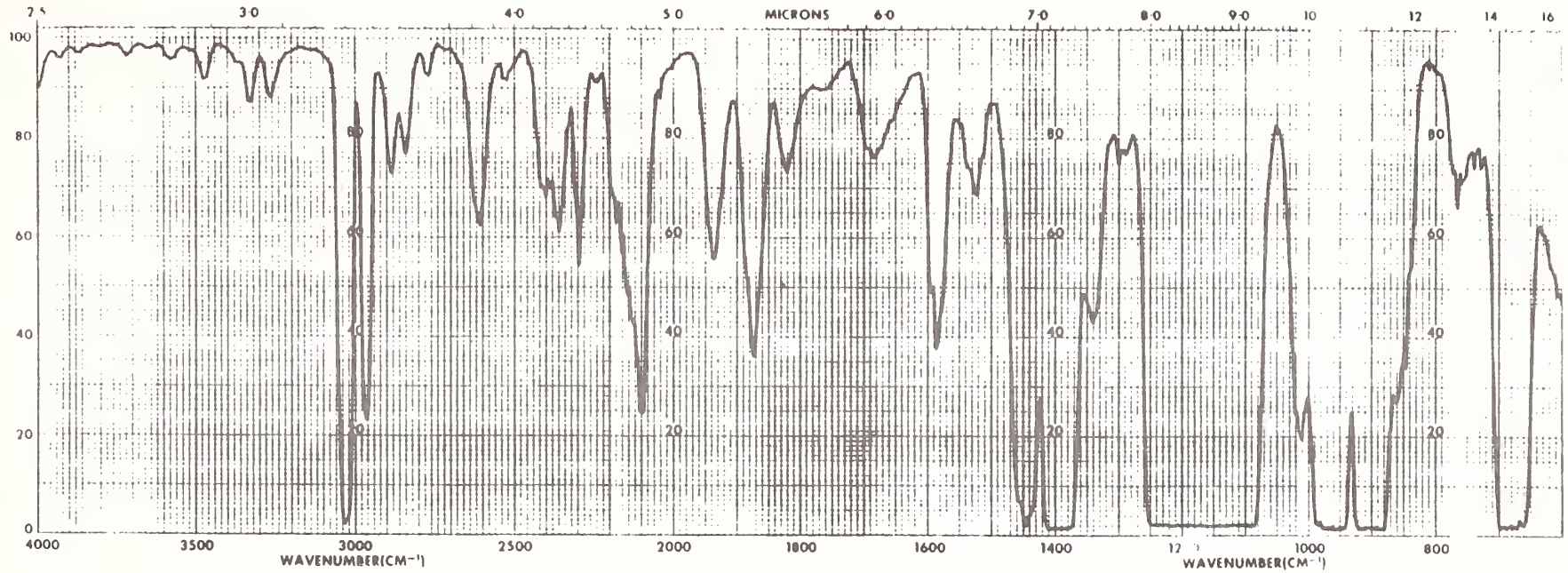
Solubilities: H_2O: 0.14 percent at 21 °C; somewhat soluble in carbon tetrachloride.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
35.00	295740	50.00	113014	66.00	127757	85.00	470406
43.00	43505	61.00	139504	79.00	25955	87.00	149087
44.00	606649	63.00	166684	80.00	25668	98.00	2635
45.00	1632008	65.00	3926336	81.00	149847	99.00	2858
46.00	102755						

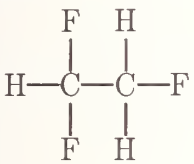
Infrared Spectrum – Gas Phase



143 1,1,2-trifluoroethane

synonyms: trifluoroethane.

structure:



C. A. S. Registry Number: 430–66–0
Relative Molecular Mass: 84.04

Normal Boiling Point: 5 °C

Melting Point: –84 °C

Density/Specific Gravity:

Critical Temperature: 71.2 °C

Refractive Index:

Critical Pressure: 4.05 MPa*

Critical Density: 0.420 g/mL*

****

Vapor Density: NA

PEL: NE

TLV: NE

Flash Point: NE

UEL: NE

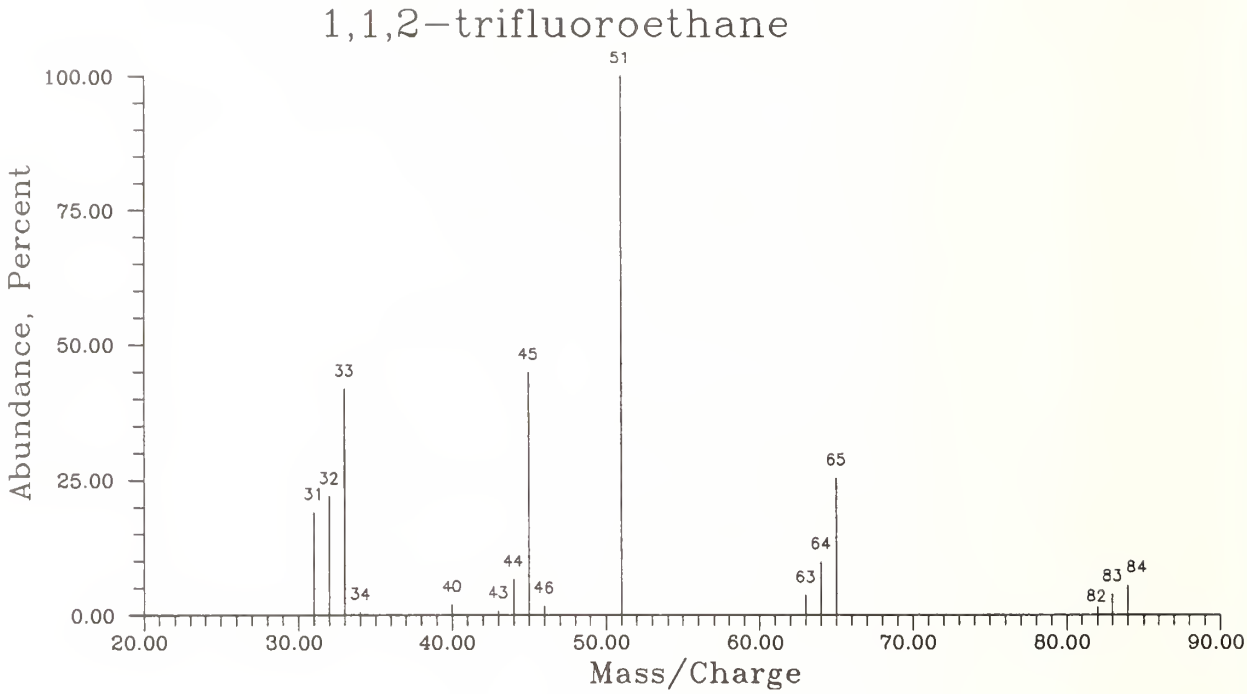
LEL: NE

Toxicology: Detailed toxicology is not available.

Reactivities and Chemical Incompatibilities: May form HF, CO, CO_2 upon thermal decomposition; avoid contact with active metals.

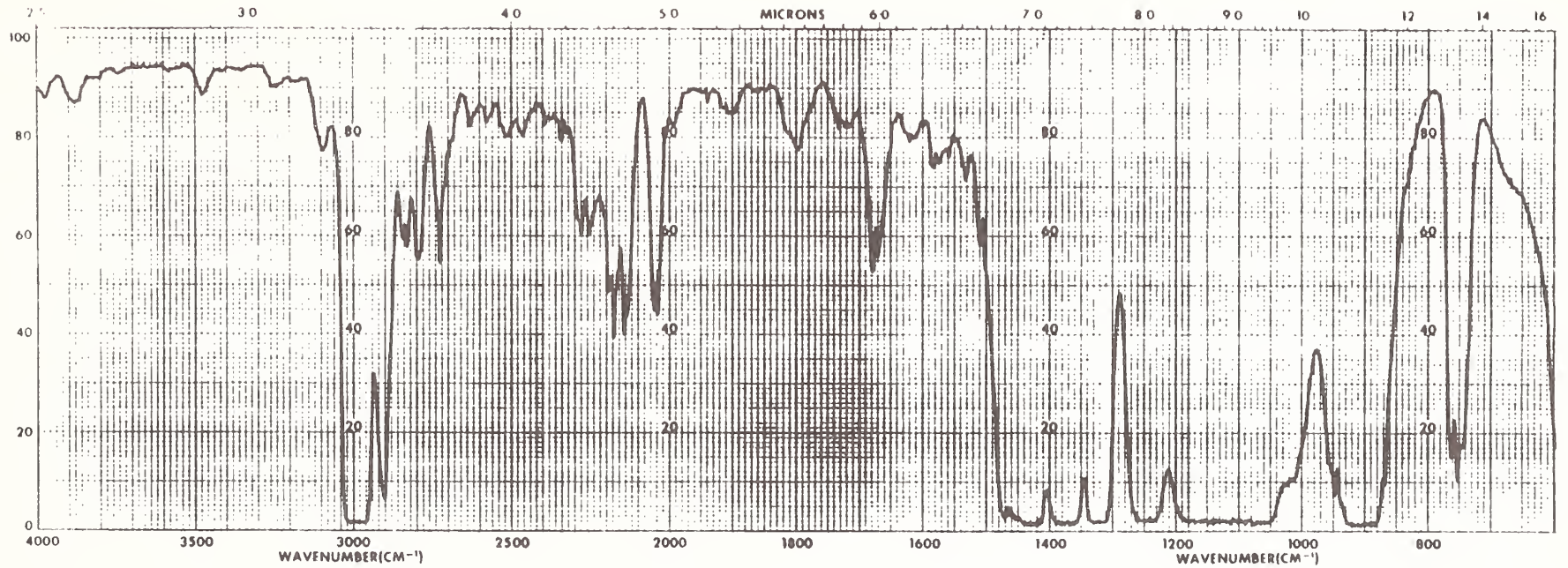
Solubilities: Slightly soluble in ether, chloroform and carbon tetrachloride; negligible solubility in H_2O.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	525936	43.00	20276	51.00	2763601	65.00	700536
32.00	605102	44.00	182810	52.00	32107	82.00	42250
33.00	1153563	45.00	1237688	63.00	101080	83.00	107193
34.00	14318	46.00	45308	64.00	270461	84.00	148307
40.00	52499						

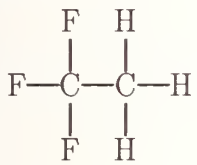
Infrared Spectrum – Gas Phase



143a 1,1,1-trifluoroethane

synonyms: trifluoroethane.

structure:



C. A. S. Registry Number: 420–46–2
Relative Molecular Mass: 84.04

Normal Boiling Point: –47.35 °C

Melting Point: –111.3 °C

Density/Specific Gravity: 0.942 g/mL, l, (30 °C)

Critical Temperature: 73.1 °C

Refractive Index:

Critical Pressure: 3.811 MPa

Critical Density: 0.434 g/mL

****

Vapor Density: NA

PEL: NA

TLV: NA

Flash Point: NA

UEL: NA

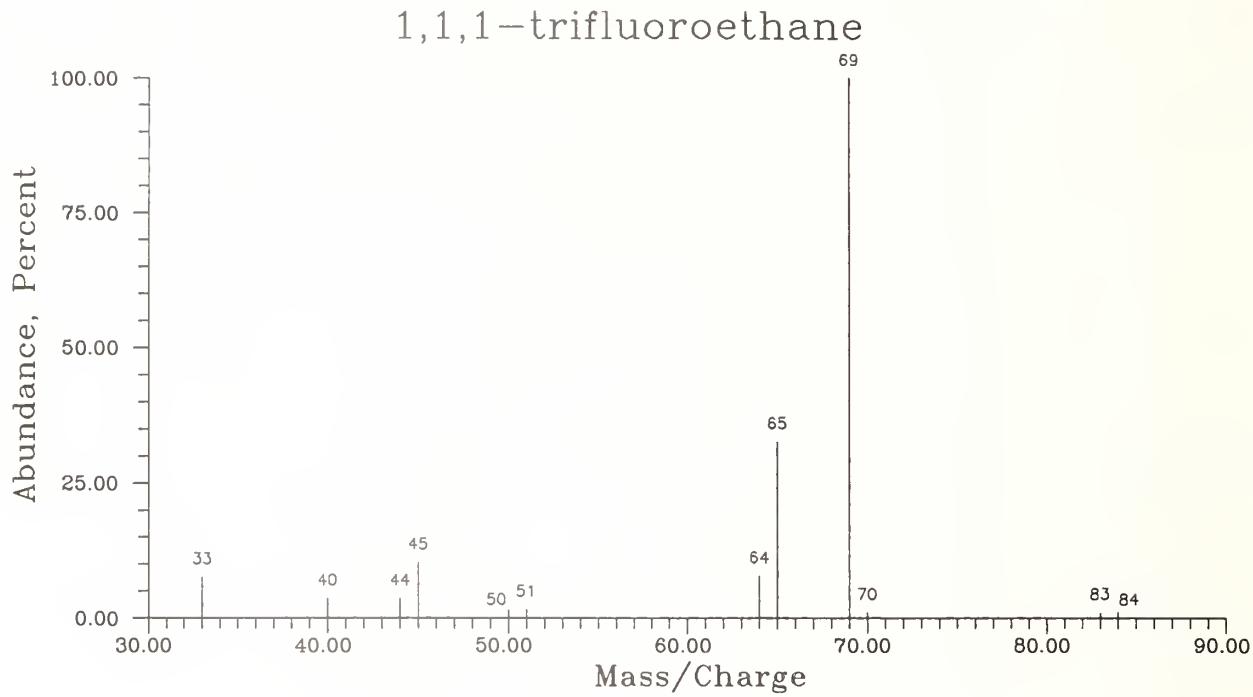
LEL: NA

Toxicology: Detailed toxicology is not available, but may be similar to other chlorofluoroethanes.

Reactivities and Chemical Incompatibilities: Details of reactivities are not known, but may be similar to other chlorofluoroethanes.

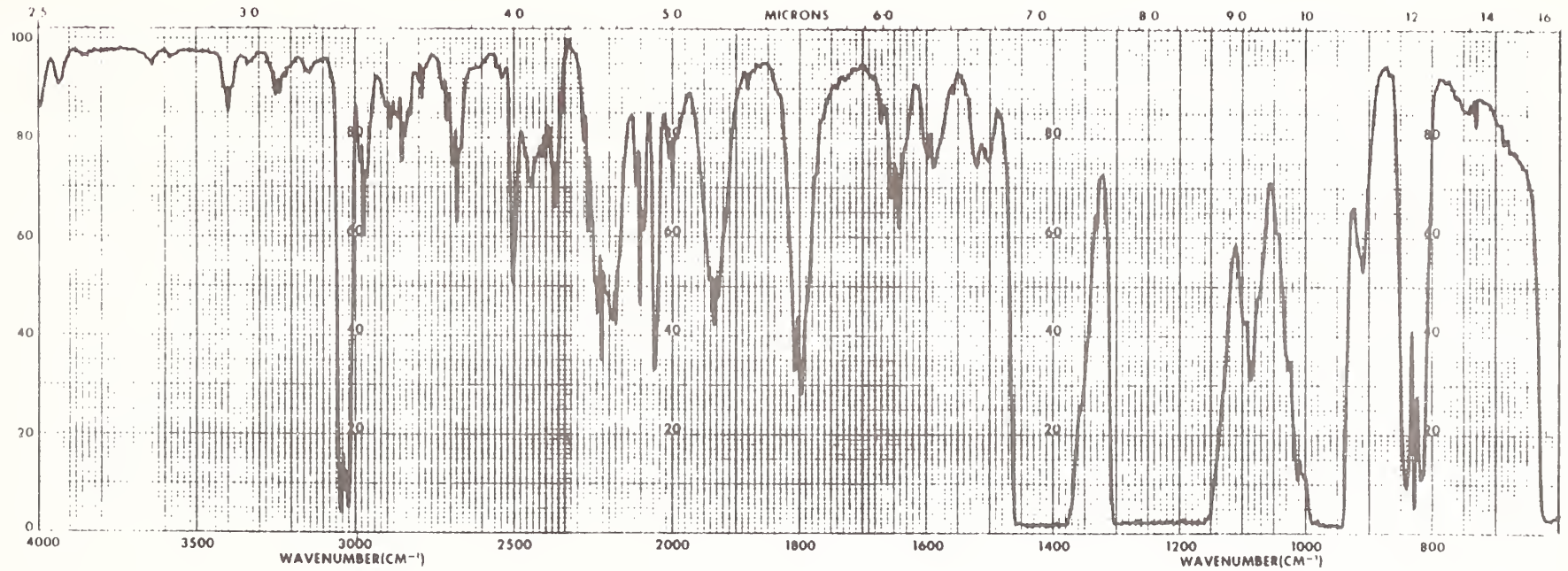
Solubilities: Soluble in ether, chloroform; negligible solubility in H_2O.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	120210	45.00	175561	64.00	133440	70.00	17439
33.00	129397	50.00	25700	65.00	555612	83.00	17311
40.00	62312	51.00	26516	69.00	1706907	84.00	16271
44.00	61732						

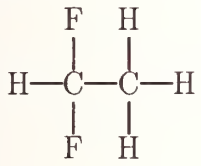
Infrared Spectrum – Gas Phase



152a 1,1-difluoroethane

synonyms: ethylidene difluoride; Algofrene type G7; UN 1030; Genetron 100.

structure:



C. A. S. Registry Number: 75–37–6
Relative Molecular Mass: 66.05

Normal Boiling Point: –24.7 °C

Melting Point: –117 °C

Density/Specific Gravity: 0.966 g/mL, l, (19 °C)

Critical Temperature: 113.5 °C

Refractive Index:

Critical Pressure: 4.52 MPa

Critical Density: 0.365 g/mL

****

Vapor Density: 2.3

PEL: NE

TLV: NE

Flash Point: NA

UEL: 18%

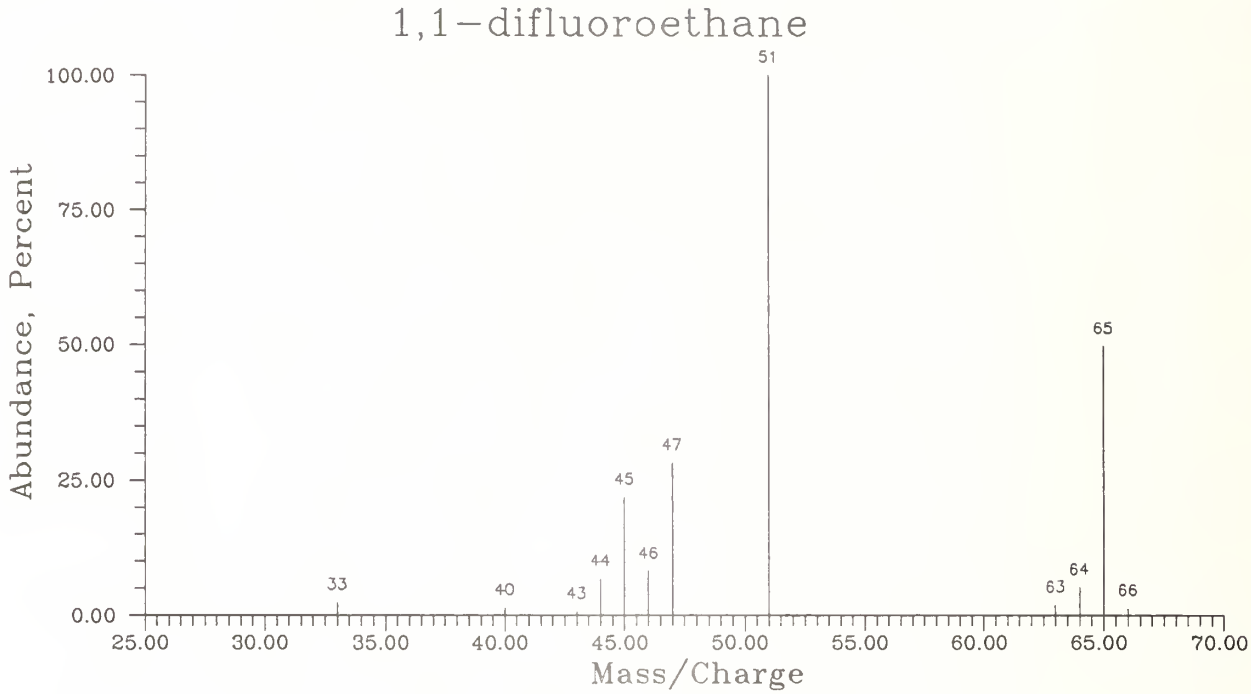
LEL: 3.7%

Toxicology: Pulmonary irritant; narcotic effects and anesthetic effects at high concentrations.

Reactivities and Chemical Incompatibilities: May produce HF, F^- upon thermal decomposition; incompatible with O_2, oxidizers, peroxidizers, active metals.

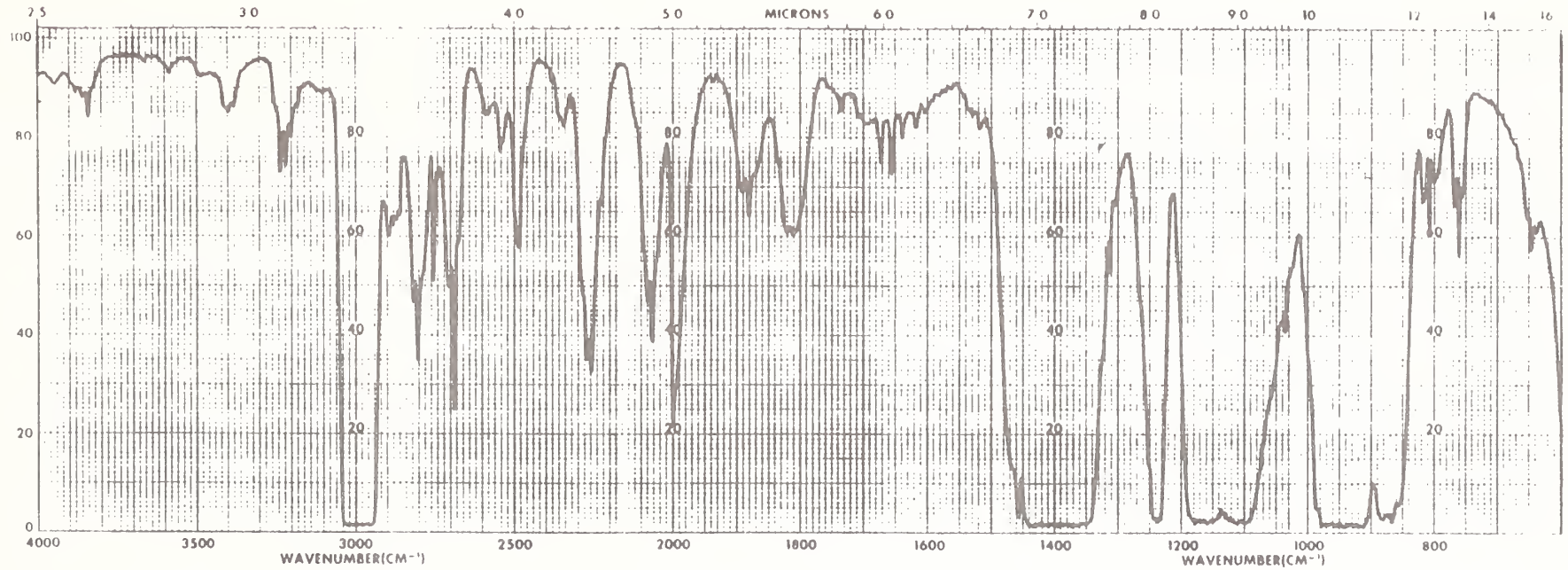
Solubilities: H_2O: 0 °C – 0.54 percent; 27.5 °C – 0.25 percent.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	335948	44.00	265459	47.00	1098537	64.00	200818
33.00	91587	45.00	851945	51.00	3914652	65.00	1945060
40.00	52435	46.00	317437	63.00	71383	66.00	49881
43.00	24575						

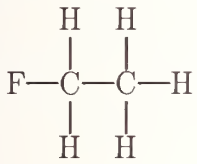
Infrared Spectrum – Gas Phase



161 fluoroethane

synonyms: ethylfluoride; UN 2453; monofluoroethane.

structure:



C. A. S. Registry Number: 353–36–6
Relative Molecular Mass: 48.06

Normal Boiling Point: –37.1 °C

Melting Point: –143.2 °C

Density/Specific Gravity:

Critical Temperature: 102.16 °C

Refractive Index: 1.2656, l, (20 °C)

Critical Pressure: 4.70 MPa*

Critical Density: 0.288 g/mL*

****

Vapor Density: 1.66

PEL: NE

TLV: NE

Flash Point: NA

UEL: NE

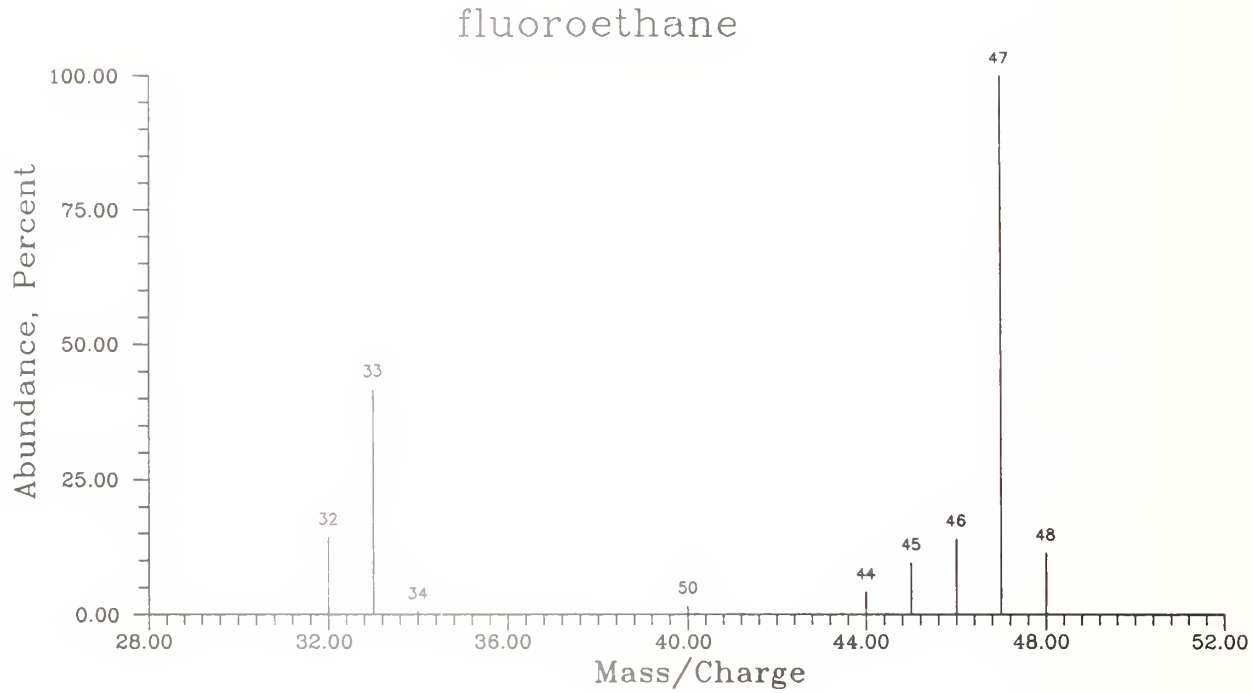
LEL: NE

Toxicology: Can cause pulmonary edema; narcotic at high concentration; simple asphyxiant.

Reactivities and Chemical Incompatibilities: Thermal decomposition can produce HF; avoid contact with active metals.

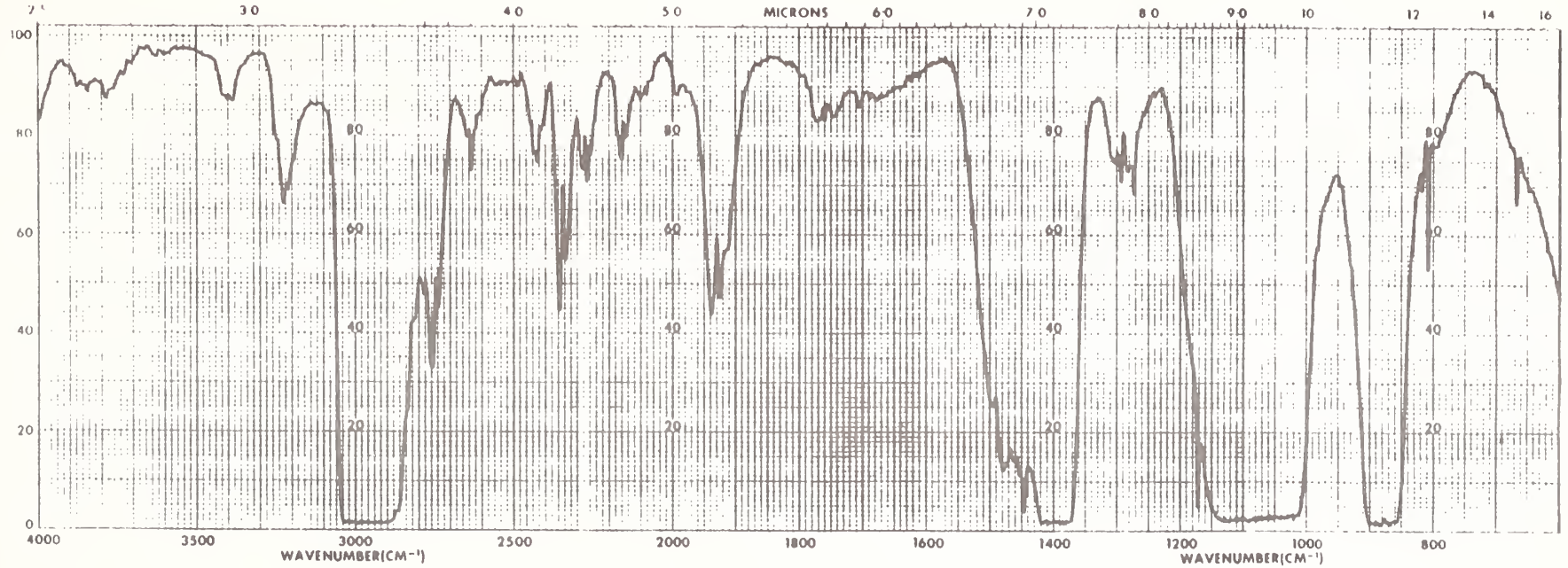
Solubilities: Slightly soluble in water; moderate solubility in alcohols, ethers, carbon tetrachloride.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
25.00	188302	32.00	471440	40.00	49517	46.00	461836
26.00	674246	33.00	1373825	44.00	135546	47.00	3305726
27.00	1739208	34.00	15966	45.00	315898	48.00	377159
31.00	102712	36.00	6925				

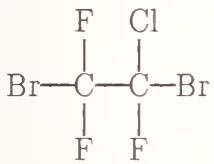
Infrared Spectrum – Gas Phase



113B2$\alpha\beta$
2-chloro-1,2-dibromo-1,1,2-trifluoroethane

synonyms: 1,2–dibromo–1–chlorotrifluoroethane.

structure:



C. A. S. Registry Number: 354–51–8
Relative Molecular Mass: 276.5

Normal Boiling Point: 93–94 °C

Melting Point:

Density/Specific Gravity:

Critical Temperature: 291.2 °C*

Refractive Index:

Critical Pressure: 5.15 MPa*

Critical Density: 0.968 g/mL*

****

Vapor Density: >1

PEL: NE

TLV: NE

Flash Point: does not flash

UEL: NA

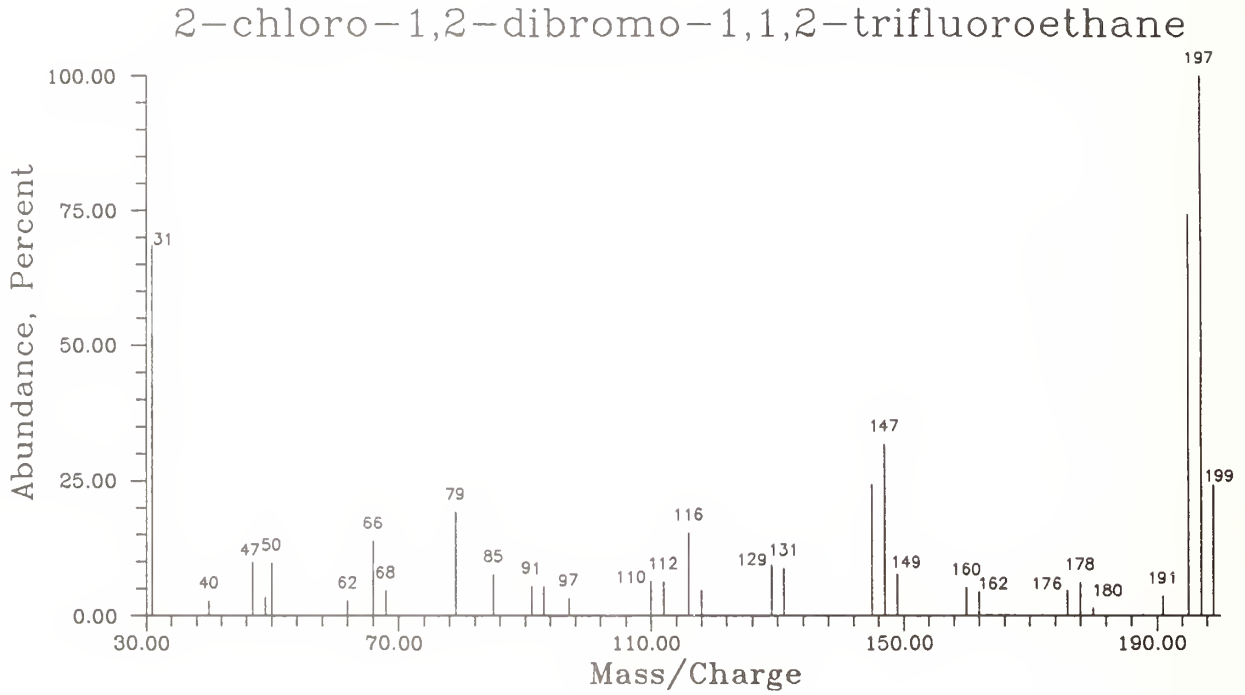
LEL: NA

Toxicology: Detailed toxicology is not available; may be harmful if inhaled or ingested through skin; may be irritating to eyes and mucous membranes.

Reactivities and Chemical Incompatibilities: Thermal decomposition can produce HF, HBr, CO, CO_2, carbonyl halides; avoid contact with oxidizing agents and halogens.

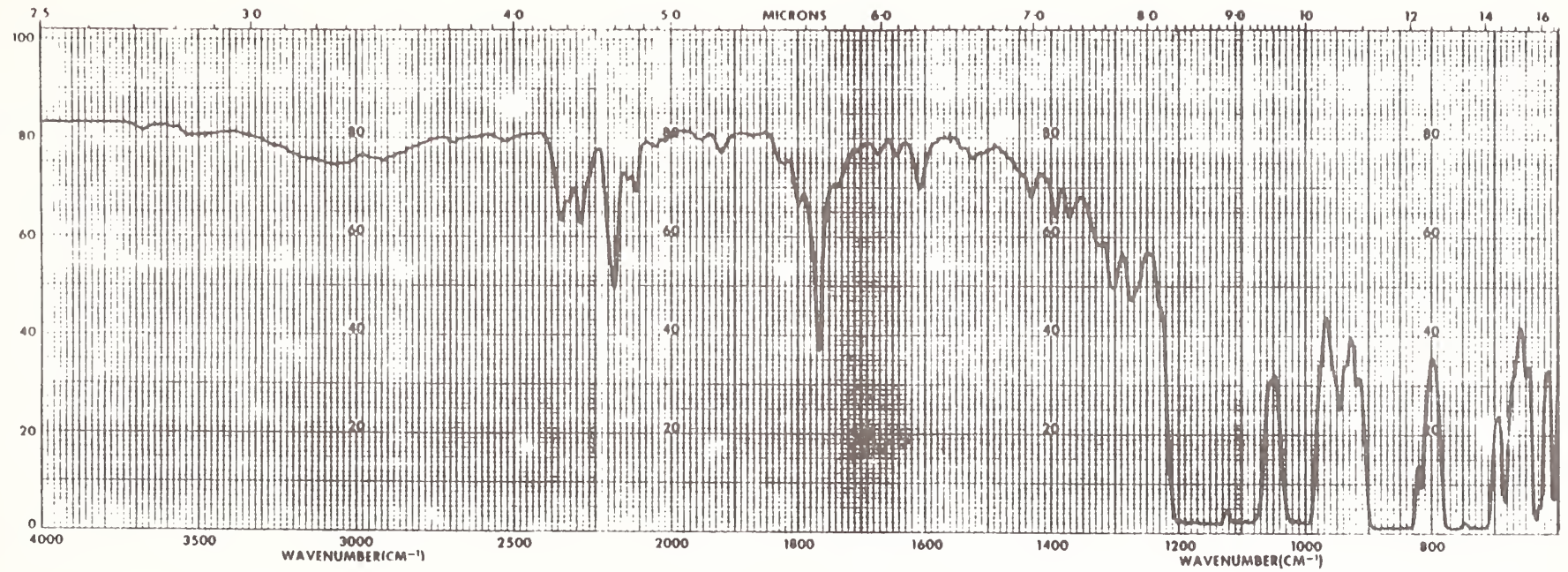
Solubilities: Somewhat soluble in carbon tetrachloride; negligible solubility in water.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	502084	81.00	144914	126.00	13323	162.00	32909
40.00	19565	85.00	55604	128.00	18875	176.00	34205
47.00	71658	91.00	39880	129.00	68609	178.00	44852
49.00	24423	93.00	38706	131.00	64411	180.00	10866
50.00	71274	97.00	22999	145.00	178443	191.00	26431
62.00	19828	110.00	46912	147.00	232601	195.00	544894
66.00	100649	112.00	45754	149.00	56657	197.00	734116
68.00	33127	116.00	112330	160.00	38107	199.00	177207
79.00	140094	118.00	35417				

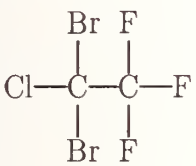
Infrared Spectrum – Liquid Phase (no solvent)



113B2 1-chloro-1,1-dibromotrifluoroethane

synonyms:

structure:



C. A. S. Registry Number: 754–17–6
Relative Molecular Mass: 275.5

Normal Boiling Point: 91–92 °C

Melting Point: 42–45 °C

Density/Specific Gravity:

Critical Temperature: 288.1 °C*

Refractive Index:

Critical Pressure: 5.1 MPa*

Critical Density: 0.973*

****

Vapor Density: >1

PEL: NE

TLV: NE

Flash Point: does not flash

UEL: NA

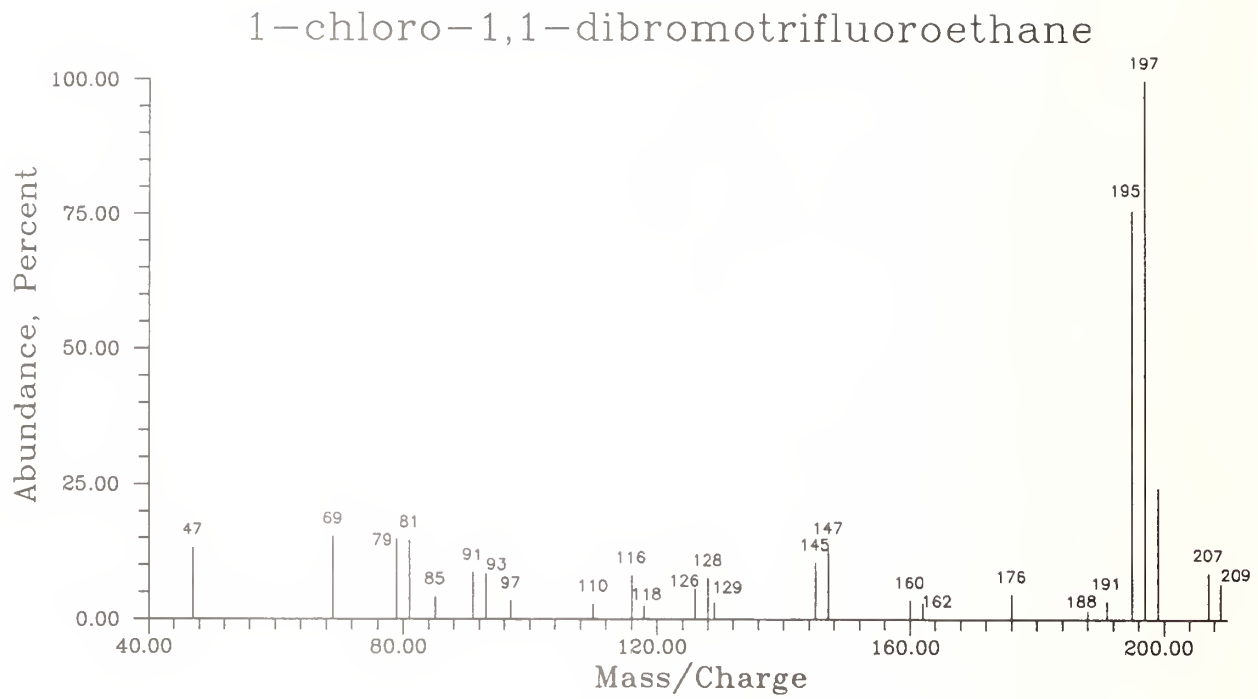
LEL: NA

Toxicology: Detailed toxicology is not available; may cause irritation to eyes, skin and mucous membranes.

Reactivities and Chemical Incompatibilities: May form HF, HBr, CO, CO_2 and carbonyl fluoride upon thermal decomposition.

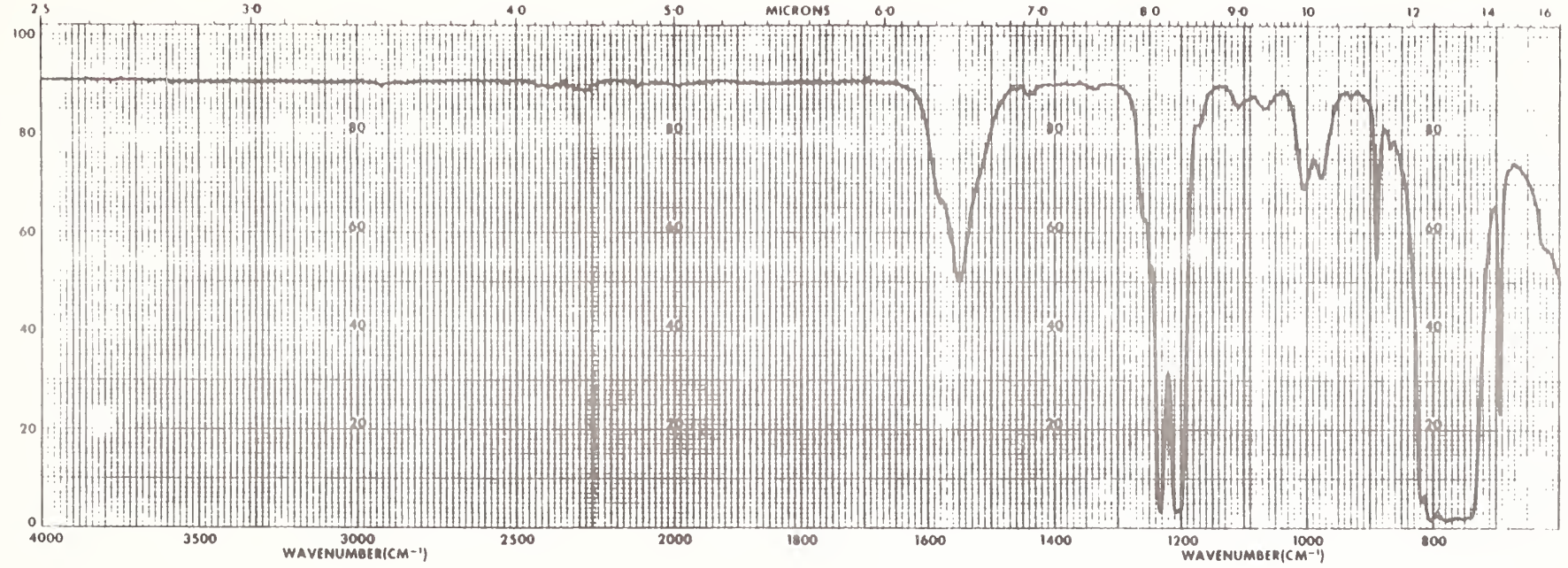
Solubilities: Somewhat soluble in carbon tetrachloride; negligible solubility in water.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	148585	81.00	98437	126.00	37968	178.00	41597
35.00	26535	85.00	27681	128.00	50789	188.00	10814
40.00	17807	91.00	57992	129.00	20423	191.00	22669
47.00	88761	93.00	56306	145.00	70706	195.00	510600
49.00	29060	97.00	15687	147.00	91496	197.00	674634
50.00	33326	110.00	18733	160.00	23360	199.00	164252
66.00	23251	116.00	53979	162.00	20259	207.00	58059
69.00	102933	118.00	16015	176.00	30863	209.00	44413
79.00	99665						

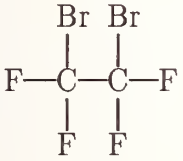
Infrared Spectrum — carbon tetrachloride solution



114B2 1,2-dibromotetrafluoroethane

synonyms: dibromotetrafluoroethane; sym–dibromotetrafluoroethane; Halon 2402.

structure:



C. A. S. Registry Number: 25497–30–7
Relative Molecular Mass: 259.82

Normal Boiling Point: 47.3 °C

Melting Point: –110.5 °C

Density/Specific Gravity: 2.163 g/mL (25 °C)

Critical Temperature: 219.4 °C*

Refractive Index:

Critical Pressure: 5.3 MPa*

Critical Density: 1.03 g/mL*

****

Vapor Density: 10 g/l (47.3 °C)

PEL: NE

TLV: NE

Flash Point: NA

UEL: NA

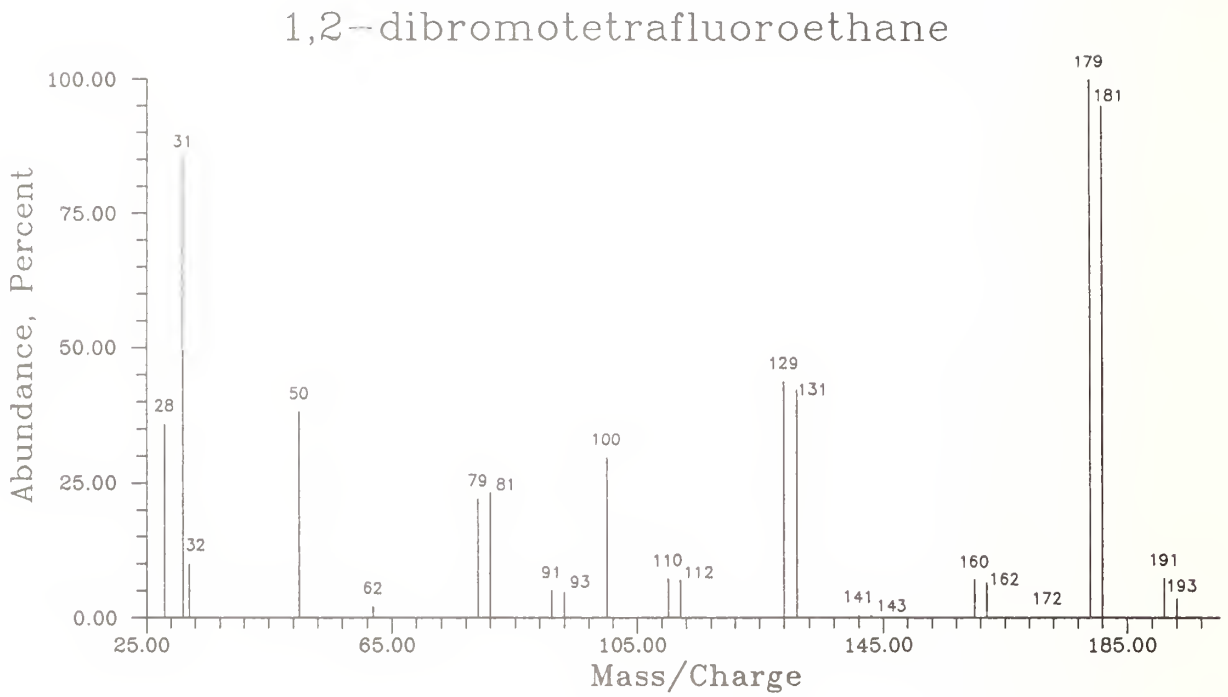
LEL: NA

Toxicology: Inhalation of concentrations in excess of 100g/m^3 (approx. 1 percent, vol/vol) for over 30 seconds depresses the central nervous system, may cause narcosis, and irreversible damage to the cardiocirculatory system. (Suggested TLV 1000 ppm for 1 minute, by NFPA.)

Reactivities and Chemical Incompatibilities: Thermal decomposition can produce HF, HBr, CO, CO_2; avoid contact with ABS resins and polystyrene.

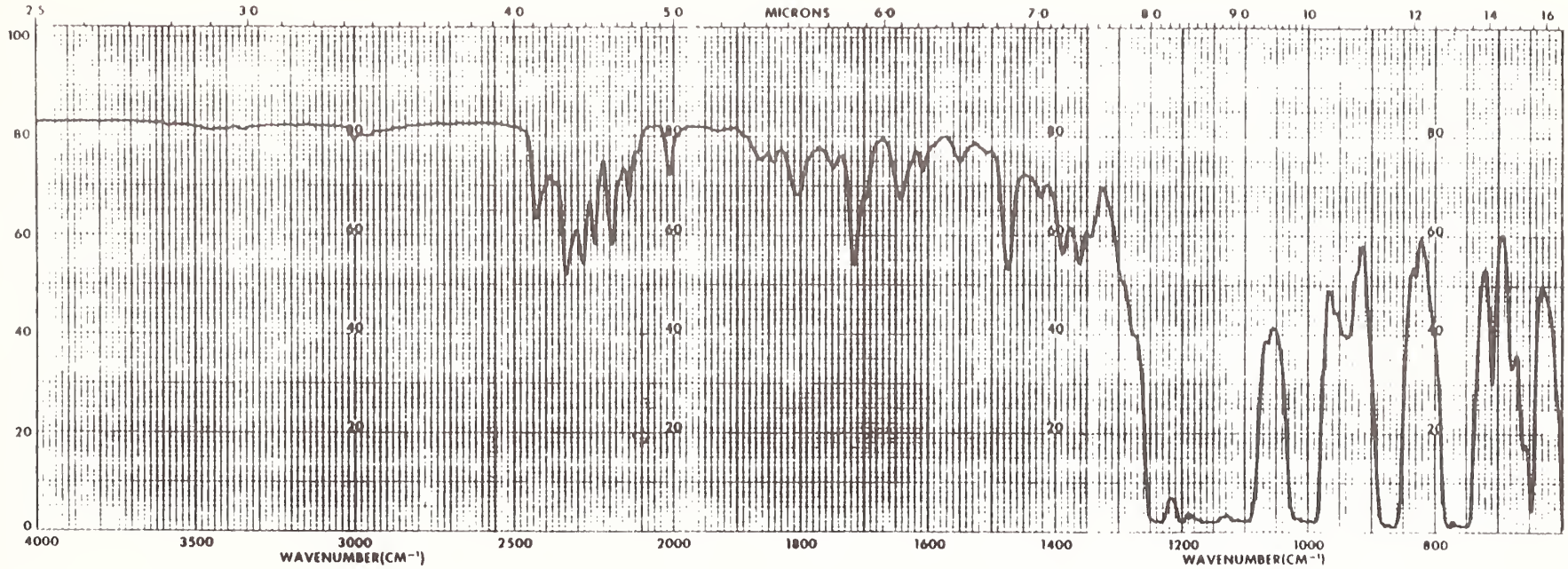
Solubilities: Negligible solubility in water.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
28.00	272202	79.00	167018	112.00	52723	162.00	49296
31.00	646049	81.00	176286	129.00	332039	172.00	1350
32.00	75637	91.00	38134	131.00	319892	179.00	760738
50.00	289411	93.00	35474	141.00	2970	181.00	724019
62.00	15350	100.00	224989	143.00	3255	191.00	55794
69.00	137368	110.00	55030	160.00	53244	193.00	26377

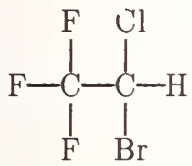
Infrared Spectrum – Liquid Phase (no solvent)



123B1 2-bromo-2-chloro-1,1,1-trifluoroethane

synonyms:

structure:



C. A. S. Registry Number: 151–67–7
Relative Molecular Mass: 197.39

Normal Boiling Point: 50.2 °C

Melting Point: NA

Density/Specific Gravity: 1.872 (20 °C)

Critical Temperature: 223.0 °C*

Refractive Index:

Critical Pressure: 4.8 MPa*

Critical Density: 0.750 g/mL*

****

Vapor Density: NA

PEL: NE

TLV: NE

Flash Point: nonflammable

UEL: NA

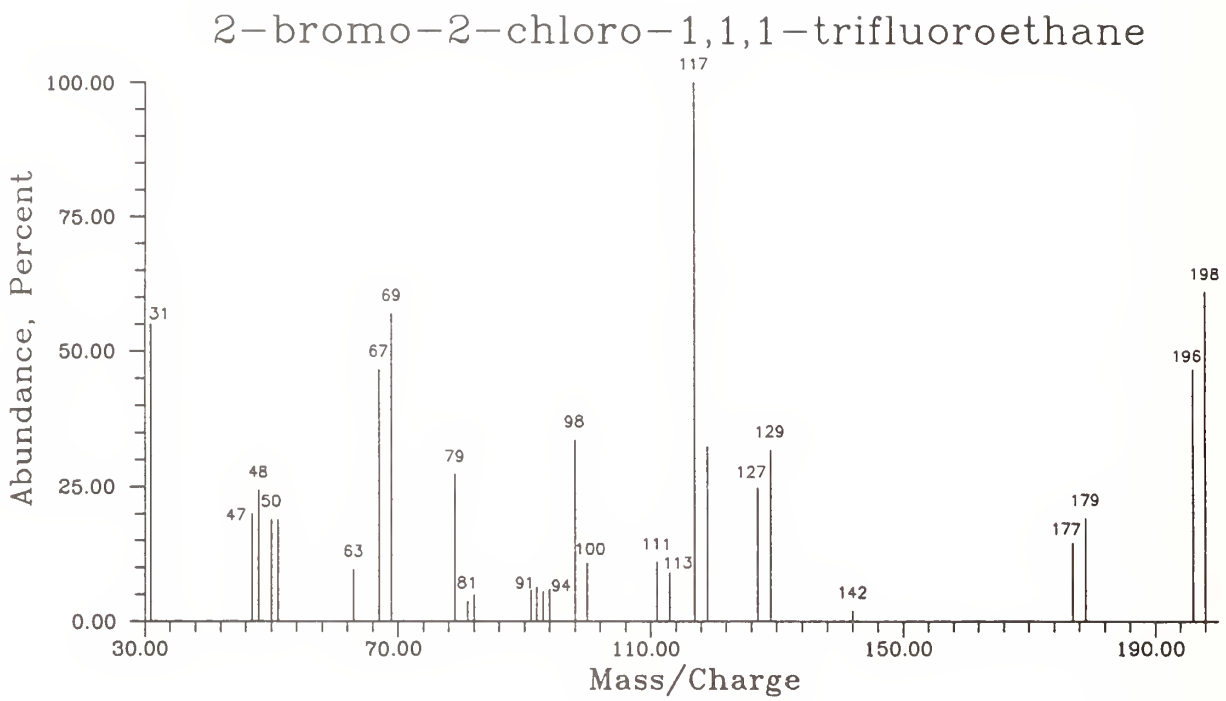
LEL: NA

Toxicology: May cause pulmonary edema and congestion, and tachycardia; anesthetic at higher concentrations.

Reactivities and Chemical Incompatibilities: Thermal decomposition may produce HF, HBr, HCl, CO, CO_2, phosgene; avoid contact with alkali metals and powdered metals.

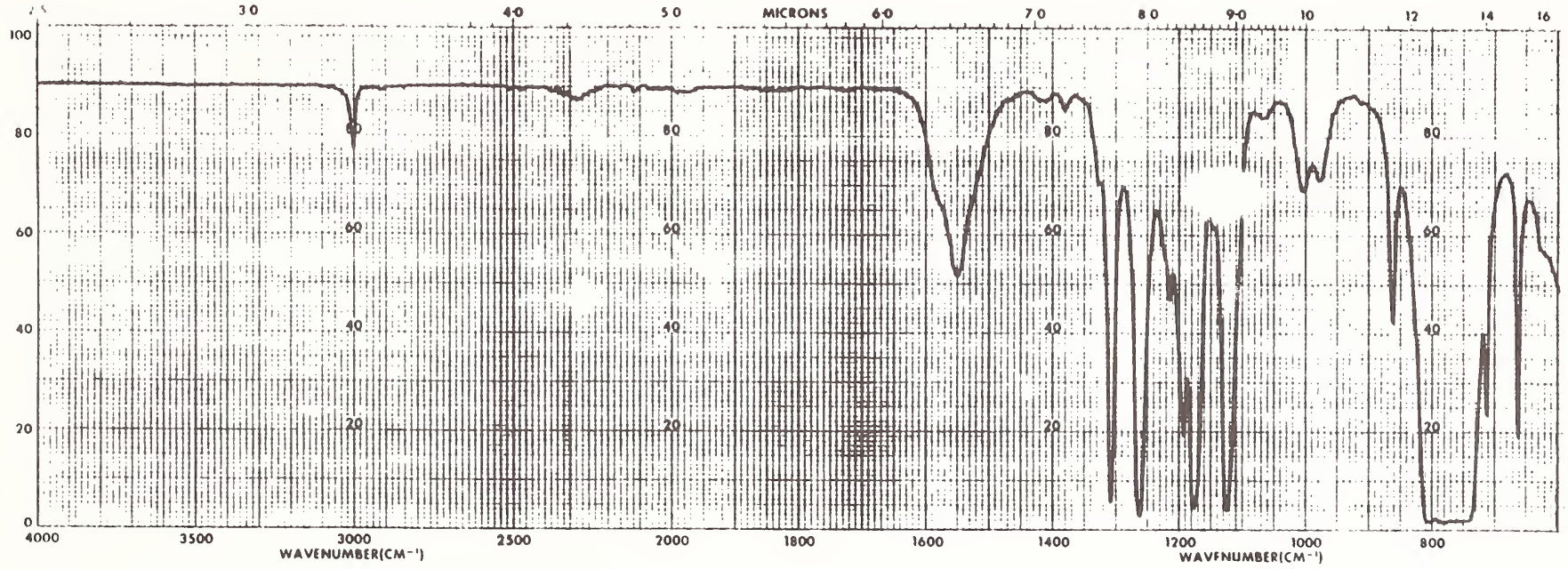
Solubilities: H_2O: 0.01 – 0.1 percent, wt/wt.

Mass Spectrum:

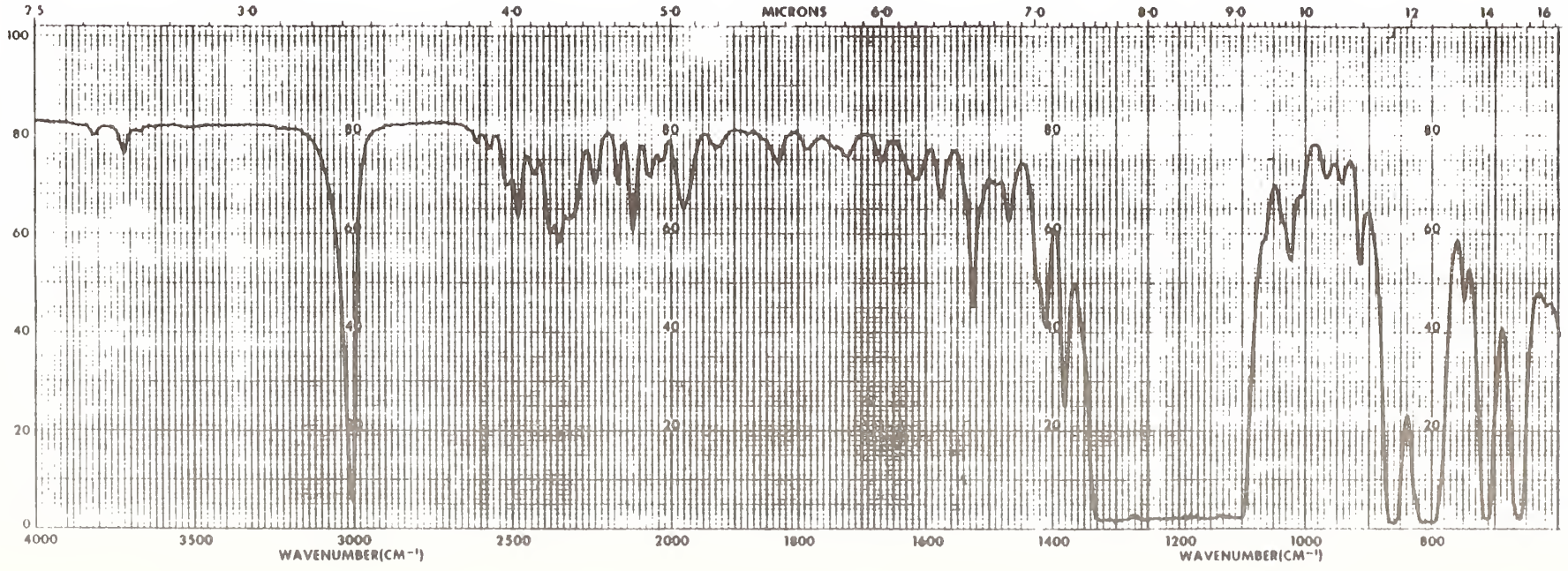


m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	326743	79.00	161308	98.00	199204	129.00	188469
47.00	118546	81.00	157911	100.00	64167	142.00	11660
48.00	144961	82.00	29146	111.00	55039	144.00	11504
50.00	111780	91.00	34091	113.00	53026	177.00	86880
51.00	111666	92.00	37651	117.00	593930	179.00	113511
63.00	56648	93.00	32711	119.00	192311	196.00	276811
67.00	276627	94.00	35901	127.00	146372	198.00	362394
69.00	337757						

Infrared Spectrum – carbon tetrachloride solution



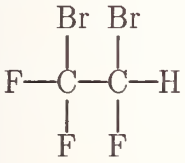
Infrared Spectrum – Liquid Phase (no solvent)



123B2 1,2-dibromo-1,1,2-trifluoroethane

synonyms:

structure:



C. A. S. Registry Number: 354–04–1
Relative Molecular Mass: 241.8

Normal Boiling Point: 76 °C

Melting Point: NA

Density/Specific Gravity:

Critical Temperature: 267.7 °C*

Refractive Index:

Critical Pressure: 4.9 MPa*

Critical Density: 0.846 g/mL*

****

Vapor Density: >1

PEL: NE

TLV: NE

Flash Point: does not flash

UEL: NA

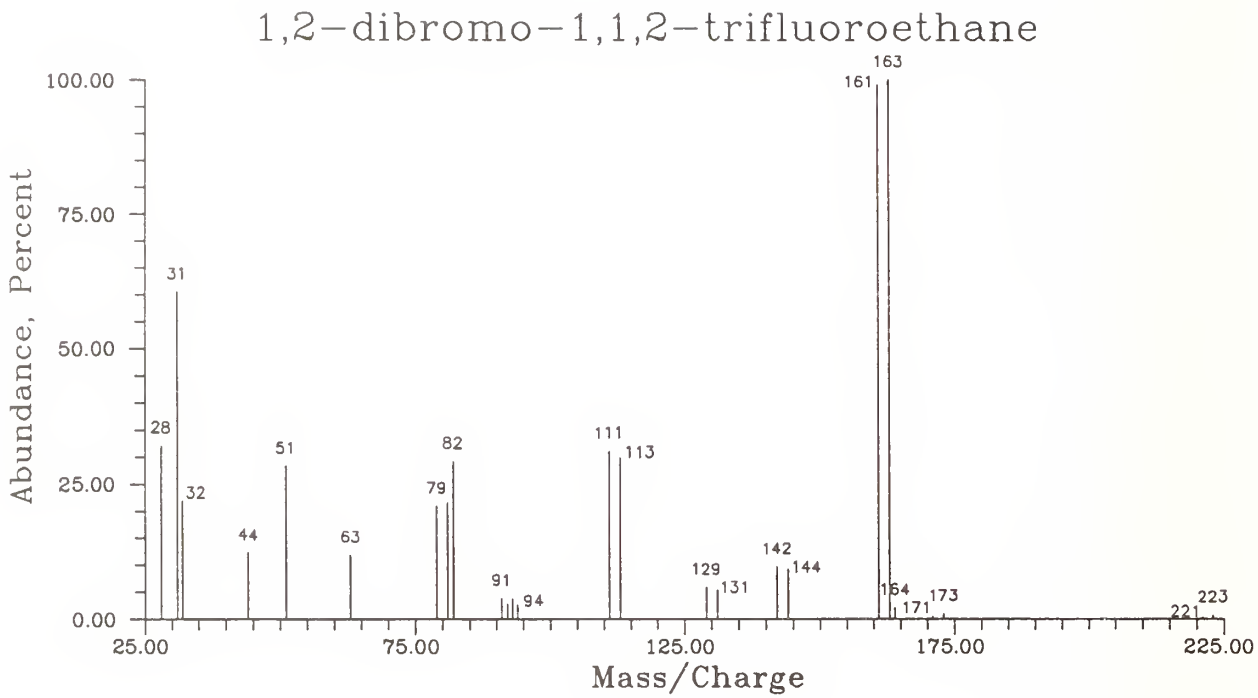
LEL: NA

Toxicology: Detailed toxicology is not available; may be harmful if inhaled or ingested through the skin; may be narcotic at higher concentrations.

Reactivities and Chemical Incompatibilities: Thermal decomposition may produce HF, HBr, Br_2, F_2, CO, CO_2.

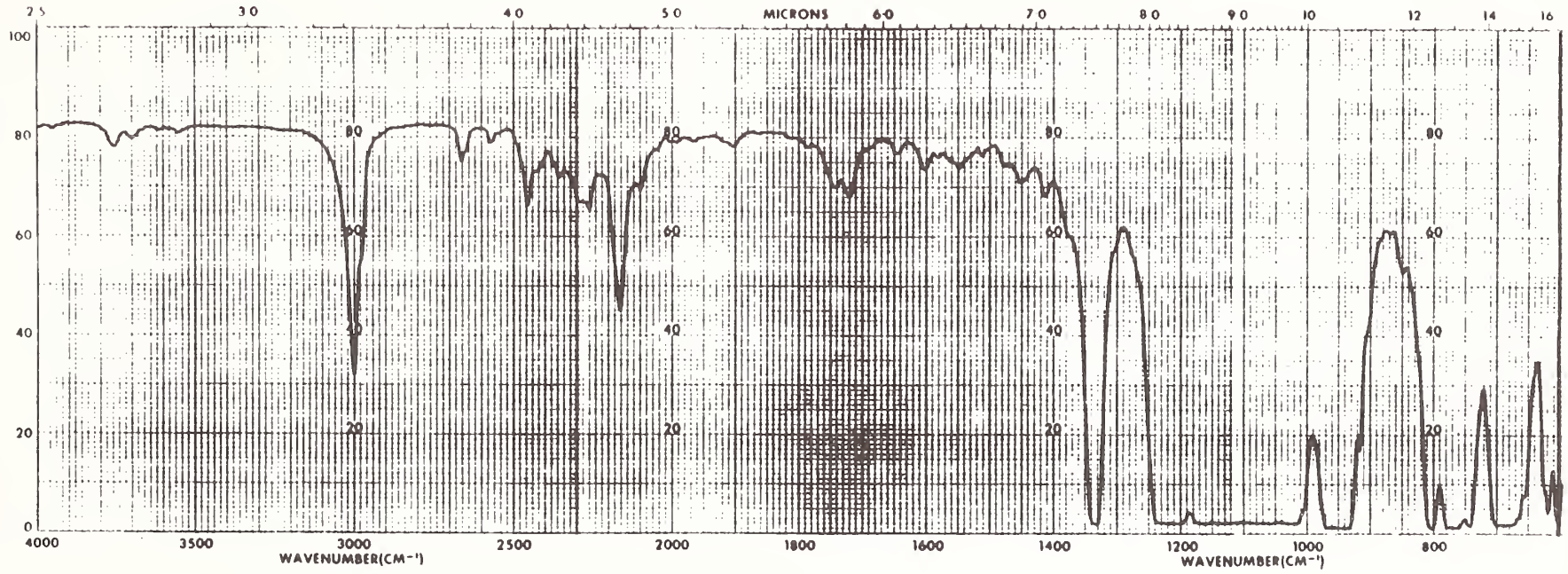
Solubilities: Negligible solubility in water.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
28.00	313245	79.00	201591	111.00	300500	163.00	967502
31.00	585547	81.00	207994	113.00	289116	164.00	20038
32.00	211288	82.00	281942	129.00	56417	171.00	4969
44.00	118593	91.00	36852	131.00	52148	173.00	9052
50.00	68169	92.00	27235	142.00	93390	221.00	3440
51.00	273007	93.00	35655	144.00	88919	223.00	6682
63.00	114024	94.00	25414	161.00	958517		

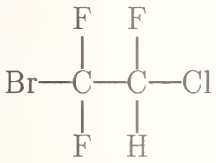
Infrared Spectrum – Liquid Phase (no solvent)



123aB1α
1-bromo-2-chloro-1,1,2-trifluoroethane

synonyms:

structure:



C. A. S. Registry Number: 354–06–3
Relative Molecular Mass: 197.4

Normal Boiling Point: 50–55 °C

Melting Point: NA

Density/Specific Gravity: 1.8636 (25 °C)

Critical Temperature: 239.4 °C*

Refractive Index:

Critical Pressure: 6.05 MPa*

Critical Density: 0.809 g/mL*

****

Vapor Density: >1

PEL: NE

TLV: NE

Flash Point: not flammable

UEL: NA

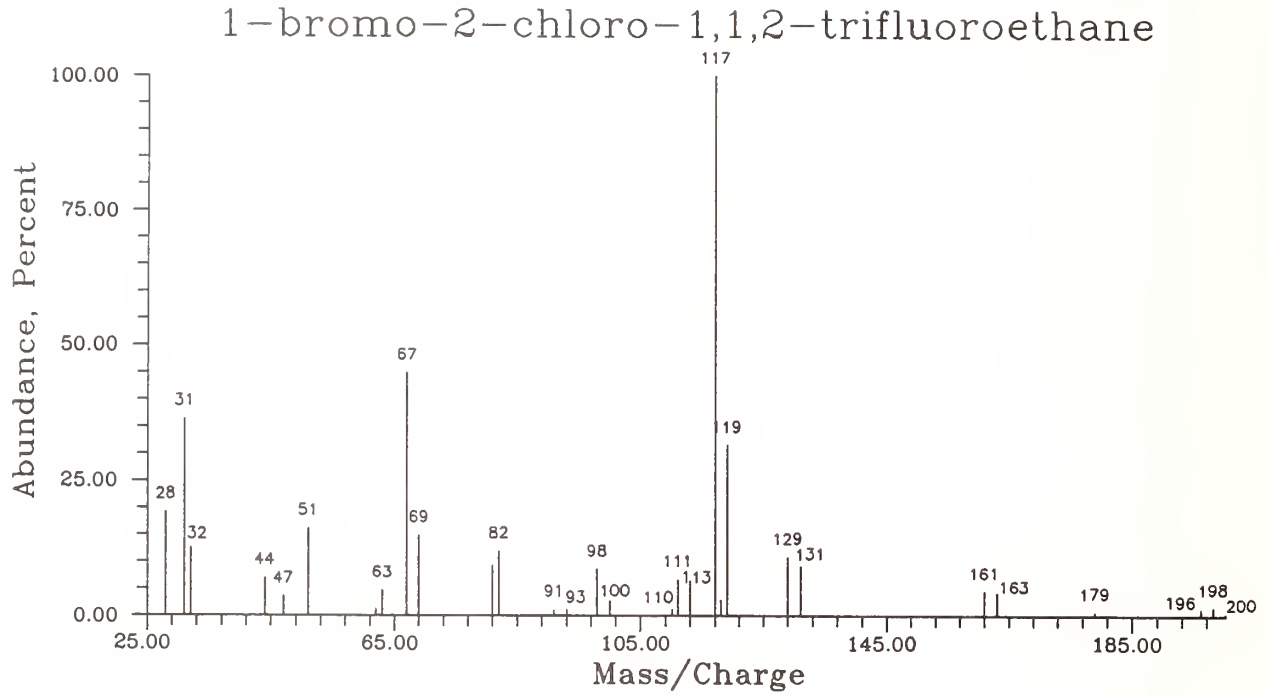
LEL: NA

Toxicology: Detailed toxicology is not available; may cause eye irritation and possible anesthesia.

Reactivities and Chemical Incompatibilities: Thermal decomposition can produce HF, HBr, and HCl.

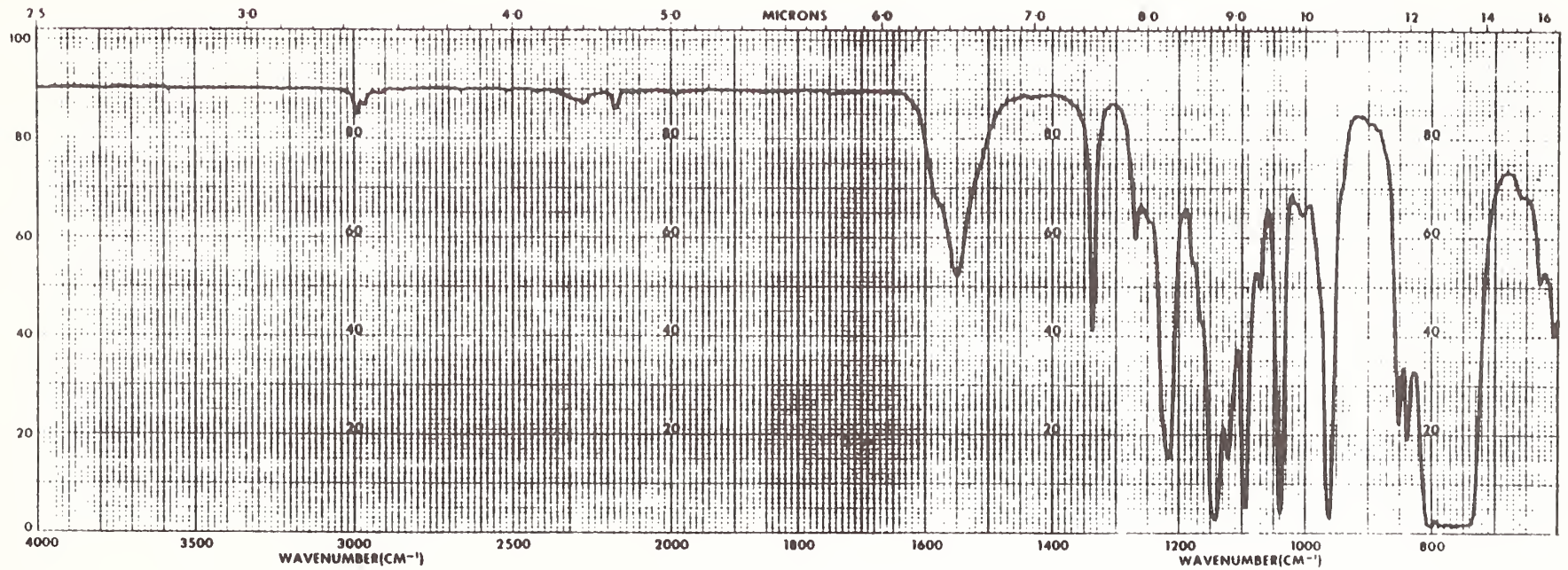
Solubilities: Negligible solubility in water.

Mass Spectrum:

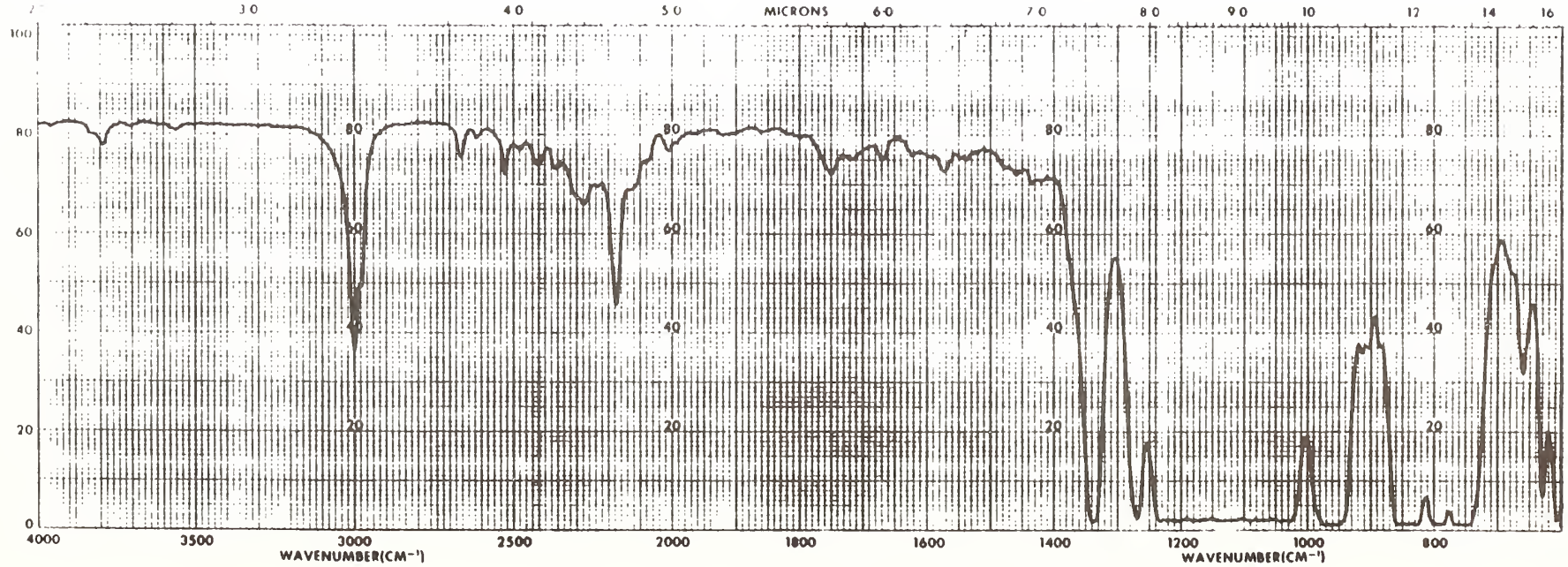


m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
28.00	272979	69.00	210798	110.00	17721	129.00	154588
31.00	517192	79.00	129713	111.00	95254	131.00	131374
32.00	179333	81.00	130636	112.00	18592	161.00	64547
44.00	99188	82.00	169759	113.00	92772	163.00	59479
47.00	50523	85.00	15316	117.00	1424313	179.00	11130
51.00	229563	91.00	16381	118.00	40755	196.00	18916
62.00	17822	93.00	15349	119.00	449633	198.00	23264
63.00	66319	98.00	122686	127.00	20694	200.00	5955
67.00	638402	100.00	39391				

Infrared Spectrum — carbon tetrachloride solution



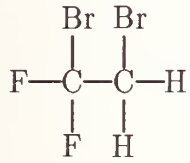
Infrared Spectrum – Liquid Phase (no solvent)



132bB2 1,2-dibromo-1,1-difluoroethane

synonyms: difluorodibromoethane; 1,1–difluoro–1,2–dibromoethane.

structure:



C. A. S. Registry Number: 75–82–1
Relative Molecular Mass: 223.86

Normal Boiling Point: 92–93 °C

Melting Point: –63.1 °C

Density/Specific Gravity: 2.2238 (20/4)

Critical Temperature: 300.7 °C*

Refractive Index:

Critical Pressure: 5.59 MPa*

Critical Density: 0.826 g/mL*

****

Vapor Density: >

PEL: NE

TLV: NE

Flash Point: NA

UEL: NA

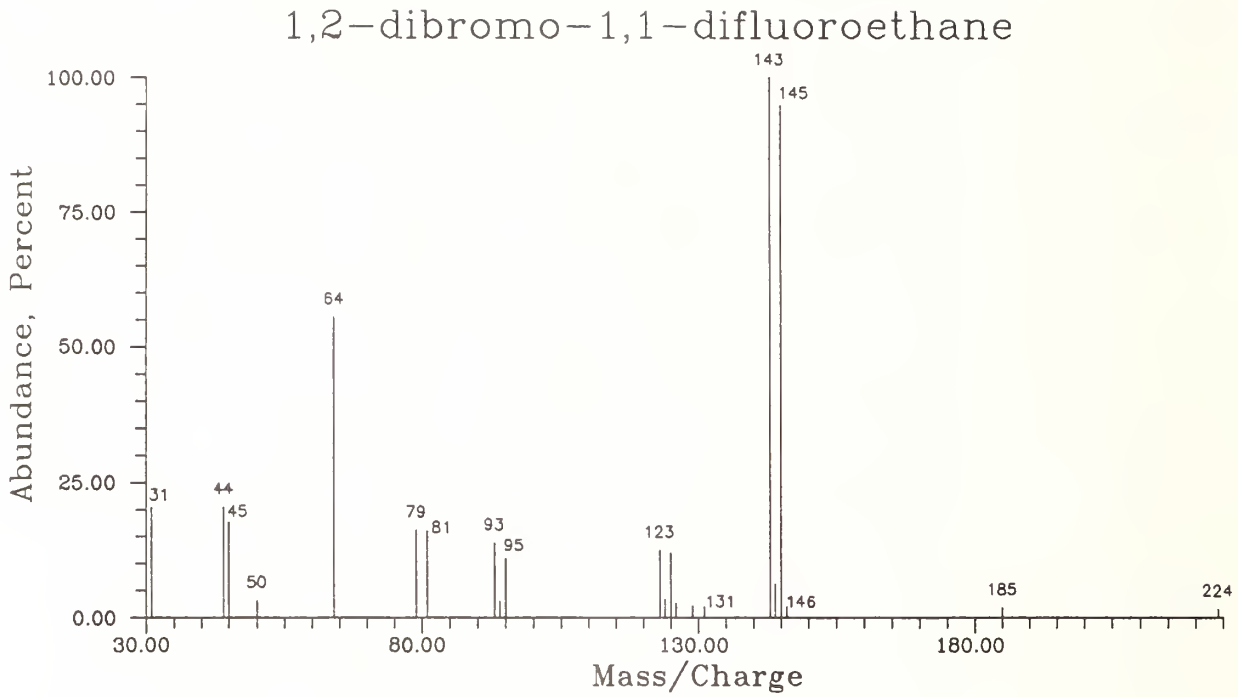
LEL: NA

Toxicology: Detailed toxicology is not available; possible pulmonary irritant.

Reactivities and Chemical Incompatibilities: Thermal decomposition can produce HF, HBr, CO, CO_2; avoid contact with active metals.

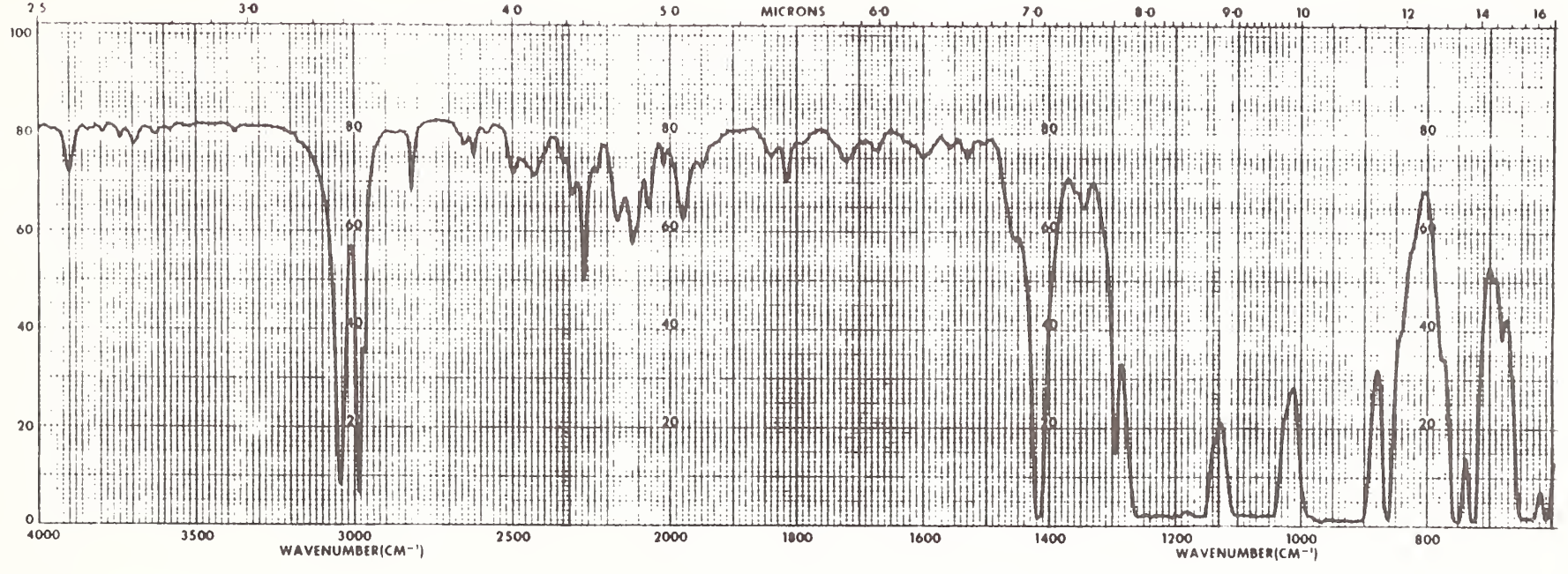
Solubilities: Negligible solubility in water.

Mass Spectrum:

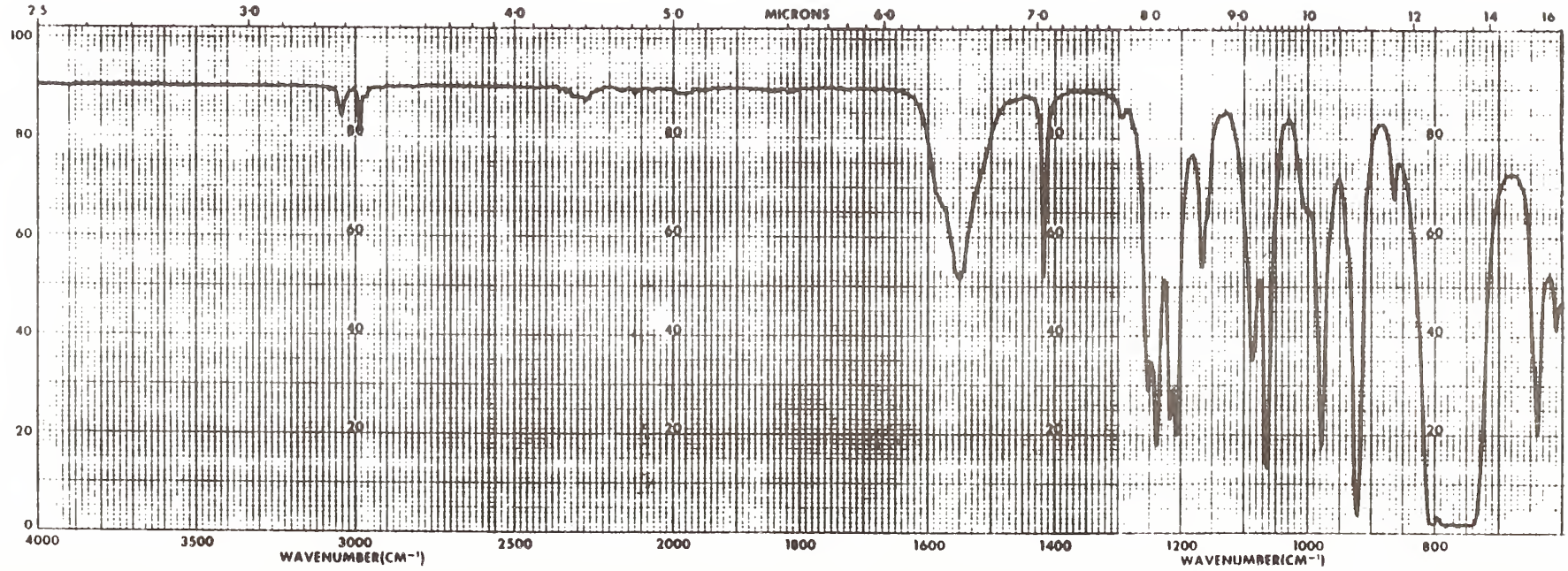


m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	152468	81.00	116715	125.00	89079	144.00	46614
44.00	152681	93.00	102832	126.00	19559	145.00	708593
45.00	131715	94.00	22218	129.00	15999	146.00	14890
50.00	23289	95.00	81022	131.00	15099	185.00	13430
64.00	414428	123.00	92725	143.00	747150	224.00	11949
79.00	120632	124.00	25248				

Infrared Spectrum – Liquid Phase (no solvent)



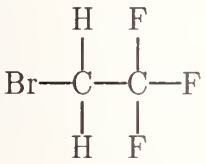
Infrared Spectrum — carbon tetrachloride solution



133aB1 2,2,2-trifluoroethyl bromide

synonyms: 1–bromo–2,2,2–trifluoroethane; 2,2,2–trifluoro–1–bromoethane.

structure:



C. A. S. Registry Number: 421–06–7
Relative Molecular Mass: 162.9

Normal Boiling Point: 26 °C

Melting Point: –94 °C

Density/Specific Gravity: 1.7881 (20/4)

Critical Temperature: 191.4 °C*

Refractive Index:

Critical Pressure: 5.46 MPa*

Critical Density: 0.744 g/mL*

****

Vapor Density: >1

PEL: NE

TLV: NE

Flash Point: NA

UEL: NA

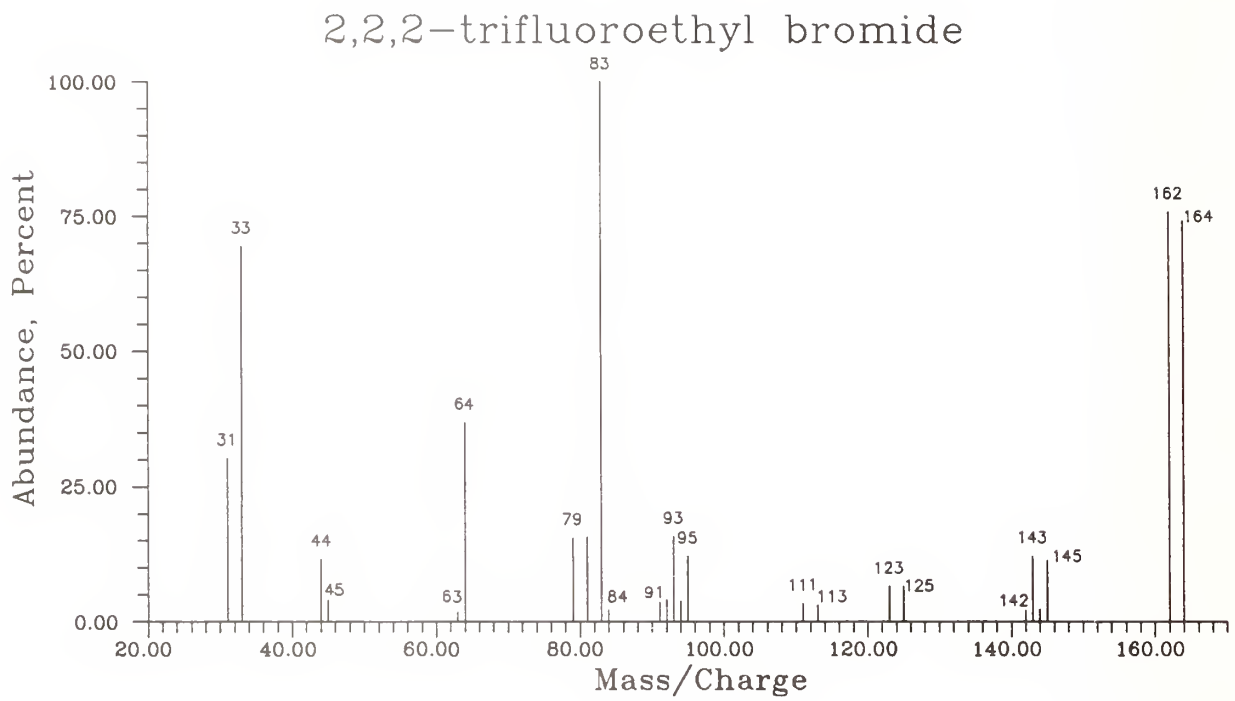
LEL: NA

Toxicology: Detailed toxicology is not available; may cause skin irritation.

Reactivities and Chemical Incompatibilities: Thermal decomposition can produce HF, HBr, CO, CO_2; avoid contact with strong oxidants.

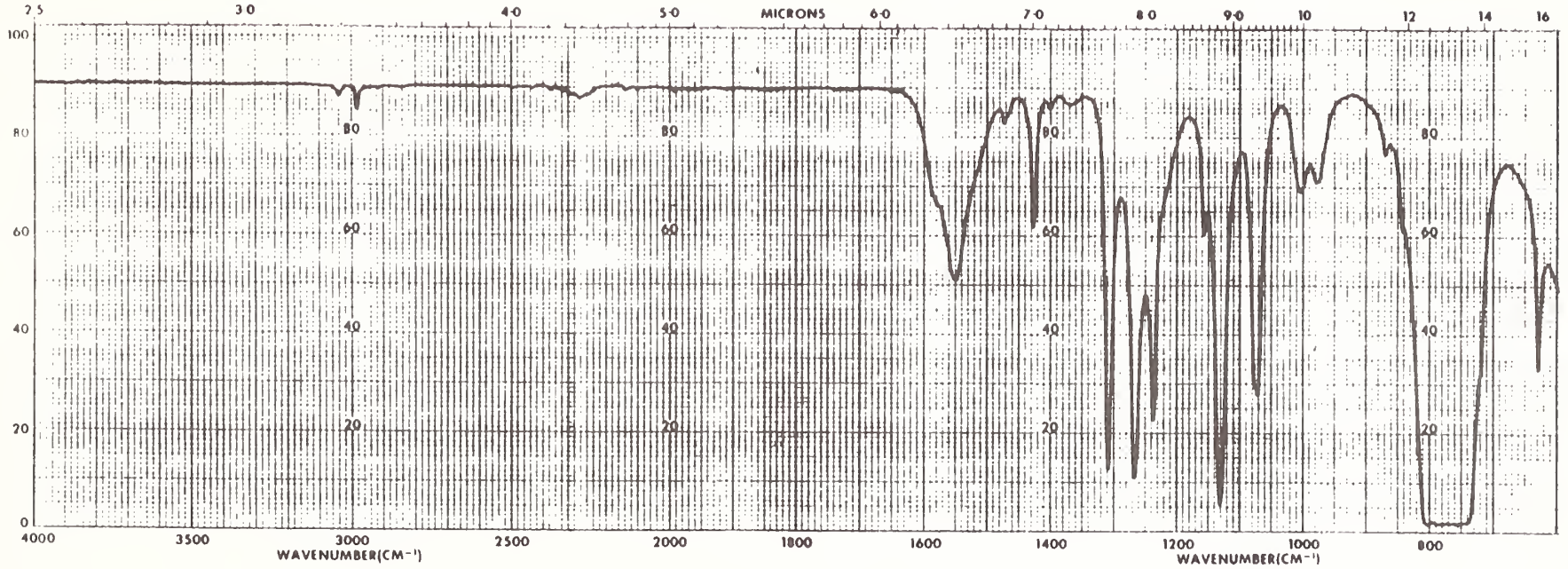
Solubilities: Negligible solubility in water; somewhat soluble in carbon tetrachloride.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	220796	64.00	268264	92.00	29540	125.00	45713
33.00	506697	69.00	208445	93.00	115203	142.00	15941
44.00	85001	79.00	113954	94.00	28411	143.00	69256
45.00	28686	81.00	114494	95.00	88612	144.00	16944
50.00	38684	83.00	730208	111.00	24890	145.00	83077
51.00	48400	84.00	15626	113.00	22142	162.00	554997
63.00	127614	91.00	26292	123.00	47899	164.00	542881

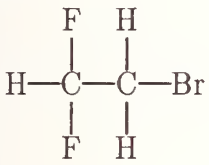
Infrared Spectrum – Gas Phase



142B1 2-bromo-1,1-difluoroethane

synonyms: bromodifluoroethane; 1–bromo–2,2–difluoroethane.

structure:



C. A. S. Registry Number: 359–07–9
Relative Molecular Mass: 144.94

Normal Boiling Point: –57.3 °C

Melting Point:

Density/Specific Gravity: 1.824 (18.5/4)

Critical Temperature: 64.7 °C*

Refractive Index:

Critical Pressure: 4.93 MPa*

Critical Density: 0.580 g/mL

****

Vapor Density: >1 **PEL:** NE **TLV:** NE

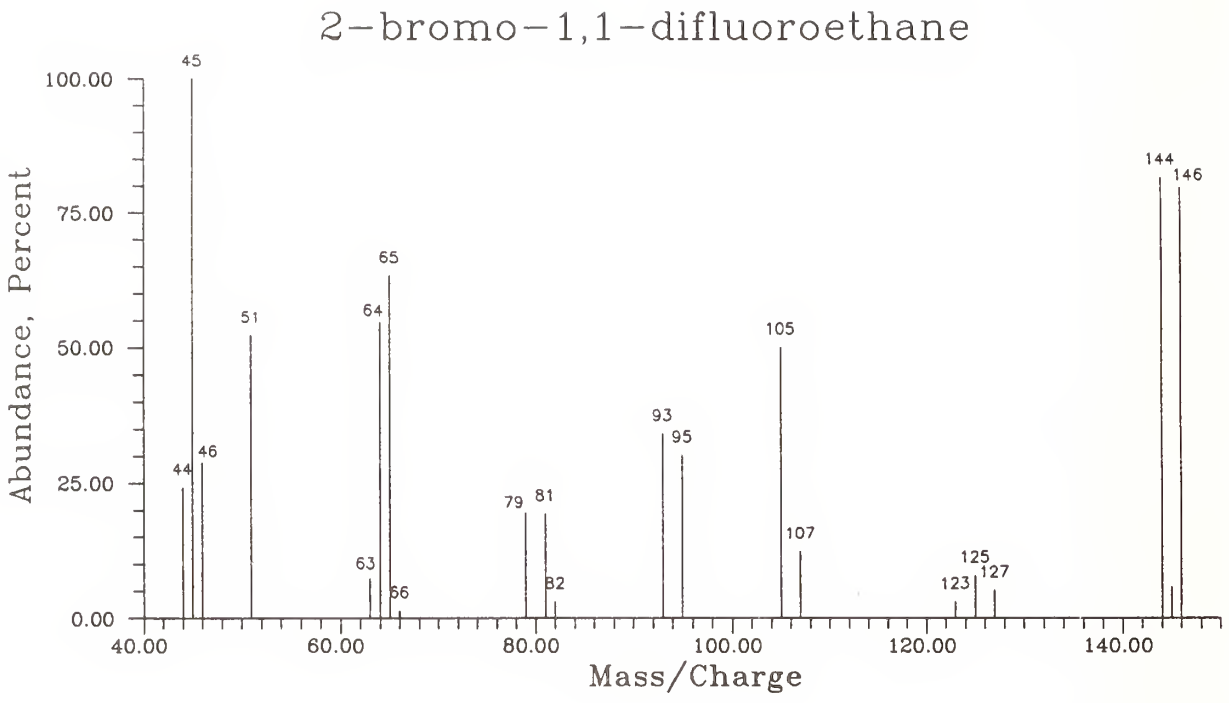
Flash Point: NA **UEL:** NA **LEL:** NA

Toxicology: Detailed toxicology is not available; may be irritating to skin, eyes, mucous membranes.

Reactivities and Chemical Incompatibilities: Thermal decomposition can result in the formation of HF, HBr, F_2, Br_2, CO, CO_2; avoid contact with oxidizing agents and halogens.

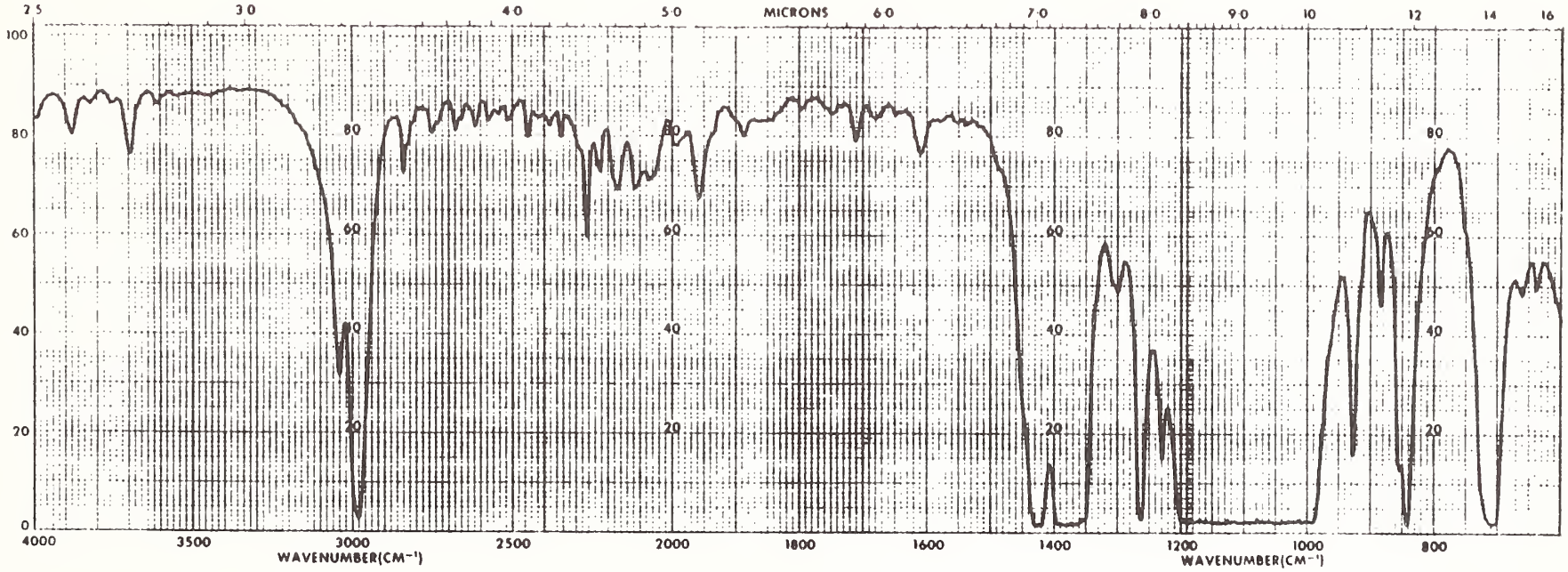
Solubilities: Somewhat soluble in carbon tetrachloride; negligible solubility in water.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	228053	64.00	436582	91.00	31508	123.00	23817
44.00	193295	65.00	506412	92.00	31845	125.00	63363
45.00	799832	66.00	10928	93.00	271936	127.00	41018
46.00	230517	79.00	155227	95.00	240789	144.00	653883
51.00	417684	81.00	154242	105.00	100140	145.00	45812
63.00	58667	82.00	24063	107.00	98191	146.00	637974

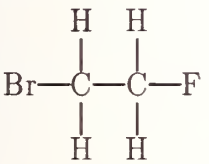
Infrared Spectrum – Liquid Phase (no solvent)



151B1 1-bromo-2-fluoroethane

synonyms: bromofluoroethane

structure:



C. A. S. Registry Number: 762–49–2
Relative Molecular Mass: 126.95

Normal Boiling Point: 71–72 °C

Melting Point: NA

Density/Specific Gravity: 1.7044 (25/4)

Critical Temperature: 273.6 °C*

Refractive Index: 1.4236 (20)

Critical Pressure: 5.6 MPa*

Critical Density: 0.533 g/mL*

****

Vapor Density: >1

PEL: NE

TLV: NE

Flash Point: NA

UEL: NA

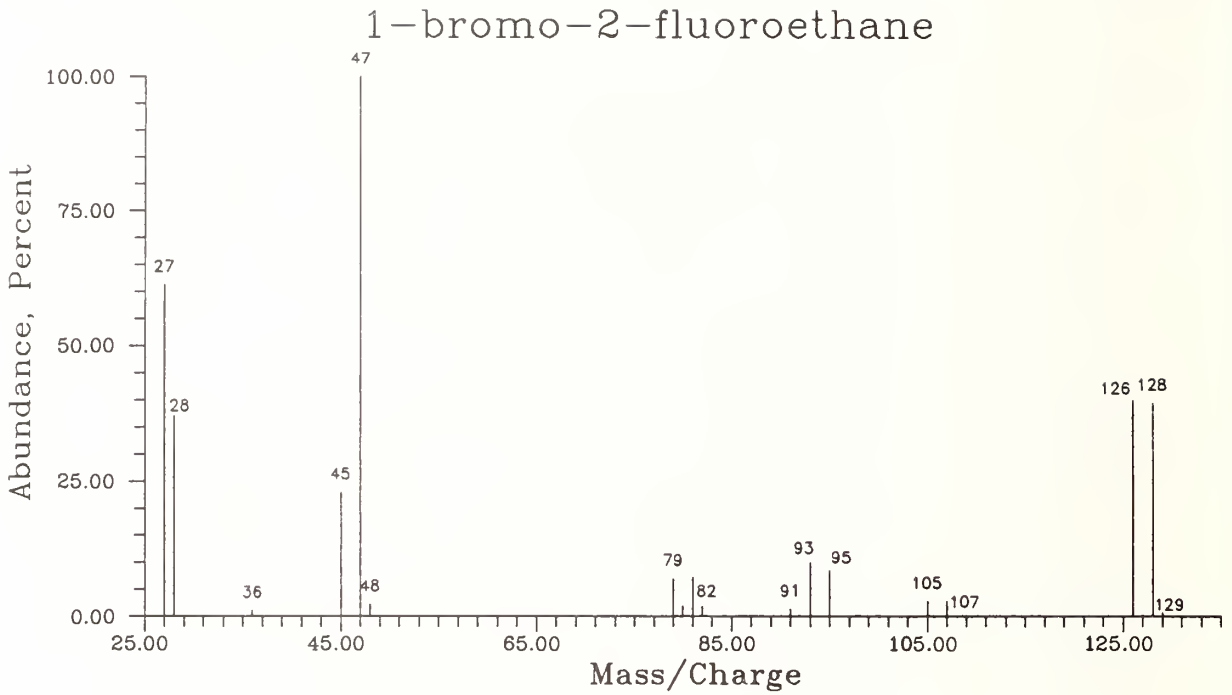
LEL: NA

Toxicology: Detailed toxicology is not available; may cause irritation to eyes, skin, mucous membranes, and upper respiratory tract.

Reactivities and Chemical Incompatibilities: Thermal decomposition may produce HF, HBr, CO, CO_2.

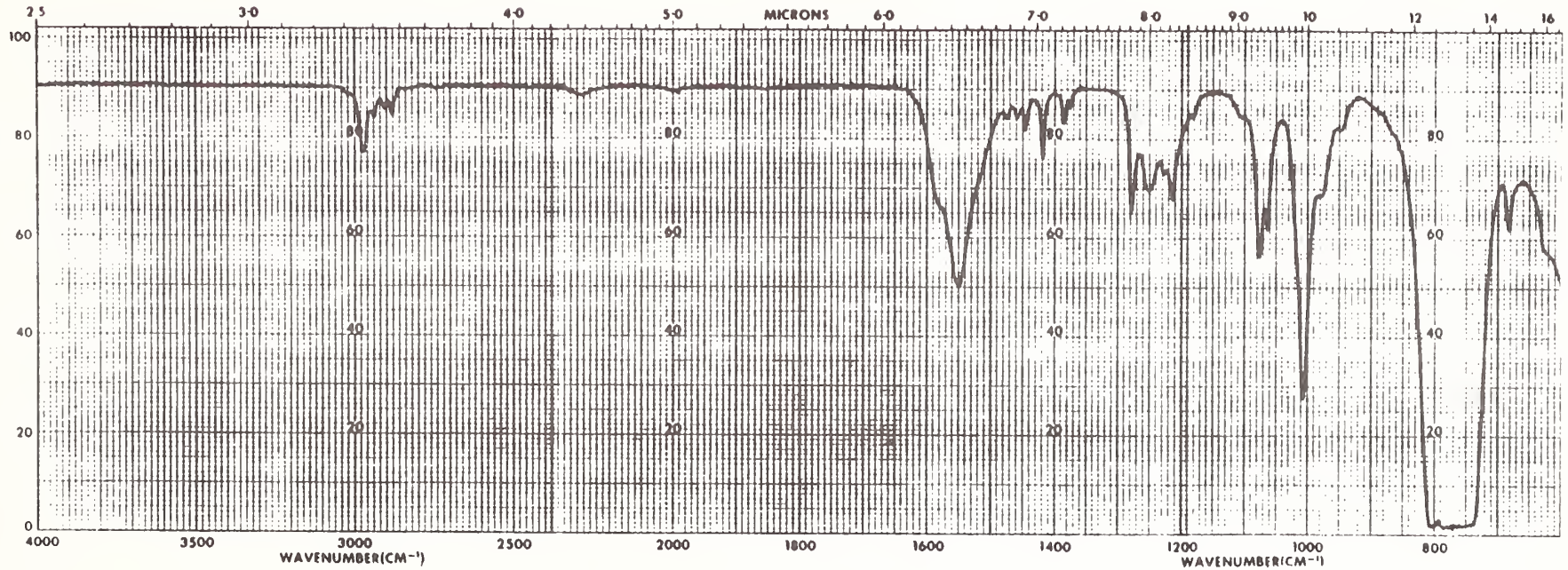
Solubilities: Somewhat soluble in carbon tetrachloride; negligible solubility in water.

Mass Spectrum:

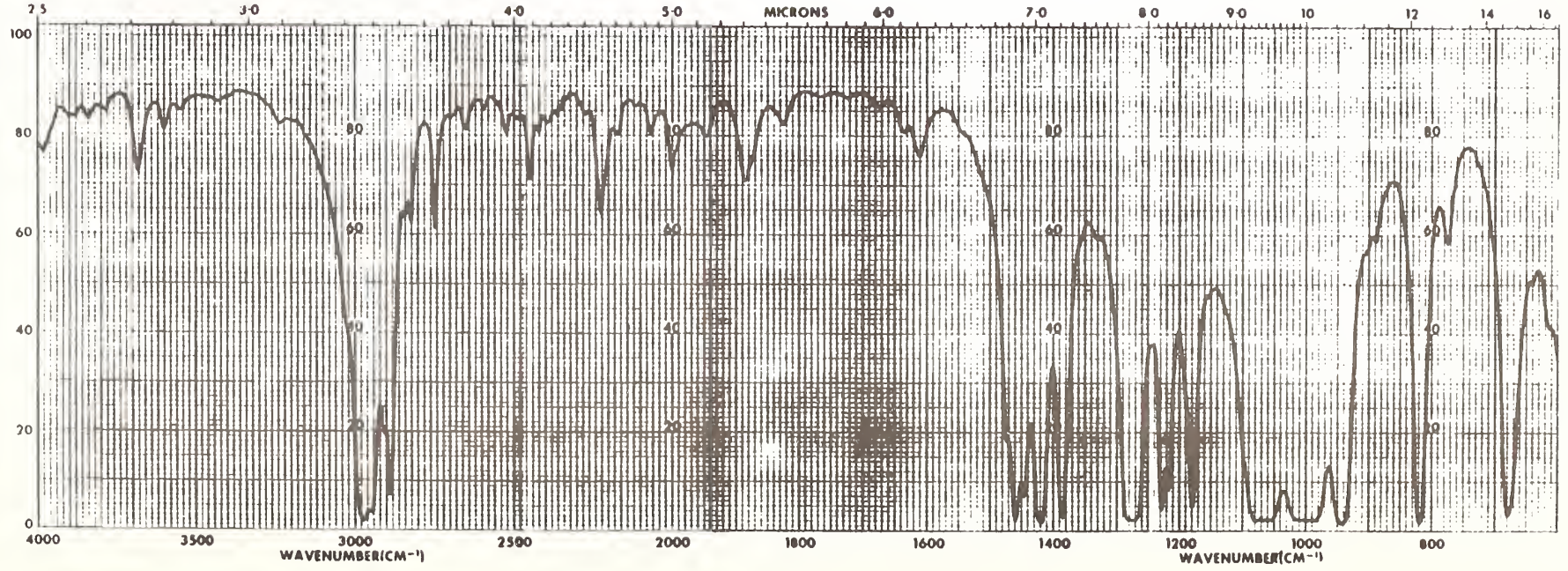


m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
27.00	660972	45.00	247226	81.00	77902	107.00	29591
28.00	399013	46.00	304329	82.00	19855	126.00	432499
33.00	97056	47.00	1080410	91.00	14765	127.00	2653
36.00	11019	48.00	23212	93.00	107307	128.00	426499
40.00	20349	79.00	75432	95.00	92496	129.00	8382
44.00	71926	80.00	19259	105.00	29881		

Infrared Spectrum – carbon tetrachloride solution



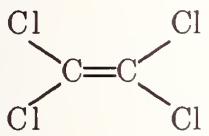
Infrared Spectrum – Liquid Phase (no solvent)



1110 tetrachloroethylene

synonyms: tetrachloroethene, carbon bichloride, carbon dichloride, perchloroethylene, ethylene tetrachloride, 1,1,2,2–tetrachloroethylene

structure:



C. A. S. Registry Number: 127–18–4
Relative Molecular Mass: 165.83

Normal Boiling Point: 121.2 °C

Melting Point: –19 °C

Density/Specific Gravity: 1.6227 (20/4)

Critical Temperature: 347.1 °C

Refractive Index: 1.5053 (20 °C)

Critical Pressure: 9.74 MPa

Critical Density: 0.703 g/mL

****

Vapor Density: 5.83

PEL: 100 ppm

TLV: 50 ppm

Flash Point: nonflammable

UEL: NA

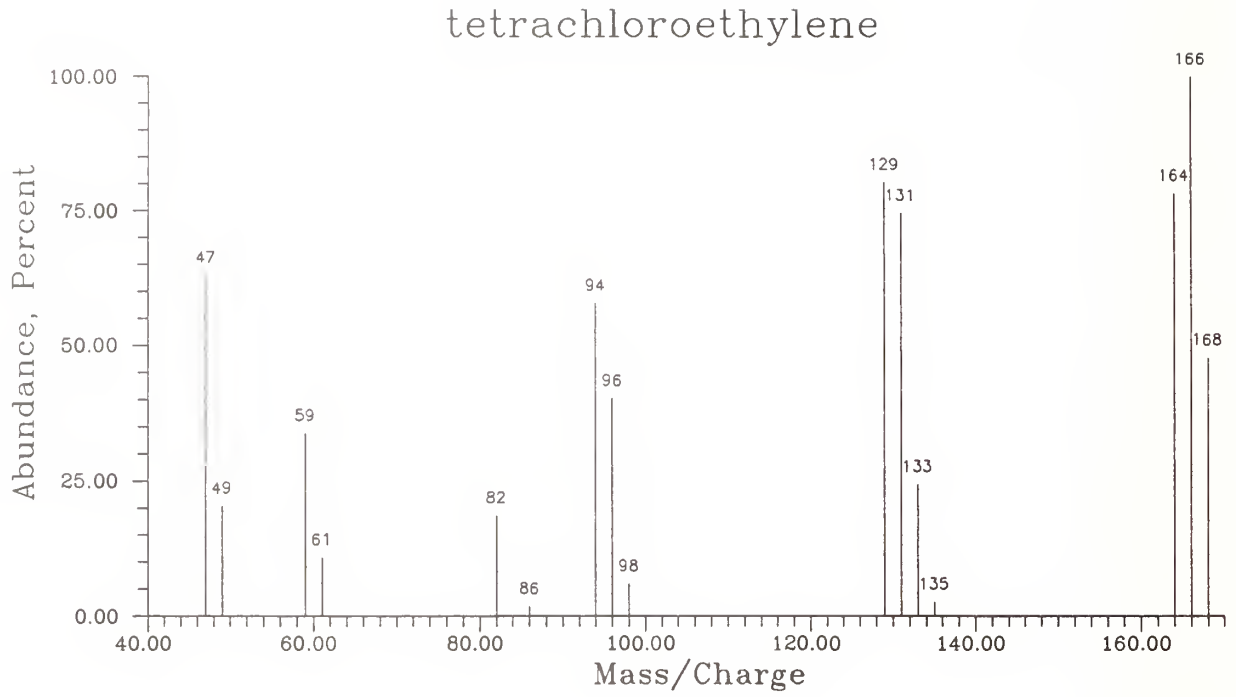
LEL: NA

Toxicology: Irritating to skin, eyes, mucous membranes; lachrymation possible at higher concentrations, as well as narcosis and dizziness; prolonged exposure can damage kidneys and liver; possible carcinogen and mutagen.

Reactivities and Chemical Incompatibilities: Thermal decomposition can produce HCl, CO, CO_2, phosgene; avoid contact with strong bases.

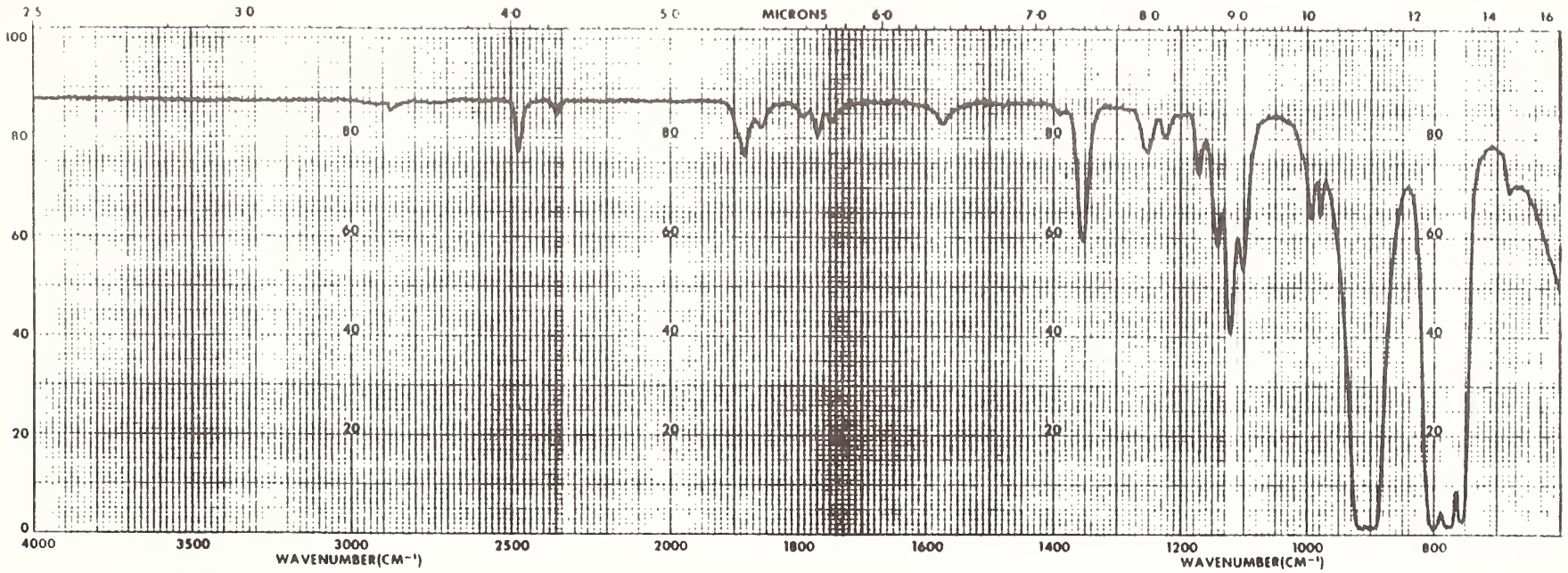
Solubilities: Alcohols, ether, benzene, carbon tetrachloride; H_2O: 0.015 g/mL (25 °C).

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
47.00	44522	70.00	9370	96.00	264311	135.00	18129
49.00	143272	82.00	130778	98.00	41944	164.00	554157
59.00	238145	84.00	85535	129.00	568487	166.00	708240
60.00	5459	86.00	12411	131.00	527589	168.00	338376
61.00	76441	94.00	408706	133.00	172194		

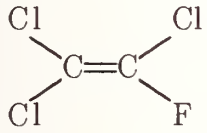
Infrared Spectrum – Liquid Phase (no solvent)



1111 trichlorofluoroethylene

synonyms: trichlorofluoroethene.

structure:



C. A. S. Registry Number: 359–29–5
Relative Molecular Mass: 149.38

Normal Boiling Point: 71 °C

Melting Point: –108.9 °C

Density/Specific Gravity: 1.5460, l, (20 °C)

Critical Temperature: 272.1 °C*

Refractive Index:

Critical Pressure: 6.52 MPa*

Critical Density: 0.729 g/mL*

****

Vapor Density: >1

PEL: NE

TLV: NE

Flash Point: does not flash

UEL: NA

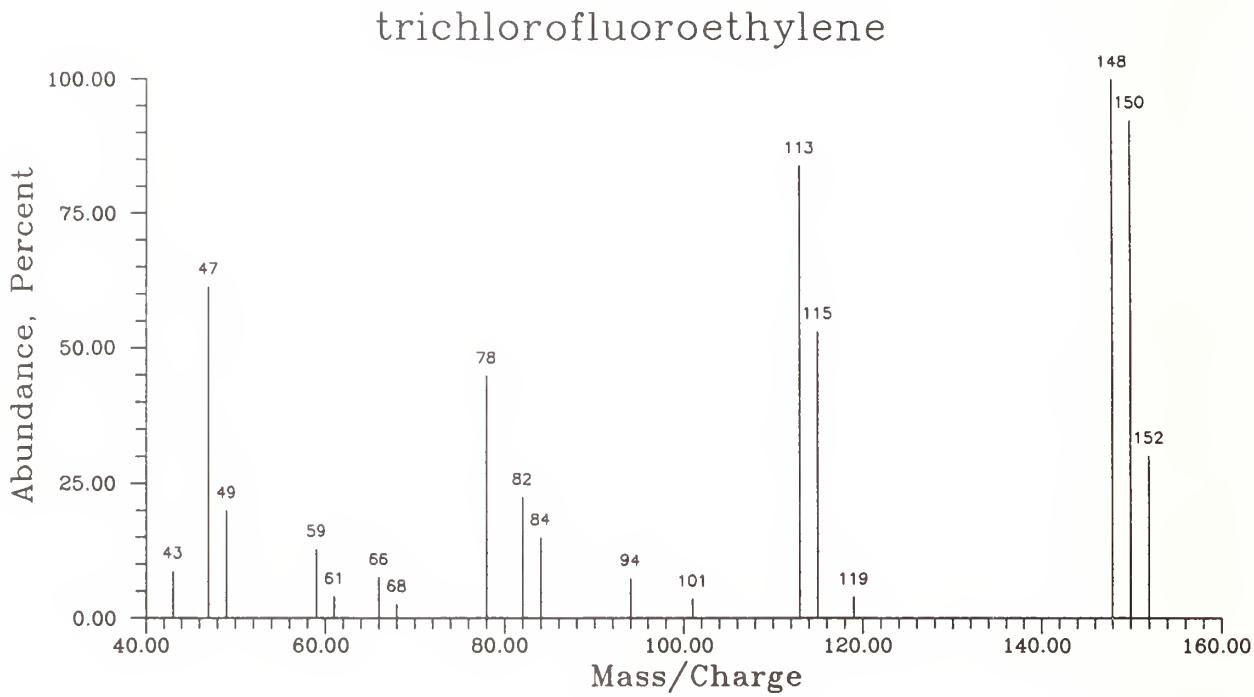
LEL: NA

Toxicology: Detailed toxicology not available; may be irritating to skin and eyes.

Reactivities and Chemical Incompatibilities: Thermal decomposition may produce HCl, HF, CO, CO_2; avoid contact with active metals, strong oxidizers.

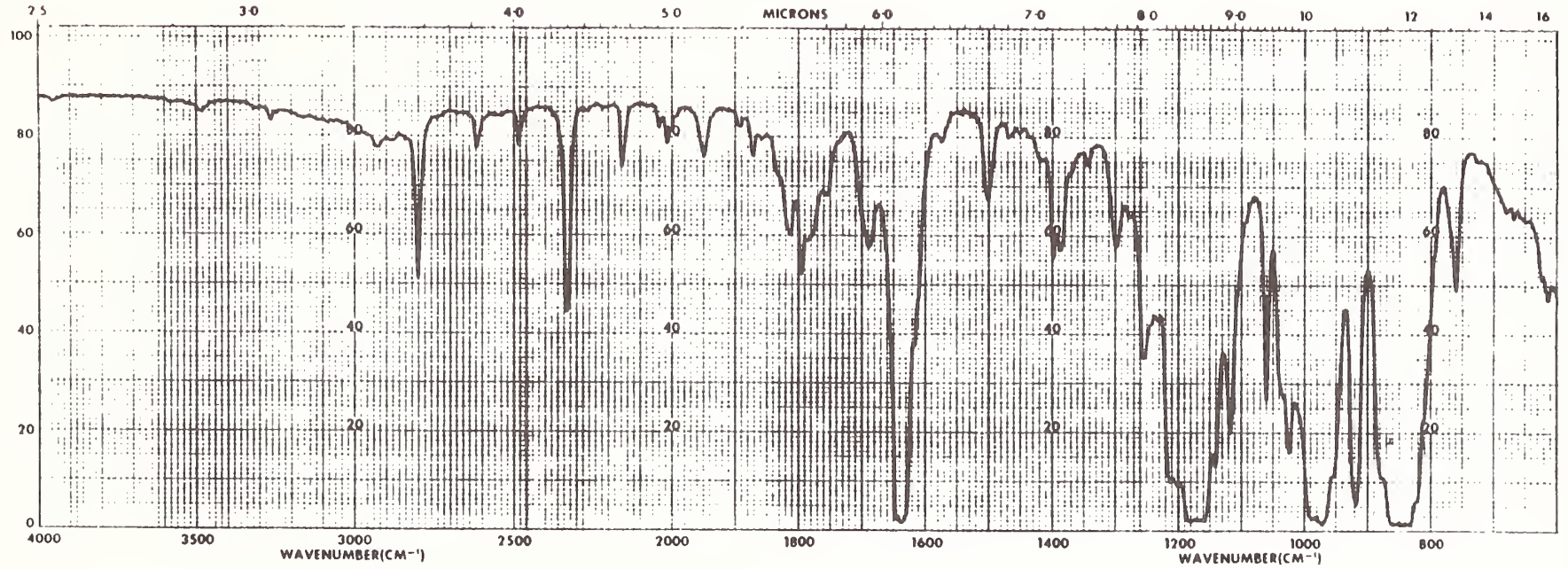
Solubilities: Somewhat soluble in carbon tetrachloride; negligible solubility in water.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
43.00	50859	66.00	44001	94.00	42417	117.00	72021
44.00	10509	68.00	14585	96.00	27780	119.00	22928
47.00	358401	74.00	10660	101.00	20473	148.00	586046
49.00	116178	78.00	261881	113.00	491082	150.00	541895
59.00	74266	82.00	130604	115.00	310443	152.00	175967
61.00	23577	84.00	86625				

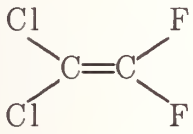
Infrared Spectrum – Liquid Phase (no solvent)



1112a 1,1-dichloro-2,2-difluoroethylene

synonyms: 1,1–dichlorodifluoroethylene; 1,1–dichloro–2,2–difluoroethene; 1,1–dichlorodifluoroethene.

structure:



C. A. S. Registry Number: 79–35–6
Relative Molecular Mass: 132.92

Normal Boiling Point: 19 °C

Melting Point: –116 °C

Density/Specific Gravity: 1.4385, l, (20 °C)

Critical Temperature: 186 °C

Refractive Index:

Critical Pressure: 6.61 MPa*

Critical Density: 0.764 g/mL*

****

Vapor Density: >1

PEL: NE

TLV: NE

Flash Point: None

UEL: NA

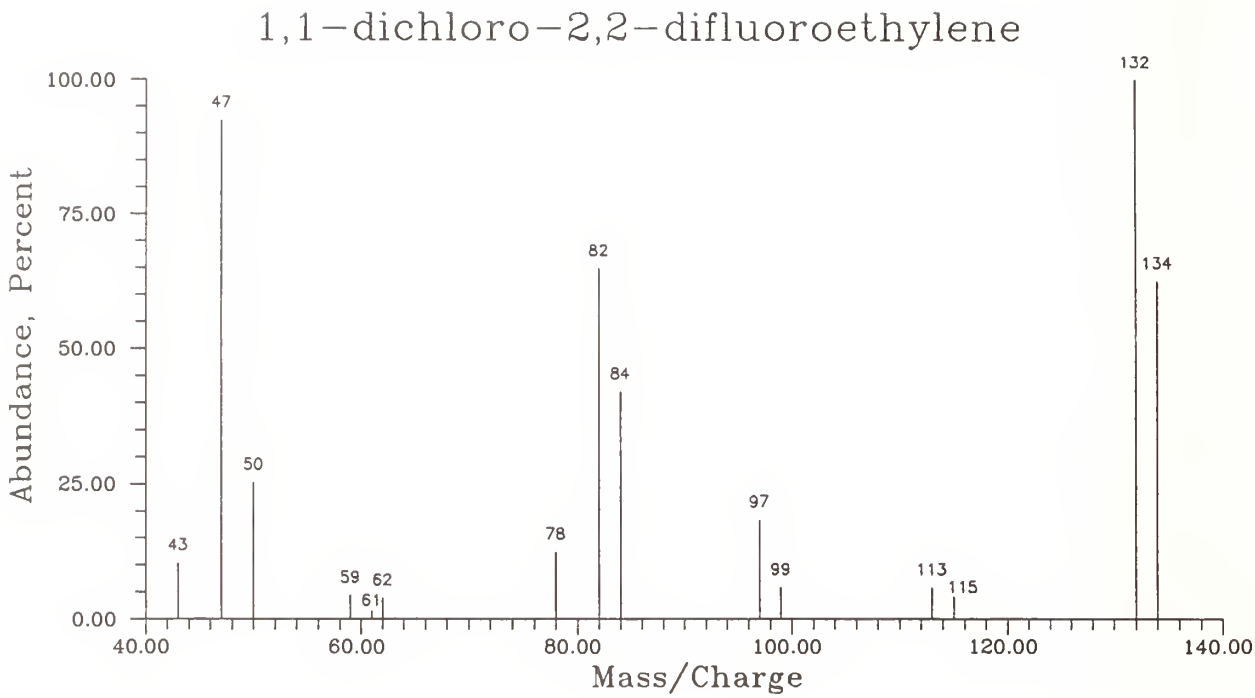
LEL: NA

Toxicology: Detailed toxicology is not available; may cause skin and eye irritation; possible pulmonary irritant.

Reactivities and Chemical **Incompatibilities:** Thermal decomposition may produce HF, HCl, CO, CO_2, and possibly carbonyl halides; avoid contact with strong oxidizers, O_2 active metals.

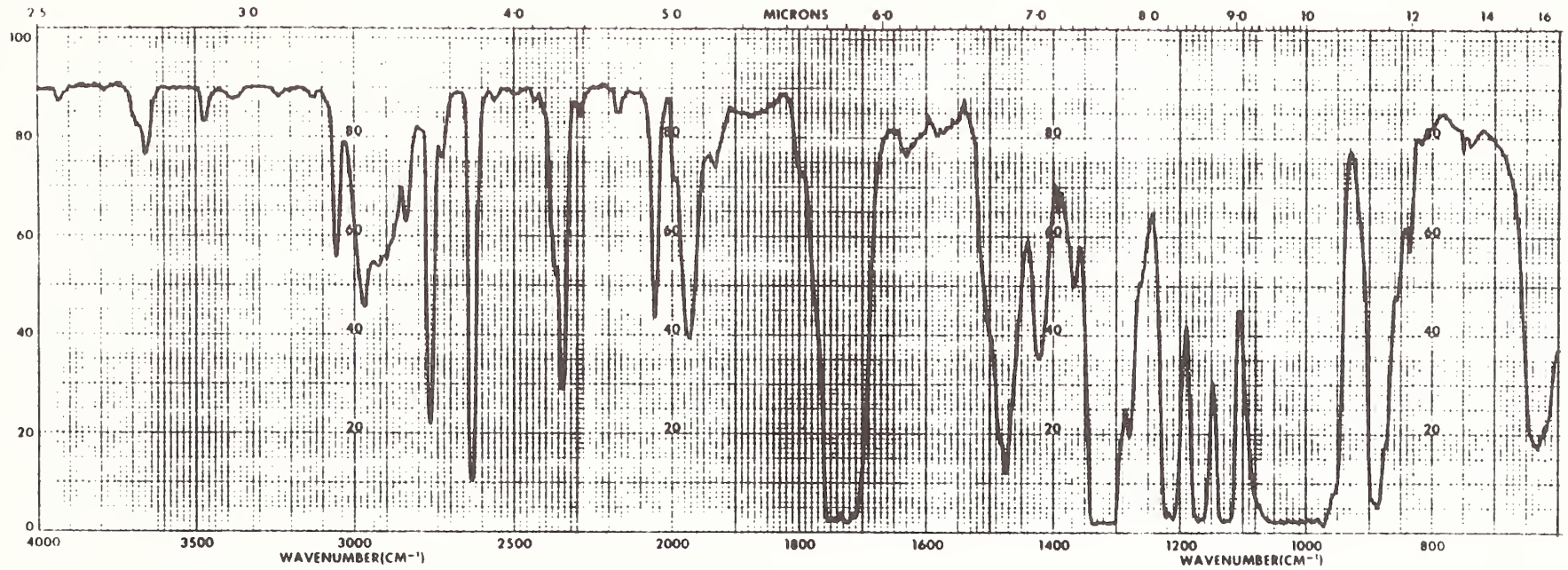
Solubilities: Somewhat soluble in carbon tetrachloride; negligible solubility in water.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
43.00	145117	66.00	77096	84.00	591322	103.00	12966
47.00	1302647	67.00	16275	85.00	38576	113.00	91085
50.00	355416	68.00	20572	97.00	257736	115.00	58451
59.00	60660	78.00	173628	99.00	81967	132.00	1411347
61.00	21502	82.00	913473	101.00	21176	134.00	882283
62.00	53676						

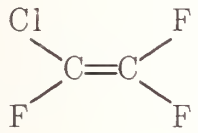
Infrared Spectrum – Gas Phase



1113 chlorotrifluoroethylene

synonyms: 1–chloro–1,2,2–trifluoroethylene; chlorotrifluoroethene; CTFE; ethylene–trifluorochloro–; 1,1,2–trifluorochloroethylene; trifluorovinylchloride; Genetron 1113.

structure:



C. A. S. Registry Number: 79–38–9
Relative Molecular Mass: 116.47

Normal Boiling Point: –26.2 °C

Melting Point: –157.5 °C

Density/Specific Gravity: 1.54 (–60/4)

Critical Temperature: 117.0 °C*

Refractive Index: 1.38 (0 °C)

Critical Pressure: 6.65 MPa*

Critical Density: 0.814 g/mL

****

Vapor Density: 4.13

PEL: NE

TLV: NE

Flash Point: –27 °C

UEL: 38.7%

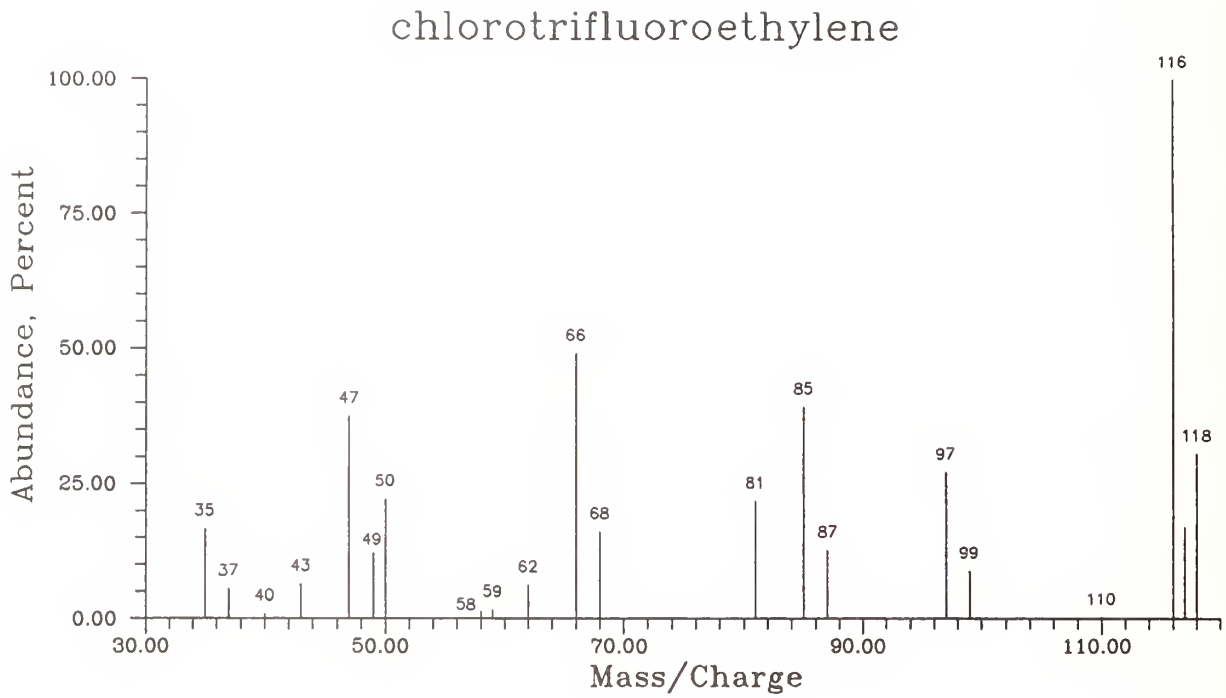
LEL: 8.4%

Toxicology: Low concentration can cause dizziness, nausea, vomiting, and possibly kidney damage. High concentrations may cause cardiac arrhythmia, asphyxia, and potentially fatal renal failure.

Reactivities and Chemical Incompatibilities: Thermal decomposition can form HF, HCl, CO, CO_2; hazardous polymerization is possible; avoid contact with strong bases, oxidants, O_2, and air.

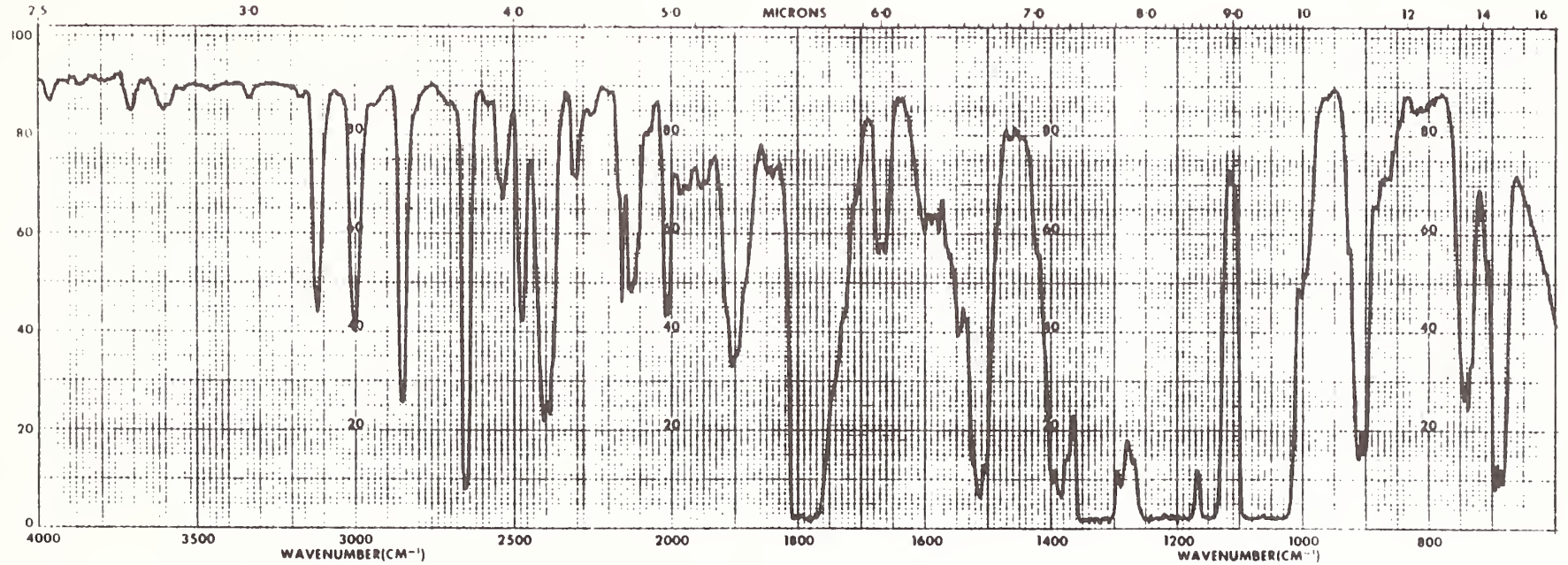
Solubilities: Somewhat soluble in carbon tetrachloride and benzene; negligible solubility in water.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	3697834	49.00	248106	68.00	318464	99.00	182122
35.00	341632	50.00	463381	81.00	446208	100.00	4663
37.00	112440	58.00	27872	85.00	804480	116.00	2056362
40.00	18318	59.00	33237	87.00	261717	117.00	36973
43.00	131618	62.00	127490	97.00	556245	118.00	627840
47.00	76891	66.00	1007274				

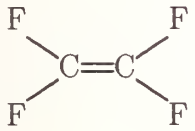
Infrared Spectrum – Gas Phase



1114 tetrafluoroethylene

synonyms: tetrafluoroethene; perfluoroethylene; perfluoroethyene; TFE; ethylene tetrafluoride.

structure:



C. A. S. Registry Number: 116–14–3
Relative Molecular Mass: 100.02

Normal Boiling Point: –75.63 °C

Melting Point: –142.5 °C

Density/Specific Gravity: 1.151 g/mL (–40 °C)

Critical Temperature: 33.3 °C

Refractive Index:

Critical Pressure: 6.63 MPa

Critical Density: 0.893 g/mL

****

Vapor Density: 3.87

PEL: NE

TLV: NE

Flash Point: flammable gas

UEL: 43

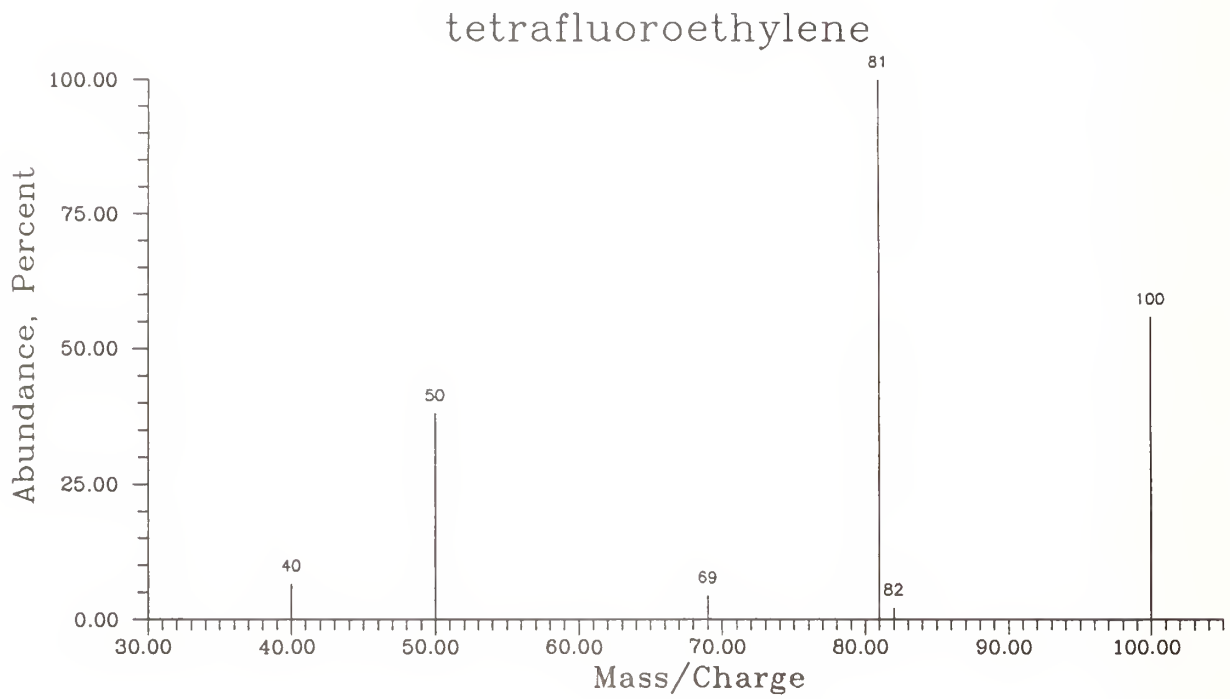
LEL: 14

Toxicology: Detailed toxicology is unknown; simple asphyxiant, may cause inflamed pharynx, difficulty in breathing, fatigue; tumorigen.

Reactivities and Chemical Incompatibilities: Thermal decomposition can produce CF_4, CO_2, COF_2, hexafluoropropene, perfluoroisobutylene; avoid contact with O_2, as explosive peroxides can form.

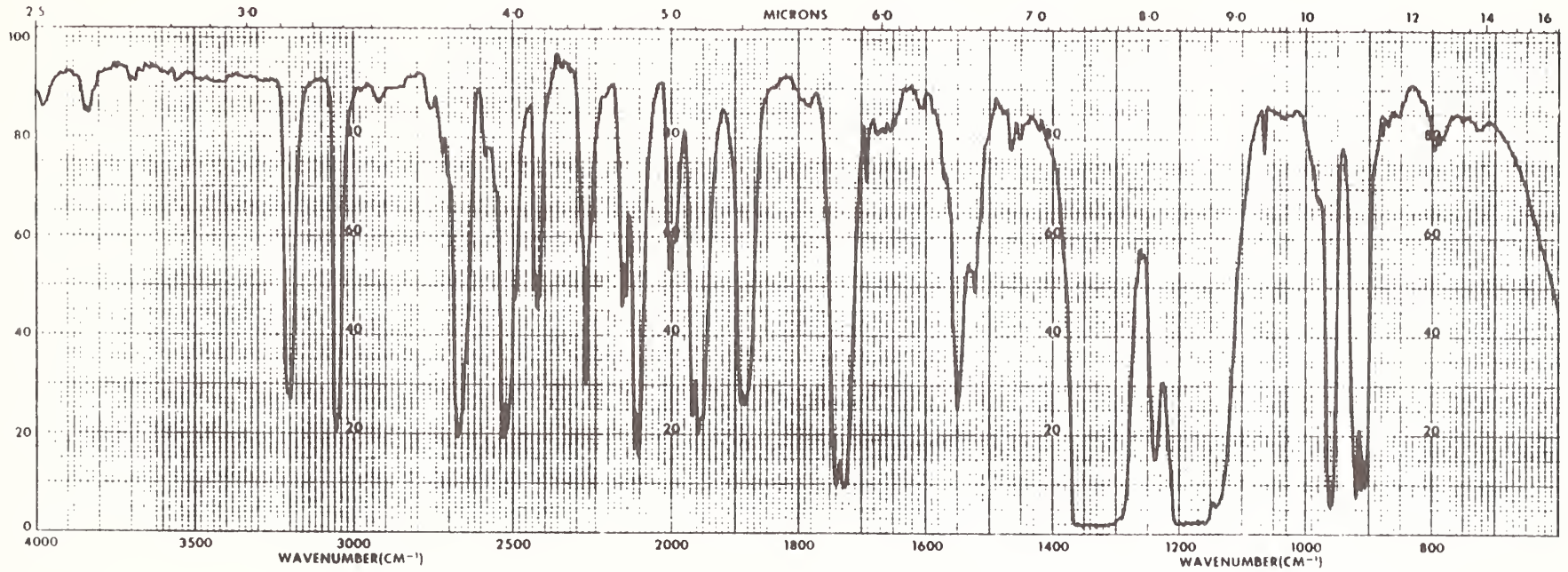
Solubilities: Somewhat soluble in carbon tetrachloride; H_2O: 0.12 g/1000 mL.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	924211	44.00	14933	69.00	39617	82.00	18870
40.00	59280	50.00	345133	81.00	910624	100.00	509062
43.00	12278						

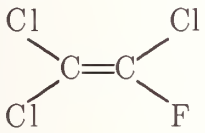
Infrared Spectrum – Gas Phase



1120 trichloroethylene

synonyms: trichloroethene; acetylene trichloride; 1–chloro–2,2–dichloroethylene; Algylen; 1,1–dichloro–2–chloroethylene; Vestrol; Tri–Clene; trichlor.

structure:



C. A. S. Registry Number: 79–01–6
Relative Molecular Mass: 131.39

Normal Boiling Point: 86.7 °C

Melting Point: –86.8 °C

Density/Specific Gravity: 1.4556 (25/4)

Critical Temperature: 271.0 °C

Refractive Index: 1.4773 (20 °C)

Critical Pressure: 5.02 MPa

Critical Density: 0.566 g/mL*

****

Vapor Density: 4.5

PEL: 50 ppm

TLV: 50 ppm

Flash Point: None

UEL: 12.5%

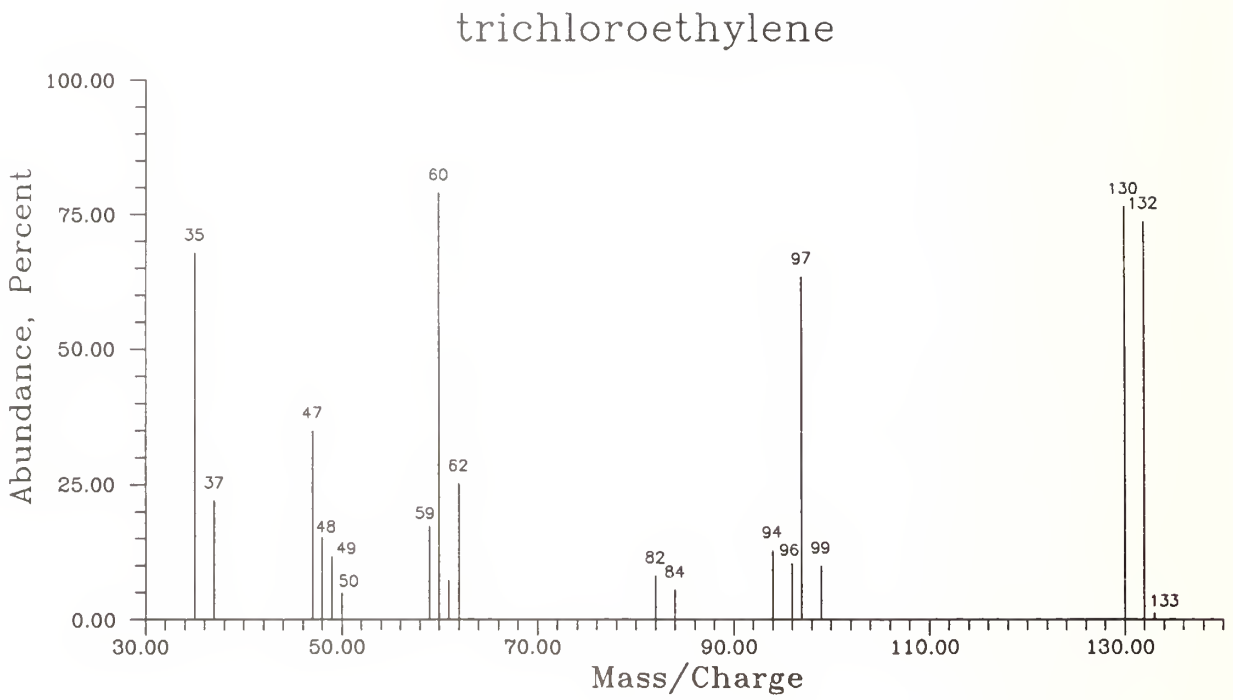
LEL: 9%

Toxicology: Possibly carcinogenic and mutagenic, narcotic, anesthetic, potentially addictive; high concentrations can cause ventricular fibrillation; eye, skin and mucous membrane irritant; may damage gastrointestinal tract, liver, and kidneys.

Reactivities and Chemical Incompatibilities: Thermal decomposition can produce HCl, CO, CO_2, phosgene; avoid contact with oxidizing and reducing agents, strong bases, Al, Mg, light.

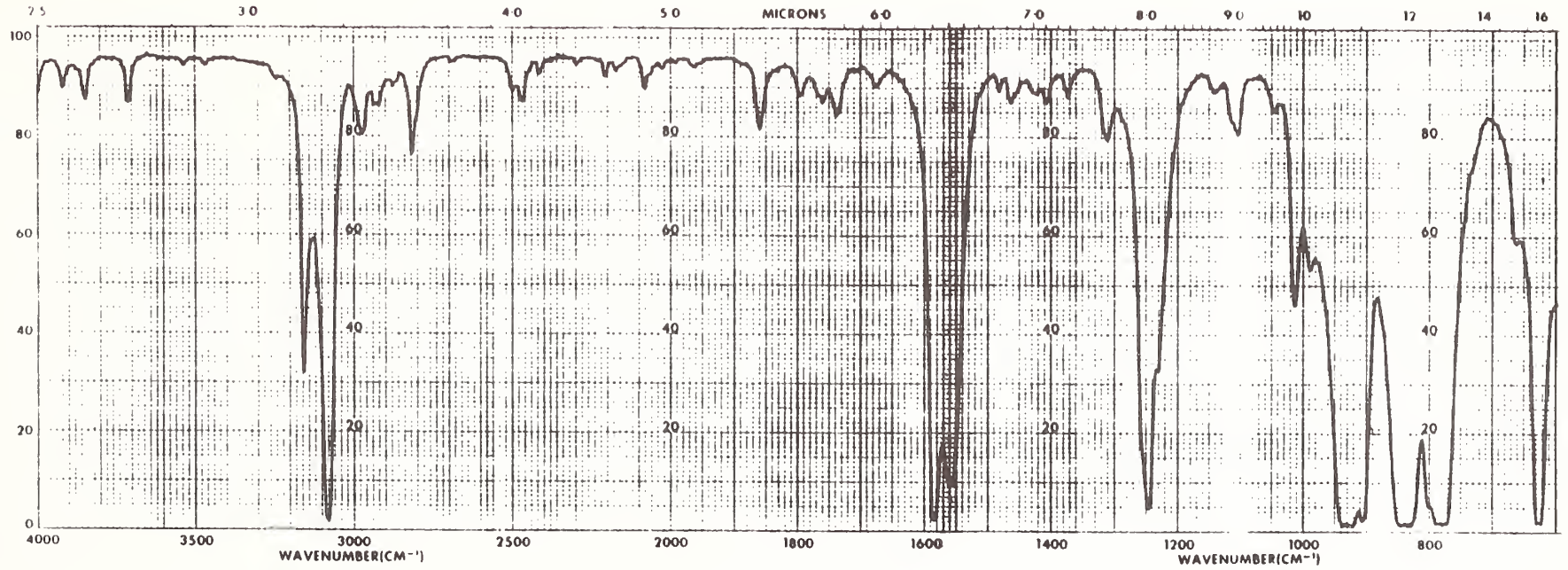
Solubilities: Soluble in alcohol, ether, acetone, benzene, carbon tetrachloride; H_2O: 0.0225 g/100 mL (20 °C).

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
35.00	816312	59.00	206692	70.00	19682	96.00	126110
36.00	69772	60.00	950936	72.00	13582	97.00	762967
37.00	263773	61.00	86905	82.00	97282	99.00	118921
47.00	419489	62.00	30149	84.00	64913	130.00	921813
48.00	182870	65.00	22222	94.00	154829	132.00	887668
49.00	139565	66.00	20437	95.00	1204437	133.00	14048
50.00	58756						

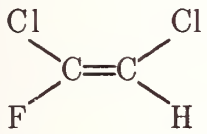
Infrared Spectrum – Liquid Phase (no solvent)



1121 1,2-dichloro-1-fluoroethylene

synonyms: 1,2–dichloro–1–fluoroethene.

structure:



C. A. S. Registry Number: 430–58–0
Relative Molecular Mass: 114.93

Normal Boiling Point: 35.1 °C

Melting Point: NA

Density/Specific Gravity: 1.4032 (16 °C)

Critical Temperature: 214.5 °C*

Refractive Index:

Critical Pressure: 5.92 MPa*

Critical Density: 0.572 g/mL*

****

Vapor Density: >1

PEL: NE

TLV: NE

Flash Point: NA

UEL: NA

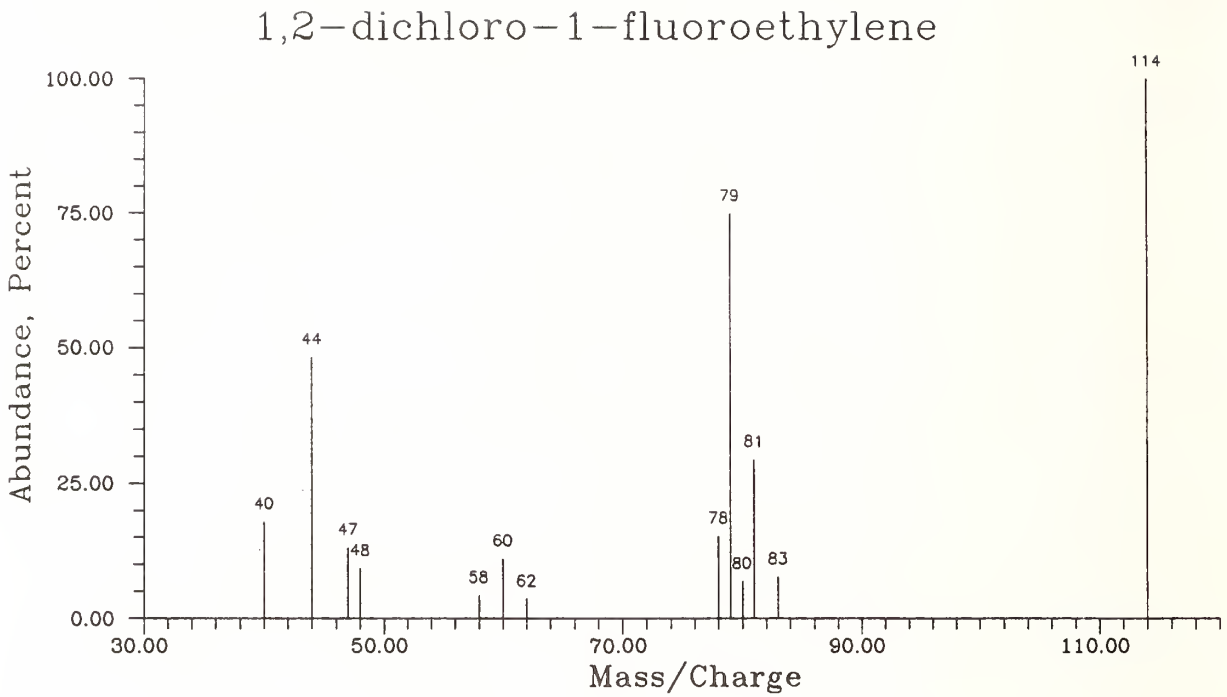
LEL: NA

Toxicology: Detailed toxicology is not available.

Reactivities and Chemical Incompatibilities: Thermal decomposition can produce HF and HCl; avoid contact with strong oxidizers.

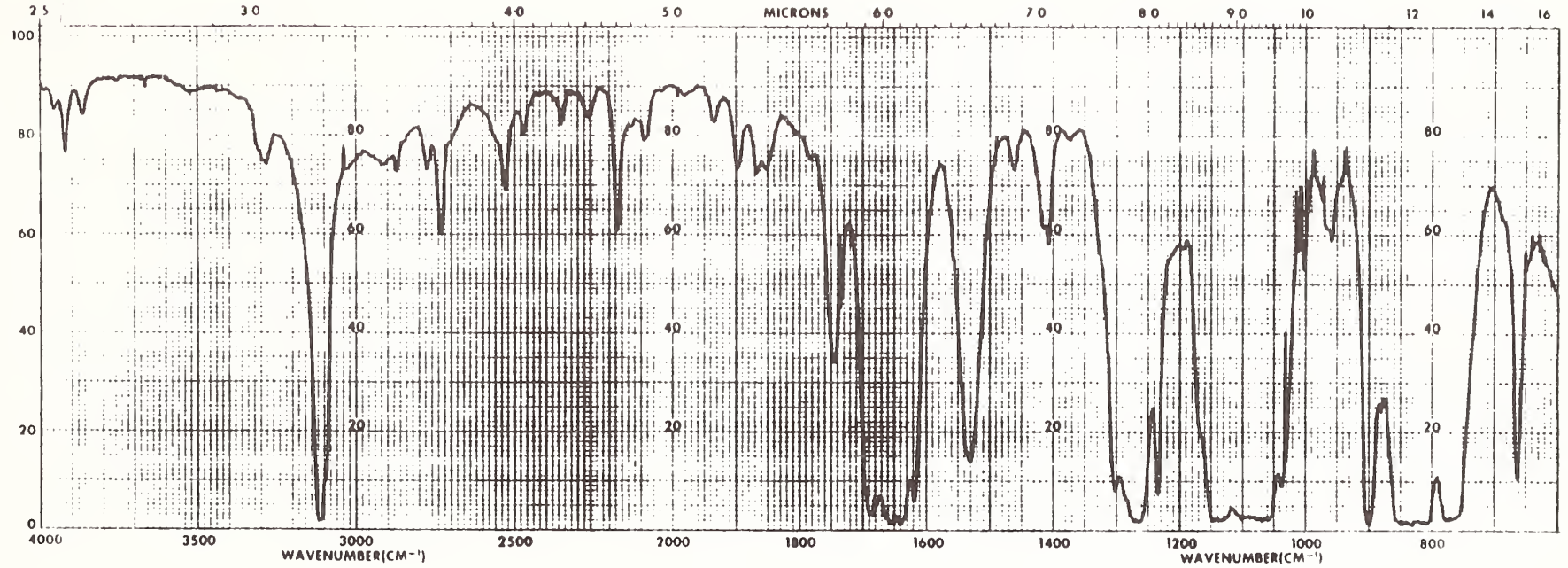
Solubilities: Somewhat soluble in carbon tetrachloride; negligible solubility in water.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
35.00	46252	48.00	27460	60.00	32978	81.00	72596
37.00	15241	49.00	13434	62.00	10583	83.00	22868
40.00	53368	50.00	8813	66.00	9681	85.00	14946
43.00	10629	57.00	4751	78.00	45389	97.00	6011
44.00	144193	58.00	3222	79.00	223866	114.00	299095
47.00	39085	59.00	12779	80.00	20337		

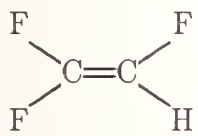
Infrared Spectrum – Liquid Phase (no solvent)



1123 trifluoroethylene

synonyms: trifluoroethene; 1,1,2–trifluoroethylene.

structure:



C. A. S. Registry Number: 359–11–5
Relative Molecular Mass: 82.03

Normal Boiling Point: –51 °C

Melting Point: –78 °C

Density/Specific Gravity: 1.265, l, (27 °C)

Critical Temperature: 77.4 °C*

Refractive Index:

Critical Pressure: 5.68 MPa*

Critical Density: 0.590 g/mL

****

Vapor Density: 2.9

PEL: NE

TLV: NE

Flash Point: NA

UEL: NA

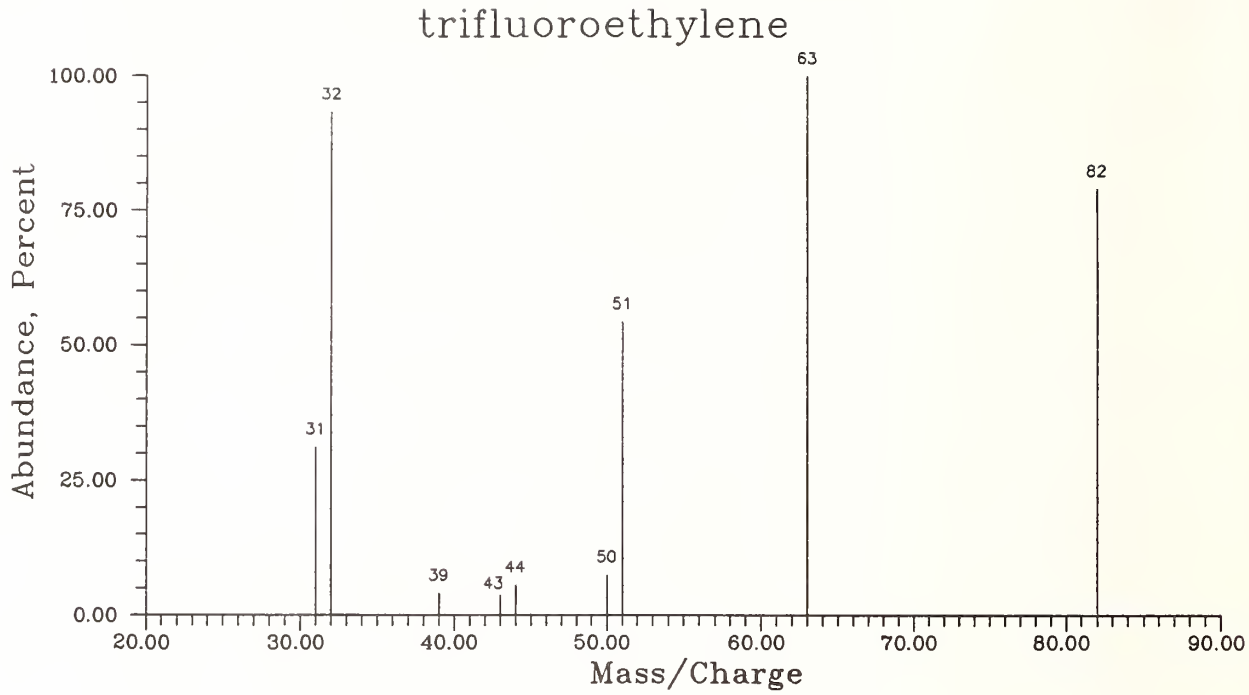
LEL: NA

Toxicology: Detailed toxicology is not available.

Reactivities and Chemical Incompatibilities: Thermal decomposition can form COF_2, HF, CO, CO_2; hazardous polymerization may occur; avoid contact with peroxides, especially under radical forming conditions.

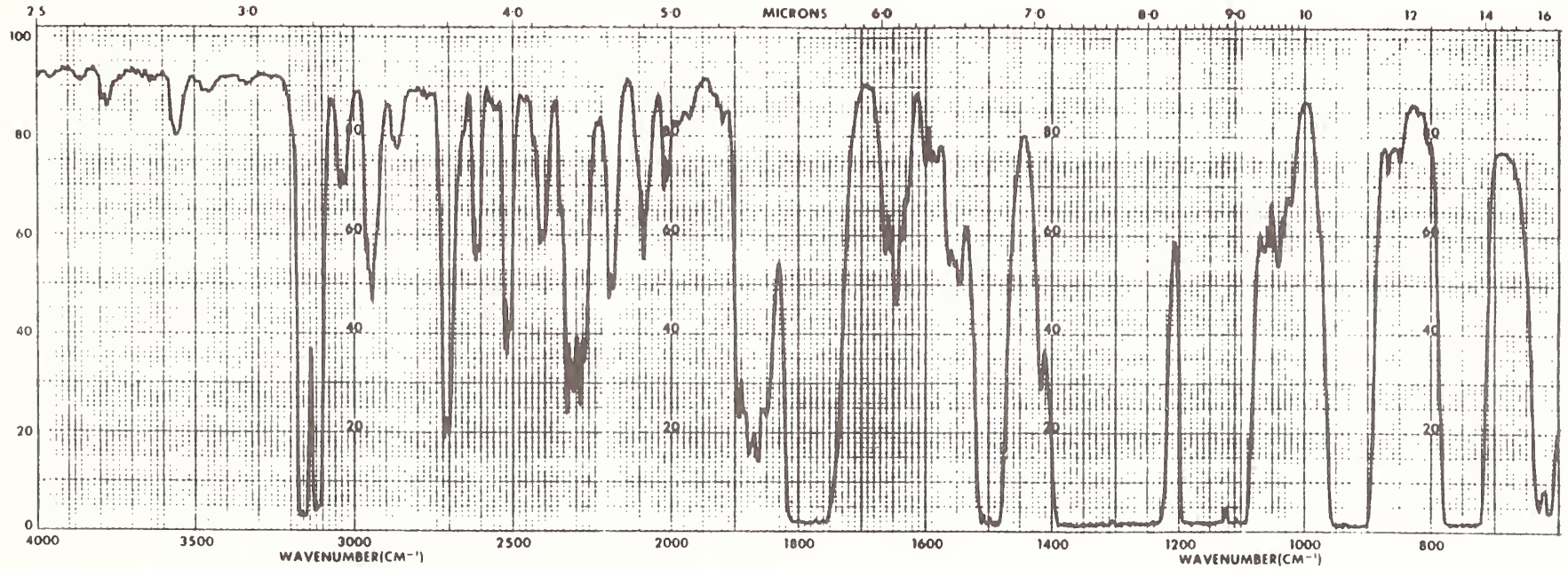
Solubilities: Somewhat soluble in carbon tetrachloride; negligible solubility in water.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	874048	43.00	50272	51.00	721152	64.00	28896
32.00	1239552	44.00	73888	63.00	1329664	82.00	1053184
40.00	53072	50.00	99024				

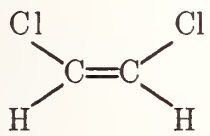
Infrared Spectrum – Gas Phase



1130 cis-1,2-dichloroethylene

synonyms: z–1,2–dichloroethylene; 1,2–dichloroethene; acetylene dichloride; Dioform; sym–dichloroethylene.

structure:



C. A. S. Registry Number: 540–59–0
Relative Molecular Mass: 96.94

Normal Boiling Point: 60.3 °C

Melting Point: –80.5 °C

Density/Specific Gravity: 1.2837 (20/4)

Critical Temperature: 234.1 °C

Refractive Index: 1.44900 (20 °C)

Critical Pressure: 5.19 MPa

Critical Density: 0.452 g/mL

****

Vapor Density: 3.34

PEL: 200 ppm

TLV: 200 ppm

Flash Point: 6 °C

UEL: 15%

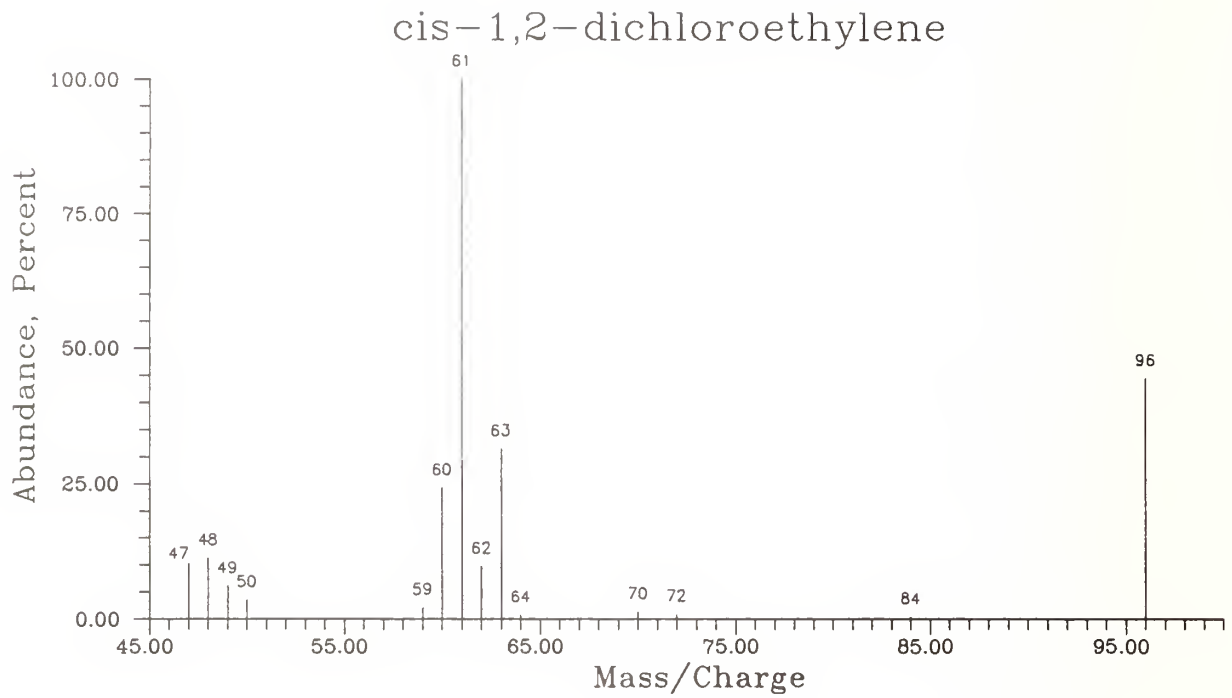
LEL: 3.3%

Toxicology: Causes respiratory irritation; prolonged exposure results in narcotic effects; possible liver and kidney damage in high concentrations.

Reactivities and Chemical Incompatibilities: Thermal decomposition may form HCl, CO, CO_2, phosgene; avoid contact with air, O_2, moisture (slow hydrolysis), light, alkali metals.

Solubilities: Somewhat soluble in carbon tetrachloride, alcohols, ether, benzene, chloroform; H_2O: 0.35–0.63 g/L, 25 °C.

Mass Spectrum:

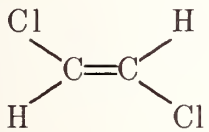


m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
35.00	1227202	49.00	190712	61.00	3136004	70.00	41405
37.00	386905	50.00	107834	62.00	304723	72.00	27800
40.00	21462	51.00	22078	63.00	885437	84.00	13401
47.00	320794	59.00	65698	64.00	21766	96.00	139451
48.00	352848	60.00	758661				

1130 trans-1,2-dichloroethylene

synonyms: E–1,2–dichloroethylene; 1,2–dichloroethene; acetylene dichloride; Dioform; sym–dichloroethylene.

structure:



C. A. S. Registry Number: 540–59–0
Relative Molecular Mass: 96.94

Normal Boiling Point: 47.5 °C

Melting Point: –50 °C

Density/Specific Gravity: 1.2565 (20/4)

Critical Temperature: 234.13 °C

Refractive Index: 1.44620 (20 °C)

Critical Pressure: 5.19 MPa

Critical Density: 0.452 g/mL

****

Vapor Density: 3.34

PEL: 200 ppm

TLV: 200 ppm

Flash Point: 2.2 °C

UEL: 12.8%

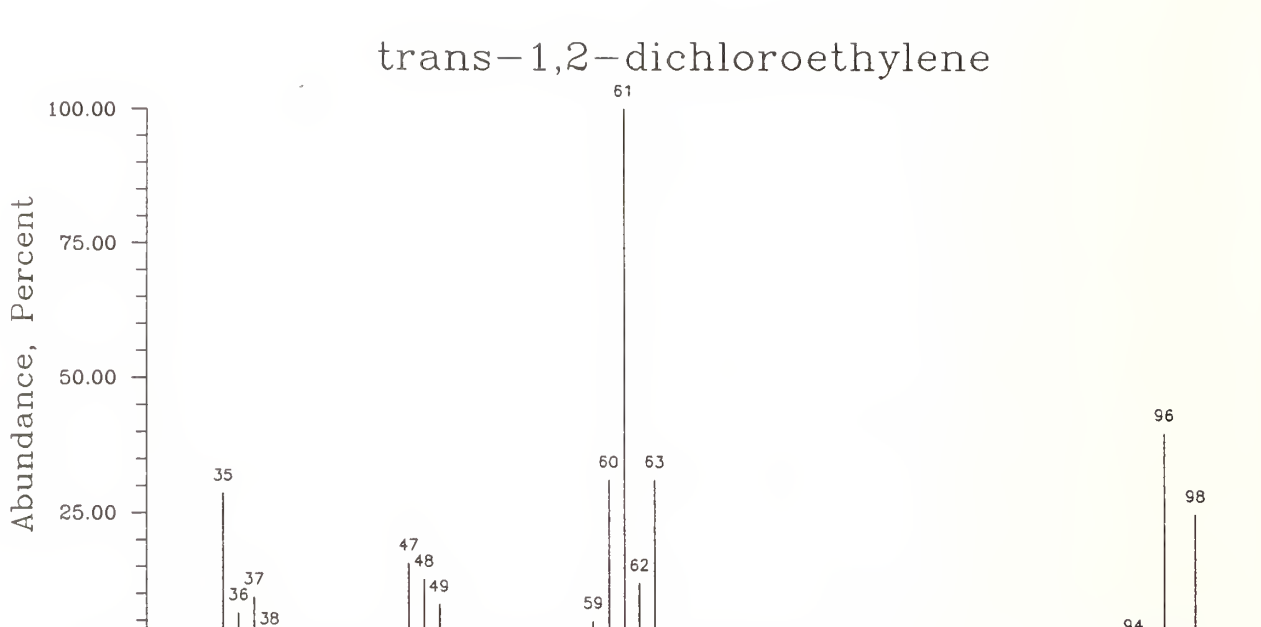
LEL: 9.7%

Toxicology: Causes respiratory irritation; prolonged exposure results in narcotic effects; possible liver and kidney damage in high concentrations.

Reactivities and Chemical Incompatibilities: Thermal decomposition may form HCl, CO, CO_2, phosgene; avoid contact with air, O_2, moisture (slow hydrolysis), light, alkali metals.

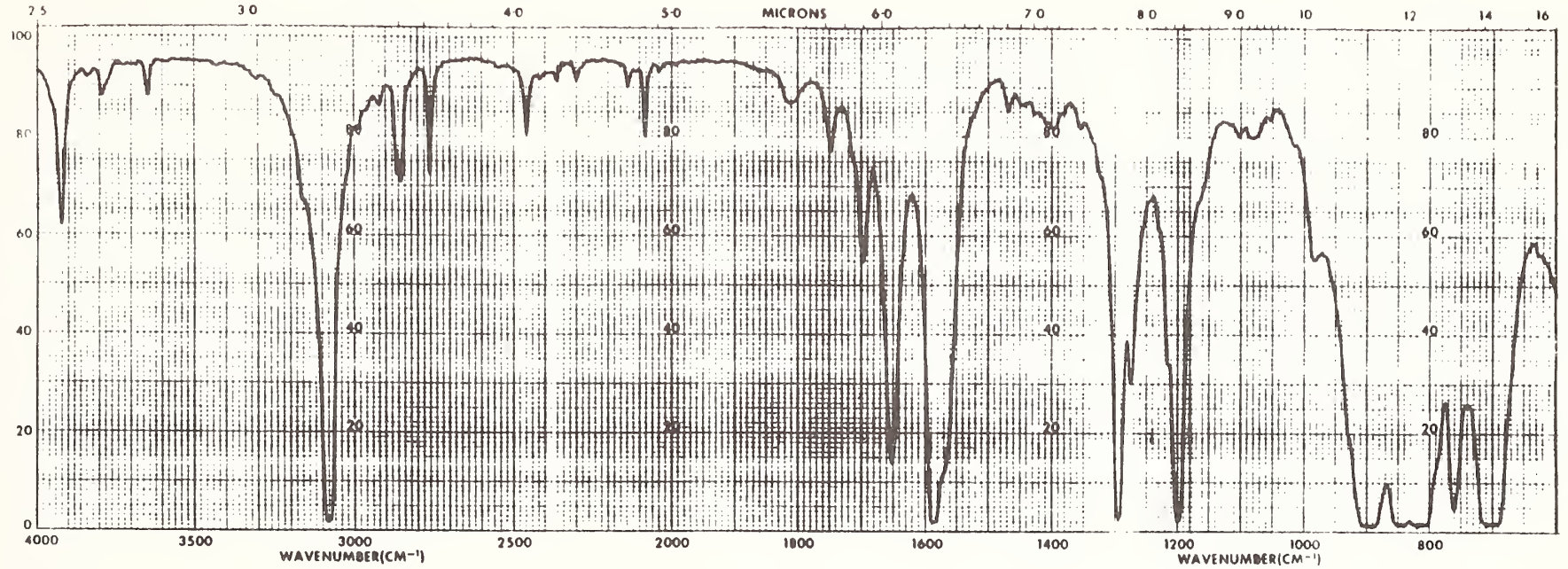
Solubilities: Somewhat soluble in carbon tetrachloride, alcohols, ether, benzene, chloroform; H_2O: 0.35–0.63 g/L, 25 °C.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
24.00	318988	38.00	72650	51.00	28500	63.00	1139067
25.00	1093777	40.00	15781	59.00	177250	94.00	27268
26.00	2107630	47.00	578094	60.00	1139635	96.00	1462681
35.00	1051874	48.00	463667	61.00	3691008	98.00	908979
36.00	233869	49.00	294114	62.00	435912	100.00	146760
37.00	346393	50.00	142307				

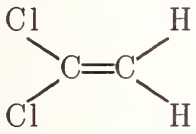
Infrared Spectrum, cis– trans– isomeric mixture – Liquid Phase (no solvent)



1130a 1,1-dichloroethylene

synonyms: 1,1–dichloroethene; vinylidene chloride; 1,1–DCE; vinylidene chloride (II); UNSYM–dichloroethylene.

structure:



C. A. S. Registry Number: 75–35–4
Relative Molecular Mass: 96.94

Normal Boiling Point: 31.6 °C

Melting Point: –122.1 °C

Density/Specific Gravity: 1.218 (20 °C)

Critical Temperature: 230.1 °C*

Refractive Index: 1.4249 (20 °C)

Critical Pressure: 7.08 MPa*

Critical Density: 0.530 g/mL

****

Vapor Density: 3.46

PEL: NE

TLV: 5 ppm

Flash Point: –22.8 °C

UEL: 15.5%

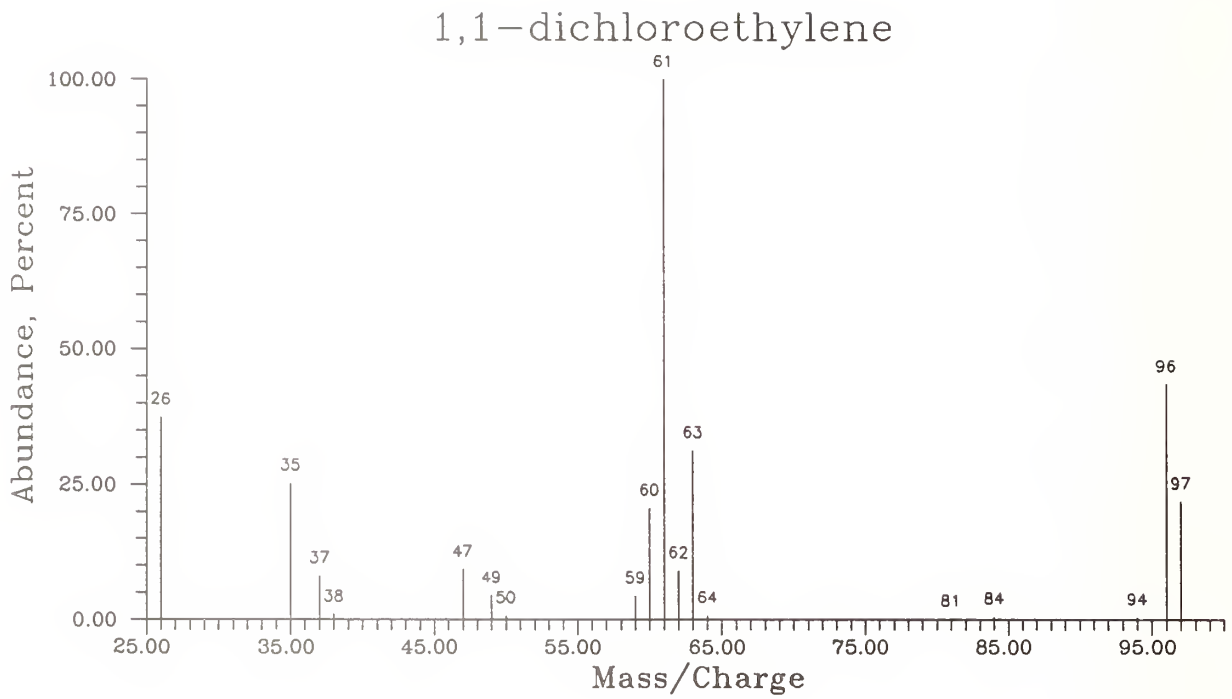
LEL: 6.5%

Toxicology: Irritating to eyes and mucous membranes and respiratory tract; possible carcinogen, possible damage to liver and kidneys; lachrymator; narcotic at high concentrations.

Reactivities and Chemical Incompatibilities: Thermal decomposition can produce HCl, CO, CO_2, phosgene; can undergo hazardous polymerization; avoid contact with strong oxidizers, air, Cu, Al; absorbs O_2, forming explosive peroxides.

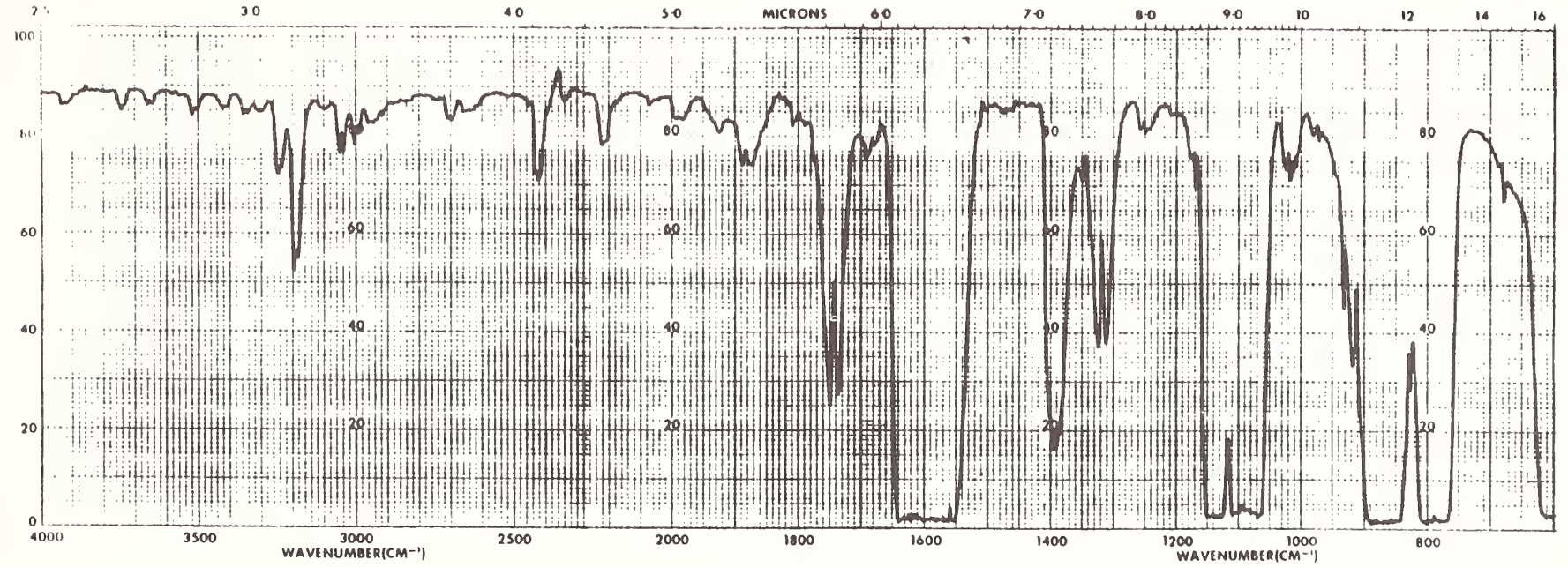
Solubilities: Alcohols (reacts), ether, benzene, acetone, chloroform, carbon tetrachloride; H_2O: 2250 mg/L (25 °C).

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
26.00	1458176	49.00	172096	62.00	351872	84.00	18192
35.00	982016	50.00	26560	63.00	1219072	94.00	15882
37.00	313984	59.00	169280	64.00	26892	96.00	1399808
38.00	36200	60.00	803712	82.00	33824	97.00	853056
47.00	359552	61.00	3907072				

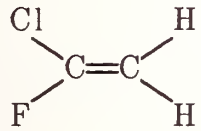
Infrared Spectrum – Gas Phase



1131a 1-chloro-1-fluoroethylene

synonyms: 1–chloro–1–fluoroethene; chlorofluoroethylene; chlorofluoroethene.

structure:



C. A. S. Registry Number: 231–79–11
Relative Molecular Mass: 80.5

Normal Boiling Point: –24 °C

Melting Point: –169 °C

Density/Specific Gravity:

Critical Temperature: 68.8 °C*

Refractive Index:

Critical Pressure: 6.97 MPa*

Critical Density: 0.530 g/mL*

****

Vapor Density: >1 **PEL:** NE **TLV:** NE

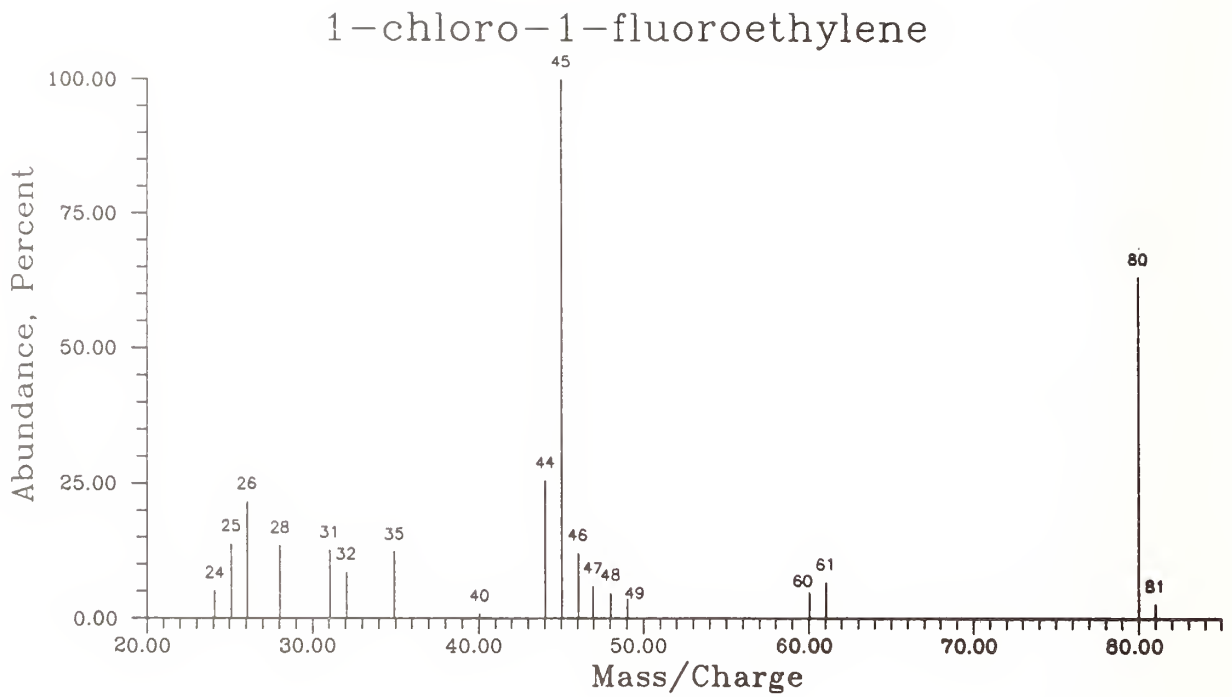
Flash Point: NA **UEL:** NA **LEL:** NA

Toxicology: Detailed toxicology is not available; possible pulmonary irritant.

Reactivities and Chemical Incompatibilities: Thermal decomposition can form HF, HCl, CO, CO_2; no known major chemical incompatibilities.

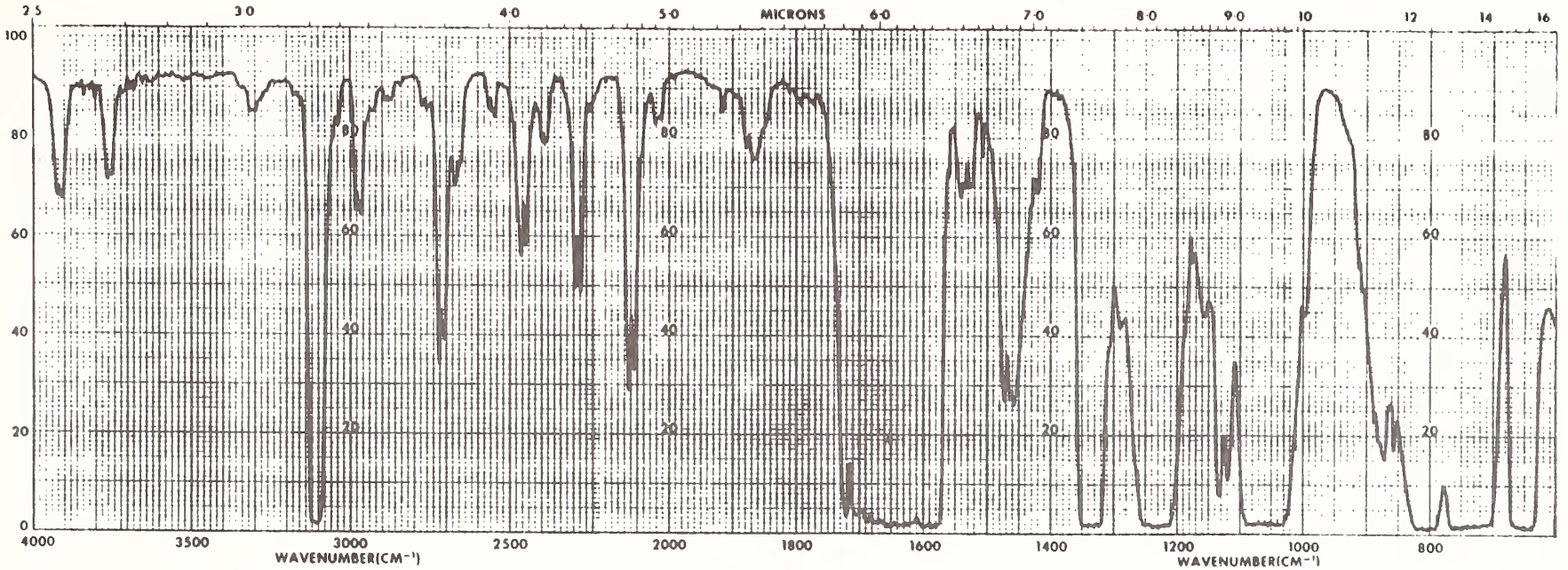
Solubilities: Somewhat soluble in carbon tetrachloride; negligible solubility in water.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
24.00	209728	32.00	351872	45.00	4135424	59.00	39056
25.00	566720	34.00	507136	46.00	94056	60.00	200256
26.00	888384	37.00	170688	47.00	242112	61.00	275008
28.00	553088	40.00	31600	48.00	189184	80.00	2616832
31.00	516864	44.00	1053184	49.00	146688	81.00	108880

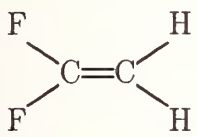
Infrared Spectrum – Gas Phase



1132a 1,1-difluoroethylene

synonyms: 1,1–difluoroethene; difluoroethylene; vinylidene fluoride; vinylidene difluoride; Genetron 1132.

structure:



C. A. S. Registry Number: 75–38–7
Relative Molecular Mass: 64.04

Normal Boiling Point: –83 °C

Melting Point: –144 °C

Density/Specific Gravity:

Critical Temperature: 30.1 °C

Refractive Index:

Critical Pressure: 4.43 MPa

Critical Density: 0.417 g/mL

****

Vapor Density: 2.21

PEL: 5 ppm

TLV: 1 ppm

Flash Point: <65 °C

UEL: 21%

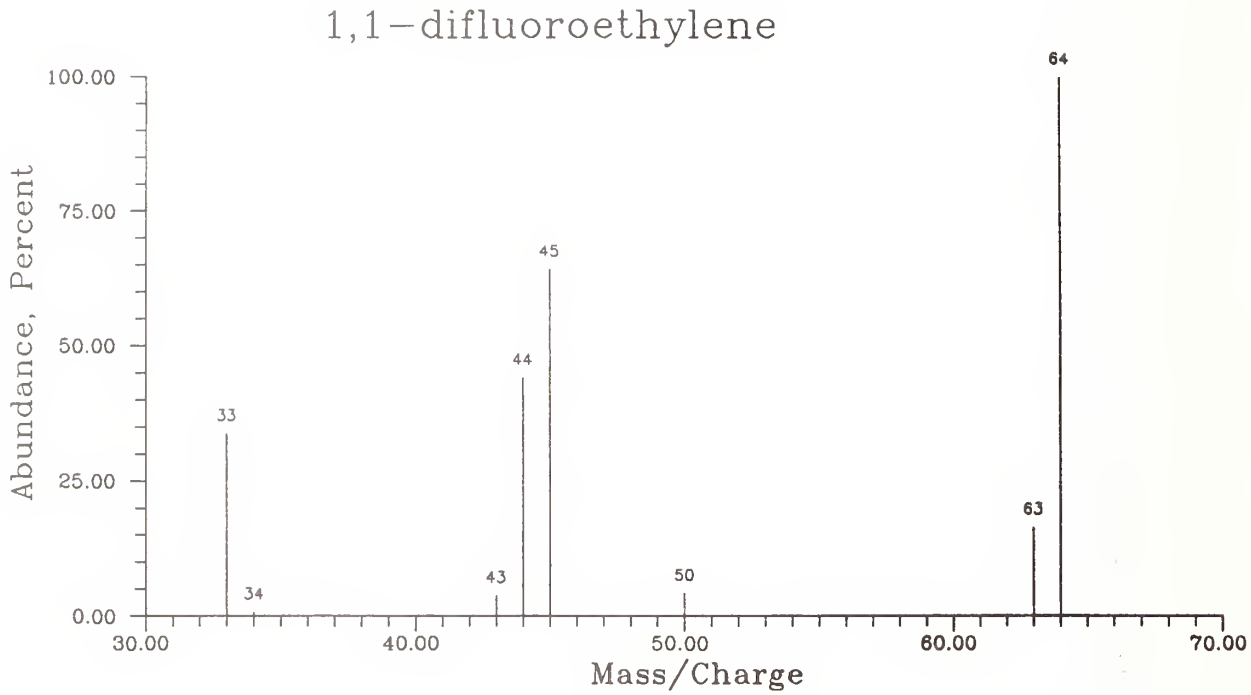
LEL: 5.5%

Toxicology: Detailed toxicology is not available; may cause slight anesthesis, difficulty in breathing, ataxia, fatigue; possible mutagen, tumorigen.

Reactivities and Chemical Incompatibilities: Thermal decomposition can produce HF, CO, CO_2; no known major chemical incompatibilities.

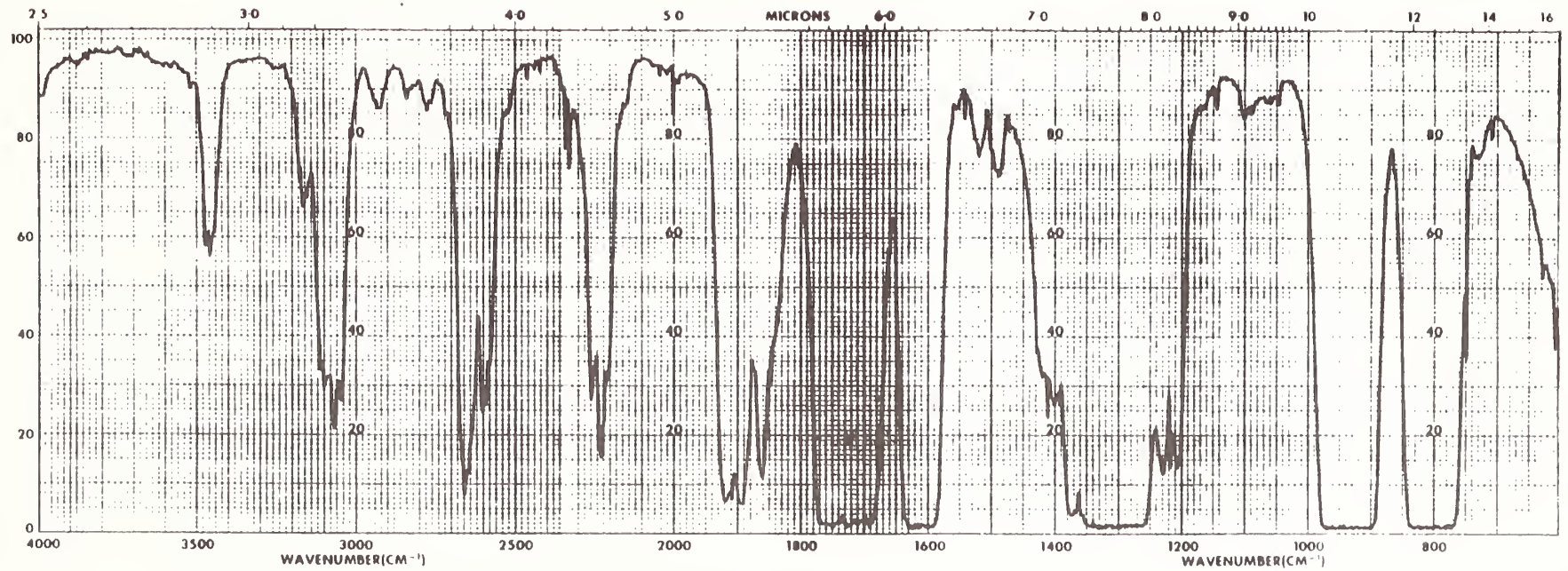
Solubilities: Somewhat soluble in carbon tetrachloride; negligible solubility in water.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
33.00	661312	43.00	67936	45.00	1158144	63.00	295872
34.00	11960	44.00	795008	50.00	75304	64.00	1805824

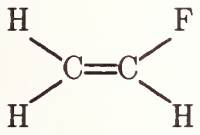
Infrared Spectrum – Gas Phase



1141 fluoroethylene

synonyms: vinyl fluoride; fluoroethene; monofluoroethene.

structure:



C. A. S. Registry Number: 75–02–5
Relative Molecular Mass: 46.04

Normal Boiling Point: –72.2 °C

Melting Point: –160.5 °C

Density/Specific Gravity: 0.615, l, (25 °C)

Critical Temperature: 54.7 °C

Refractive Index:

Critical Pressure: 5.54 MPa

Critical Density: 0.320 g/mL

****

Vapor Density: 1.6

PEL: NE

TLV: NE

Flash Point: flammable gas

UEL: 29%

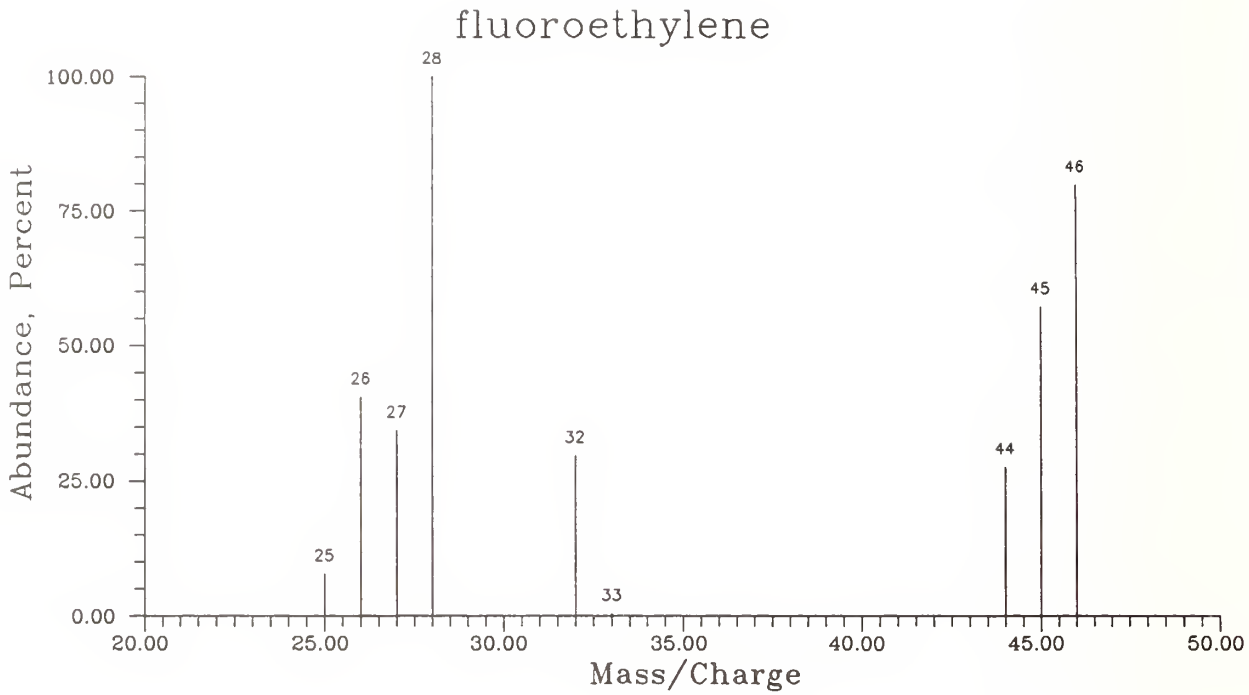
LEL: 2.6%

Toxicology: Moderate level of toxicity, causing light–headedness at low levels; at higher concentrations, eye and respiratory irritation, and narcosis is possible; possible mutagen.

Reactivities and Chemical Incompatibilities: Thermal decomposition can produce HF, CO, CO_2; avoid contact with alkali and alkaline earth metals, powdered Al, Zn, Be, azo compounds, peroxides, uv radiation, oxygen.

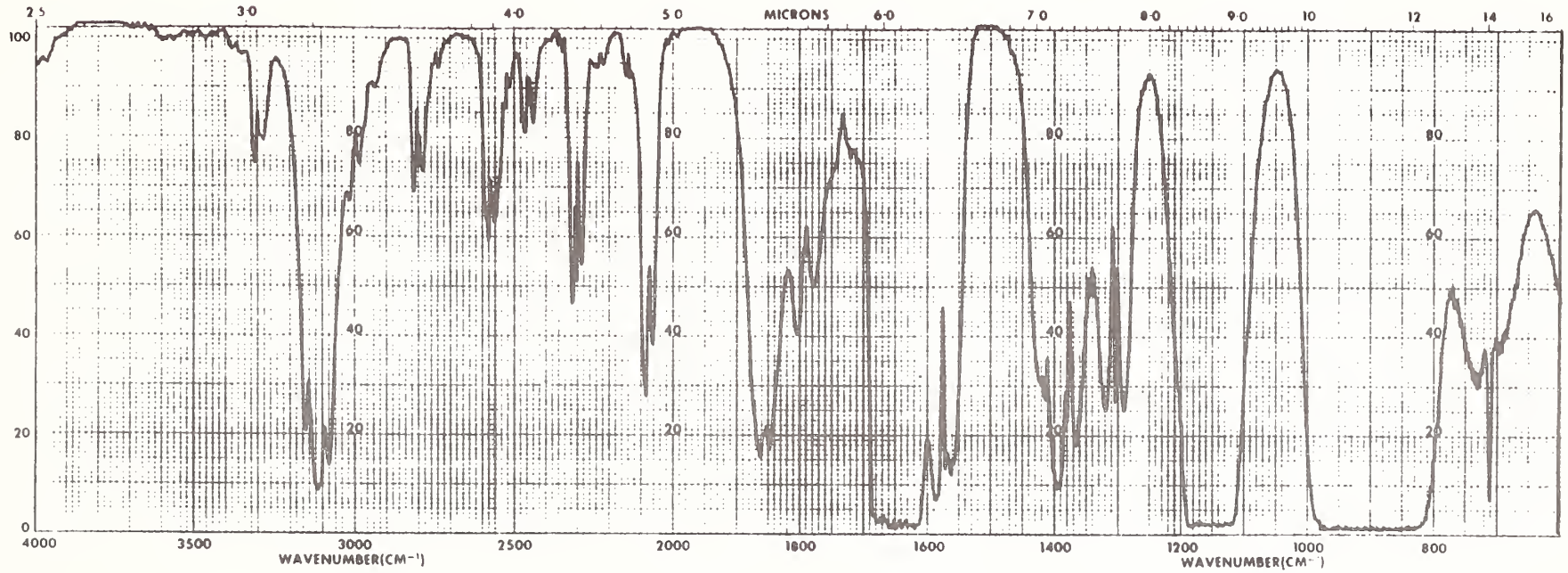
Solubilities: Alcohols, ether, carbon tetrachloride; H_2O: 1.1 percent wt/wt.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
25.00	230592	28.00	2956288	33.00	12528	45.00	1692160
26.00	1196544	32.00	876416	44.00	816832	46.00	2367488
27.00	1011712						

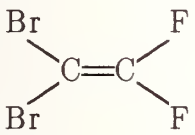
Infrared Spectrum – Gas Phase



1112aB2 1,1-dibromodifluoroethylene

synonyms: 1,1–dibromodifluoroethylene; 2,2–difluoroethylene.

structure:



C. A. S. Registry Number: 430–85–3
Relative Molecular Mass: 222

Normal Boiling Point: 68–69 °C

Melting Point:

Density/Specific Gravity:

Critical Temperature: 292.9 °C*

Refractive Index:

Critical Pressure: 9.2 MPa*

Critical Density: 1.12 g/mL*

****

Vapor Density: >1 **PEL:** NE **TLV:** NE

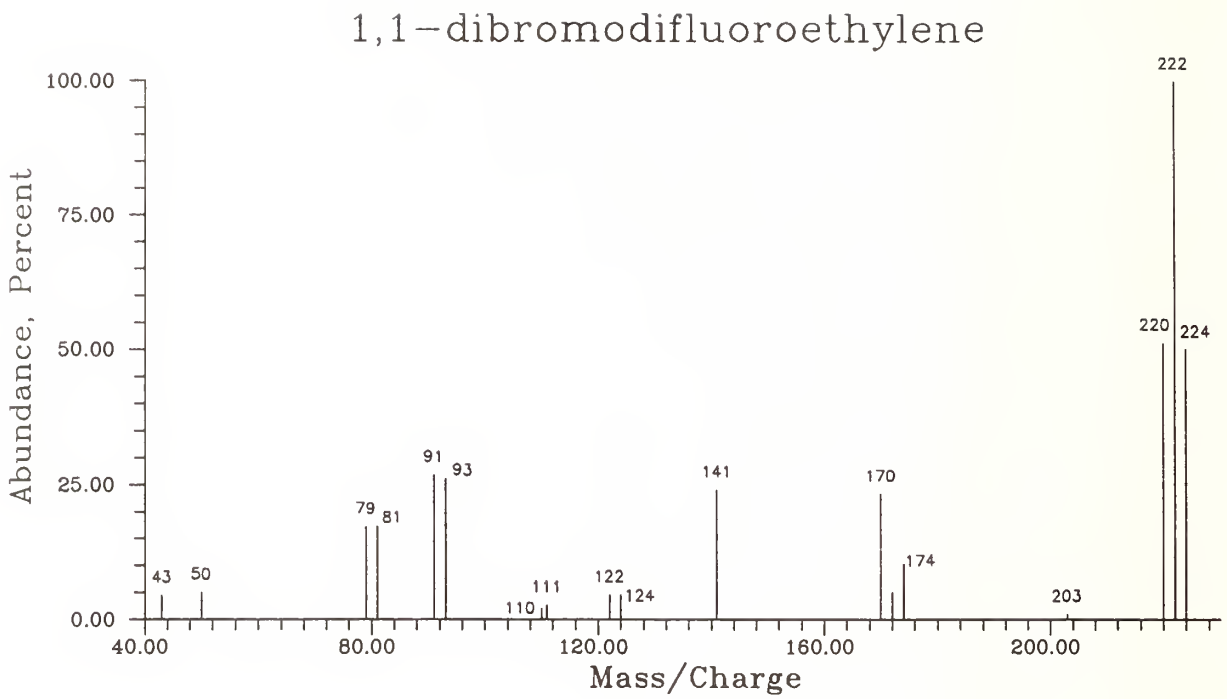
Flash Point: nonflammable **UEL:** NA **LEL:** NA

Toxicology: Detailed toxicology not available; possible skin, eye irritation; possible pulmonary edema.

Reactivities and Chemical Incompatibilities: Thermal decomposition can produce HBr, HF, CO, CO_2, COF, COBr; avoid contact with O_2, strong oxidizers, and active metals.

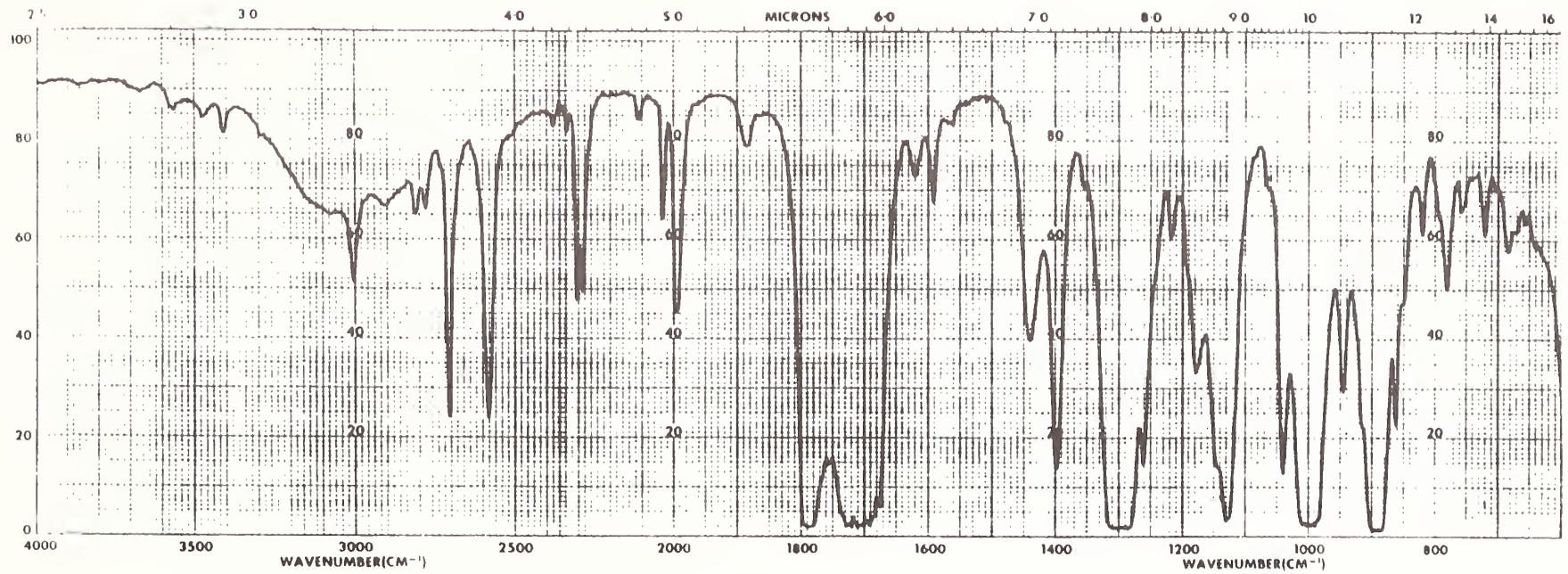
Solubilities: Somewhat soluble in carbon tetrachloride; negligible solubility in water.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
29.00	18188	81.00	101558	124.00	26951	174.00	28523
32.00	650545	91.00	158686	141.00	141954	203.00	5905
34.00	2757	93.00	154064	143.00	137556	220.00	303395
43.00	26269	110.00	12298	170.00	29599	222.00	592184
50.00	30081	111.00	15748	172.00	60688	224.00	296319
79.00	101473	122.00	26909				

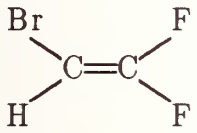
Infrared Spectrum — Liquid Phase (no solvent)



1122B1 1-bromo-2,2-difluoroethylene

synonyms: 1–bromo–2,2 difluoroethene.

structure:



C. A. S. Registry Number: NA
Relative Molecular Mass: 142.91

Normal Boiling Point: 6 °C

Melting Point: NA

Density/Specific Gravity: 1.82 g/mL (0.5 °C)

Critical Temperature: 183.8 °C*

Refractive Index:

Critical Pressure: 6.56 MPa*

Critical Density: 0.786 g/mL*

****

Vapor Density: 4.9

PEL: NE

TLV: NE

Flash Point: NA

UEL: NA

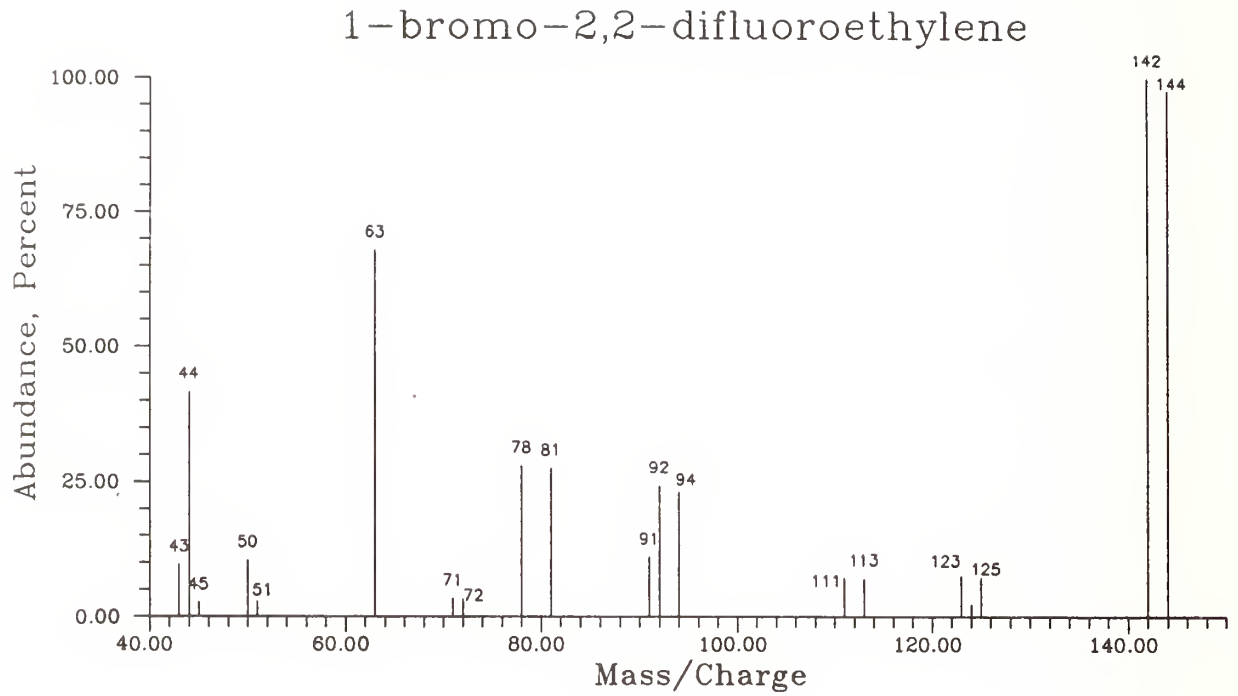
LEL: NA

Toxicology: Detailed toxicology is unknown; assume material to be highly toxic.

Reactivities and Chemical Incompatibilities: Avoid contact with oxidizing agents, halogens; thermal decomposition not investigated.

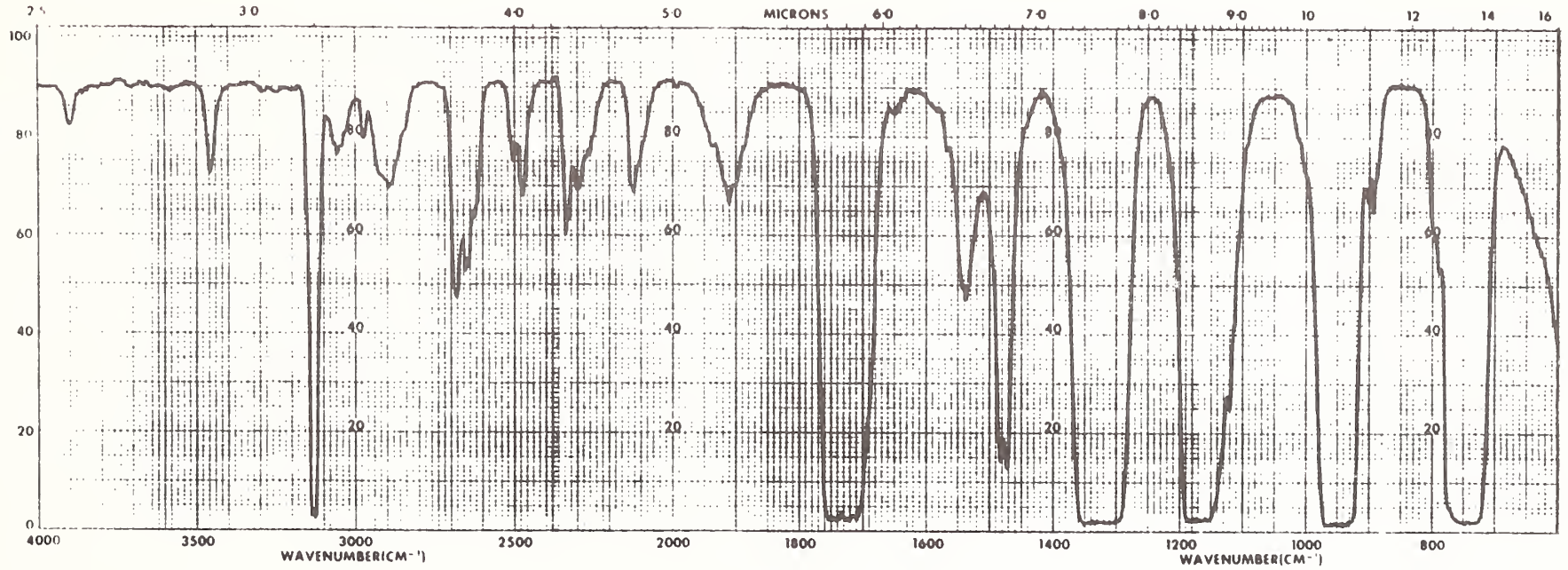
Solubilities: Somewhat soluble in carbon tetrachloride; negligible solubility in water.

Mass Spectrum:



m/e	Abund.	m/e	Abund.	m/e	Abund.	m/e	Abund.
31.00	1019546	63.00	748152	91.00	121403	123.00	82537
43.00	106084	64.00	20319	92.00	266633	124.00	25061
44.00	458099	71.00	37746	94.00	254655	125.00	80657
45.00	28605	72.00	35239	111.00	79481	142.00	1101913
50.00	114993	78.00	306360	113.00	77786	144.00	1077849
51.00	30979	81.00	302267				

Infrared Spectrum – Gas Phase



Active Metal – A metallic element (or alloy of elements) that reacts easily with a wide range of chemical compounds. Examples of active metals are the alkali and alkaline earth metals.

Addictive (substance) – A material for which a chemical or psychological dependence may develop upon slight to moderate exposure. (See narcotic, narcosis.)

Anesthesia – A temporary, reversible loss of sensation without necessarily a loss of consciousness.

Anesthetic – A chemical compound that causes temporary and reversible light–headedness, giddiness, symptoms of intoxication, and some degree of loss of sensory perception.

Ataxia – An inability to coordinate voluntary muscle movement, bearing similarity to the symptoms of a nervous disease.

Cardiac Sensitizer – A chemical compound that causes tachycardia, or causes an increase in sensitivity toward epinephrine (adrenaline).

Carcinogen – A substance which can produce cancer in organisms. Carcinogens may be confirmed or suspected.

Combustible Material – Any material that will burn, regardless of its autoignition temperature. All flammable materials are also considered combustible, but the term "combustible" strictly refers to materials that are difficult to ignite or that burn relatively slowly. A more exact quantification of this term is not possible since many regulatory agencies impose different limits of combustibility on materials.

Compatibility (chemical) – The ability of two or more chemical compounds to coexist intact, in an intimately mixed condition, without inducing chemical decomposition or reaction of any chemical species present in the mixture. In general, physical changes do not affect chemical compatibility. Thus, if moisture induces a change in crystal structure of a solid, the two are not considered incompatible.

Conjunctivitis – An inflamation of the conjunctiva, the delicate membrane that lines the eyelids, often associated with a discharge.

Critical Density – The density of a fluid at its critical temperature.

Critical Pressure – The pressure of a fluid at its critical temperature.

Critical Temperature – The temperature above which a fluid cannot be liquefied by the application of additional pressure.

Detonation – A rapid reaction of an explosive compound characterized by a high energy pressure–temperature wave that propagates at sonic velocity or greater.

Dyspnea – Difficulty with or labor in breathing.

Explosive Material – A chemical compound that easily detonates as a result of shock, heat, or chemical initiation.

Flammable Material – Any solid, liquid, vapor, or gas which will ignite and burn easily and rapidly, but not involving a shock wave that propagates at sonic velocity. It should be noted that the terms "flammable," "explosive," etc., are difficult to quantify with any degree of precision or uniformity. Any material that will burn at any temperature in any atmosphere is considered "combustible" by definition. The term flammable applies only to materials that ignite and burn easily. The distinction between nonflammable and noncombustible follows from these criteria as well. For example, sodium chloride is noncombustible, sucrose is nonflammable.

Hazardous Polymerization – A polymerization reaction that can release large amounts of energy, cause fires, or burst typical chemical containers. Chemicals capable of hazardous polymerization usually contain an inhibitor which slows or prevents the polymerization reaction.

Lachrymator – A gas or vapor that is strongly irritating to the eyes, usually producing increased tear flow (lachyrimation).

Mutagen – A chemical that can change the genetic material of an organism.

Narcosis – A reversible condition in an organism characterized by immobility or significantly reduced or impaired mobility, stupor, insensibility, and a general attitude of irresponsibility.

Narcotic – A natural or synthetic material that induces coma, produces unconsciousness, or relieves pain, and that is potentially addictive. While many chemical compounds can have the biological effects of narcotics (such as chloroform, benzene, etc.), the element of addiction is present in the case of a narcotic.

Neat Sample – A sample which is not diluted with a solvent.

Pulmonary Edema – An abnormal, diffuse extravascular accumulation of fluid in the pulmonary tissues and air spaces of organisms due to changes in the hydrostatic pressure inside the capillaries or changes in the permeability of the capillaries.

Reproductive Affector – A chemical that can cause birth defects or spontaneous abortion of a fetus.

Tachycardia – Excessive rapidity in the action of the heart, usually characterized by a heart rate above 100 beats per minute.

Tumorigen – A chemical that can produce tumor; oncogenic compound.

Ventricular Fibrillation – Arrhythmia characterized by fibrillary contractions of the ventricular muscle due to rapid repetitive excitation of the myocardial fiber, without the coordinated concentration of the ventricle.

Appendix 1: Lydersen's Method of Critical Property Estimation

This method of critical property estimation is based upon additive group contributions for the major functionalities [1]. The only required inputs are the chemical structure of the chemical, the relative molecular mass, and the normal boiling point. The critical parameters are determined from:

$$T_c = T_b(0.567 + \Sigma\Delta_T - (\Sigma\Delta_T)^2)^{-1} \quad \text{(A1.1)}$$

$$P_c = M(0.34 + \Sigma\Delta_p)^{-2} \quad \text{(A1.2)}$$

$$V_c = 40 + \Sigma\Delta_v \quad \text{(A1.3)}$$

In the equations above, T_c is the critical temperature (in K), P_c is the critical pressure (in atmospheres), V_c is the critical volume (in cm^3/mol), T_b is the normal boiling point (in K), and M is the relative molecular mass. The relevant group increments are summarized in table A1.1:

Table A1.1

Group	Δ_T	Δ_p	Δ_v
CH_3—	0.020	0.227	55
—CH_2—	0.020	0.227	55
—CH<	0.012	0.210	51
CH_2=	0.018	0.198	45
CH=	0.018	0.198	45
—F	0.018	0.224	18
—Cl	0.017	0.320	49
—Br	0.010	0.5*	70*

* based on too few experimental data to be reliable.

The errors associated with using this method to estimate the critical temperature are usually less than 2 percent. For fluids of relative molecular mass of 100 or higher, and for increasingly polar compounds, the error can be expected to increase to approximately 5 percent. Uncertainties are greater for molecules having multifunctional polar groups, such as glycols. The errors in the critical pressures determined using A1.2 are between 4 and 10 percent, with the higher figure applicable for heavier and more polar molecules. The errors associated with the determination of the critical volume (and therefore the critical density) using A1.3 are probably between 5 and 15 percent, since there is much less data available upon which to base the group contributions.

Reference

[1] Lydersen, A. L., Estimation of Critical Properties of Organic Compounds, University of Wisconsin College of Engineering Experiment Station Report 3, Madison, WI, April 1965.

Appendix 2: Sources of Toxicology and Physical Properties

1. Toxic and Hazardous Industrial Chemicals Safety Manual, The International Technical Information Institute, Tokyo, Japan, 1975.

2. Matheson Gas Data Book, The Matheson Company, East Rutherford, NJ.

3. Sax, N. I., Dangerous Properties of Industrial Materials, 6th ed., Van Nostrand Reinhold, New York, NY, 1984.

4. Verschueren, K., Handbook of Environmental Data on Organic Chemicals, Van Nostrand Reinhold Co., New York, NY, 1977.

5. Weast, R., CRC Handbook of Chemistry and Physics, 69th ed., CRC Press, Boca Raton, FL, 1988.

6. Sax, N. I., Cancer Causing Chemicals, Van Nostrand Reinhold, New York, NY, 1981.

7. The Condensed Chemical Dictionary, 8th ed., Van Nostrand Reinhold Co., New York, NY, 1966.

8. Threshold Limit Values and Biological Exposure Indices for 1988–1989, American Conference of Governmental Industrial Hygienists, Cincinnati, OH, 1988.

9. Dorland's Illustrated Medical Dictionary, 28th ed., W. B. Saunders Co., Philadelphia, PA, 1989.

10. Weiss, G., ed., Hazardous Chemicals Data Book, 2nd ed., Noyes Data Corp., Park Ridge, NJ, 1986.

11. The Merck Index, Merck and Co., Inc., Rahway, NJ, 1983.

The following DIALOG databases have been used in the preparation of this Technical Note:

Chemname
Chemical Abstracts
Occupational Safety and Health
Registry of Toxic Effects of Chemical Compounds.

The following BRS database was used in the preparation of this Technical Note:

Hazardline

Appendix 3: Refrigerant Code Numbers for Ethane and Ethylene–Based Compounds

The digits in the ANSI/ASHRAE coding system [1] are determined from the right–hand side of the number.

1. The first digit on the right is the number of fluorine atoms on the molecule. When there are no fluorines on the molecule, such as in methylene chloride, a zero is assigned to this position.

2. The second digit from the right is one more than the number of hydrogen atoms on the molecule.

3. The third number from the right is one less than the number of carbon atoms in the compound. When this digit is zero, as in the case of methane–based fluids, it is omitted.

4. The number of chlorines is found by substracting the sum of the number of fluorine and hydrogen atoms from the total of the number of atoms that can be connected to the carbon atoms.

5. For cyclic compounds, an upper case "C" is placed before the identifying number.

6. In those instances where bromine is present in place of several or all of the chlorine atoms, the same rules apply except that the letter B after the number for the parent refrigerant shows the presence of bromine. The number to the right of the "B" indicates the number of bromine atoms present. When isomers of brominated compounds exist, the position of the bromine atoms are indicated by the Greek letters α and β. The Greek letters indicate the carbon atoms of the backbone chain, starting from the end carbon having the largest sum of atomic weights bonded to it. If more than one bromine is bonded to the same carbon, the Greek letter identifying that carbon is repeated for each bromine atom.

7. In the case of isomers, each isomer carries the same number. The different isomers are then indicated by appending lower case a, b, c, etc., to the extreme right–hand side of the code. The most symmetrical isomer does not have a letter appended. The letters are appended to the isomers as they become more and more unsymmetrical. The symmetry is determined by adding the atomic weights of the atoms bonded to each carbon, and subtracting one sum from another.

8. Unsaturated compounds are indicated by the fourth number from the right, which indicates the number of double bonds.

<u>Reference</u>

[1] Number Designation and Safety Classification of Refrigerants, ASHRAE standard, ANSI/ASHRAE 34–1989, American Society of Heating, Refrigerating and Air–Conditioning Engineers, Atlanta, GA, 1989.

Appendix 4: Unit Conversions

The international system of units is described in detail in NBS Special Publication 330 [1] and lists of physical constants and conversion factors are tabulated by Mechtly [2]. The American Society for Testing and Materials (ASTM), American National Standards Institute (ANSI), and the Institute of Electrical and Electronics Engineers (IEEE) have published a joint standard for metric practice [3]. The most recent guidelines for use of the metric system are given in References 1,2, and 3. Selected unit conversions, [1,4,5] are given in the following tables. The conversions are presented in matrix format when all of the units are of a convenient order of magnitude. When some of the unit conversions are of little value (such as the conversion between metric tons and grains), tabular form is followed, with the less useful units omitted.

References:

[1] The International System of Units (S.I.), National Bureau of Standards (U.S.) Special Publication SP-330 (July 1986).

[2] Mechtly, E.A., The International System of Units, Physical Constants and Conversion Factors, NASA Special Publication SP-7012, 1964.

[3] Standard for Metric Practice, ANSI/ASTM E-380-76, IEEE Std. 268-1976 (Jul. 1976).

[4] Chiu, Y., A Dictionary for Unit Conversion, School of Engineering and Applied Science, The George Washington University, Washington, DC, 20052.

[5] Bruno, T.J., Svoronos, P.D.N., CRC Handbook of Basic Tables for Chemical Analysis, CRC Press, Boca Raton 1989.

Area

MULTIPLY	BY	TO OBTAIN
square millimeters	0.00155	square inches (U.S.)
	1×10^{-6}	square meters
	0.01	square centimeters
	1.2732	circular millimeters
square centimeters	1.196×10^{-4}	square yards
	0.00108	square feet
	0.15500	square inches
	1×10^{-4}	square meters
	100	square millimeters
square kilometers	0.38610	square miles (U.S.)
	1.1960×10^{6}	square yards
	1.0764×10^{7}	square feet
	1×10^{6}	square meters
	247.10	acres (U.S)
square inches (U.S)	0.00694	square feet
	0.00077	square yards
	6.4516×10^{-4}	square meters
	6.4516	square centimeters
	645.15	square millimeters
square feet (U.S.)	3.5870×10^{-8}	square miles
	0.11111	square yards
	144	square inches
	0.09290	square meters
	929.03	square centimeters
	2.2957×10^{-5}	acres
square miles	640	acres
	3.0967×10^{6}	square yards
	2.7878×10^{7}	square feet
	2.5900	square kilometers

Density

kg/m^3	g/cm^3	lb/ft^3
16.018	0.016018	1
1	0.001	0.062428
1 000	1	62.428
2 015.9	2.0159	125.85

Enthalpy, Heat of Vaporization, Heat of Conversion, Specific Energies

kJ/kg (J/g)	cal/g	Btu/lb
2.3244	0.55556	1
1	0.23901	0.43022
4.1840	1	1.8

Length

MULTIPLY	BY	TO OBTAIN
angstroms	1×10^{-10}	meters
	3.9370×10^{-9}	inches (U.S.)
	1×10^{-4}	micrometers
	1×10^{-8}	centimeters
	0.1	nanometers
nanometers	1×10^{-9}	meters
	1×10^{-7}	centimeters
	10	angstroms
micrometers (μm)	3.9370×10^{-5}	inches (U.S.)
	1×10^{-6}	meters
	1×10^{-4}	centimeters
	1×10^{4}	angstroms
millimeters	0.03937	inches (U.S.)
	1000	micrometers
centimeters	0.39370	inches (U.S.)
	1×10^{4}	micrometers (μm)
	1×10^{7}	nanometers
	1×10^{8}	angstroms
meters	6.2137×10^{-4}	miles (statute)
	1.0936	yards (U.S.)
	39.370	inches (U.S.)
	1×10^{9}	millimicrons
	1×10^{10}	angstroms
kilometers	0.53961	miles (nautical)
	0.62137	miles (statute)
	1093.6	yards
	3280.8	feet
inches	0.02778	yards
	2.5400	centimeters
	2.5400×10^{8}	angstroms
feet (U.S.)	0.30480	meters
	30.480	centimeters

Length (cont.)

yards (U.S.)	5.6818×10^{-4}	miles
	0.91440	meters
	91.440	centimeters
miles (nautical)	1.1516	statute miles
	2026.8	yards
	1.8533	kilometers
miles (U.S. statute)	320	rods
	0.86836	nautical miles
	1.6094	kilometers
	1609.4	meters

Parts Per Million

PARTS PER MILLION	vs.	PERCENT
1 ppm	=	0.0001%
10 ppm	=	0.001%
100 ppm	=	0.01%
1 000 ppm	=	0.1%
10 000 ppm	=	1.0%
100 000 ppm	=	10.0%
1 000 000 ppm	=	100.0%

Pressure

MPa	atm	Torr (mm Hg)	bar	lbs/in^2 (psi)
6.8948×10^{-3}	0.068046	51.715	6.8948×10^{-2}	1
1	9.8692	7,500.6	10.0	145.04
0.101325	1	760.0	1.01325	14.696
1.3332×10^{-4}	1.3158×10^{-3}	1	1.332×10^{-3}	0.019337
0.1	0.98692	750.06	1	14.504

Specific Heat, Entropy

kJ/(kg-k) J/(g-K)	Btu (°R·lb)
4.184	1
1	0.23901

Specific Volume

m^3/kg (L/g)	cm^3/g	ft^3/lb
0.062428	62.428	1
1	1 000	16.018
0.001	1	0.016018

Surface Tension

N/m	dyne/cm	lb/in
175.13	175.13×10^3	1
1	1 000	5.7102×10^{-6}
0.001	1	5.7102×10^{-3}

Temperature

T(rankine) = 1.8T(kelvin)
T(celsius) = T(kelvin) - 273.15
T(fahrenheit) = T(rankine) - 459.67
T(fahrenheit) = 1.8T(celsius) + 32

Thermal Conductivity

mW/(cm-K)	J/(s-cm-K)	cal/(s-cm-K)	Btu/(ft-hr-°R)
17.296	0.017296	0.0041338	1
1	0.001	2.3901×10^{-4}	0.057816
1 000	1	0.23901	57.816
4 184	4.184	1	241.90

Velocity

MULTIPLY	BY	TO OBTAIN
feet per minute	0.01136	miles per hour
	0.01829	kilometers per hour
	0.5080	centimeter per second
	0.01667	feet per second
feet per second	0.6818	miles per hour
	1.097	kilometers per hour
	30.48	centimeter per second
	0.3048	meters per second
	0.5921	knots
knots (Br.)	1.0	nautical miles per hour
	1.6889	feet per second
	1.1515	miles per hour
	1.8532	kilometers per hour
	0.5148	meters per second
meters per second	3.281	feet per second
	2.237	miles per hour
	3.600	kilometers per hour
miles per hour	1.467	feet per second
	0.4470	meters per second
	1.609	kilometers per hour
	0.8684	knots

Velocity of Sound

m/s	ft/s
0.3048	1
1	3.2808

Viscosity

kg/(m-s) (N-s/m^2, Pa·s)	cP (10^{-2}g/(cm-s))	lb-s/ft^2 (slug/(ft-s))	lb/(ft-s)
1.48816	1 488.16	0.31081	1
1	1 000	0.020885	0.67197
0.001	1	2.0885×10^{-5}	6.7197×10^{-4}
47.881	4.7881×10^{-4}	1	32.175

Volume

MULTIPLY	BY	TO OBTAIN
barrels (pet)	42	gallons (U.S.)
	34.97	gallons (Br.)
cubic centimeters	10^{-3}	liters
	0.0610	cubic inches
cubic feet	28317	cubic centimeters
	1728	cubic inches
	0.03704	cubic yards
	7.481	gallons (U.S., liq.)
	28.317	liters
cubic inches	16.387	cubic centimeters
	0.016387	liters
	4.329×10^{-3}	gallons (U.S., liq.)
	0.01732	quarts (U.S., liq.)
gallons, imperial	277.4	cubic inches
	1.201	U.S. gallons
	4.546	liters
gallons, U.S. (liquid)	231	cubic inches
	0.1337	cubic feet
	3.785	liters
	0.8327	imperial gallons
	128	fluid ounces (U.S.)
ounces, fluid	29.57	cubic centimeters
	1.805	cubic inches
liters	0.2642	gallons
	0.0353	cubic feet
	1.0567	quarts (U.S., liq.)
	61.025	cubic inches
quarts, U.S. (liquid)	0.0334	cubic feet
	57.749	cubic inches
	0.9463	liters

Mass (weight)

MULTIPLY	BY	TO OBTAIN
milligrams	2.2046×10^{-6}	pounds (avoirdupois)
	3.5274×10^{-5}	ounces (avoirdupois)
	0.01543	grains
	1×10^{-6}	kilograms
micrograms	1×10^{-6}	grams
grams	0.00220	pounds (avoirdupois)
	0.03527	ounces (avoirdupois)
	15.432	grains
	1×10^{6}	micrograms
kilograms	0.00110	tons (short)
	2.2046	pounds (avoirdupois)
	35.274	ounces (avoirdupois)
	1.5432×10^{4}	grains
grains	1.4286×10^{-4}	pounds (avoirdupois)
	0.00229	ounces (avoirdupois)
	0.06480	grams
	64.799	milligrams
ounces (avoirdupois)	3.1250×10^{-5}	tons (short)
	0.06250	pounds (avoirdupois)
	437.50	grains
	28.350	grams
pounds (avoirdupois)	5×10^{-4}	tons (short)
	16	ounces (avoirdupois)
	7000	grains
	0.45359	kilograms
	453.59	grams
tons (short, U.S.)	2000	pounds (avoirdupois)
	3.200×10^{4}	ounces (avoirdupois)
	907.19	kilograms
tons (long)	2240	pounds (avoirdupois)
	1016	kilograms
tons (metric)	1000	kilograms
	2205	pounds (avoirdupois)
	1.102	tons (short)

Prefixes for SI Units

Fraction	Prefix	Symbol
10^{-1}	deci	d
10^{-2}	centi	c
10^{-3}	milli	m
10^{-6}	micro	μ
10^{-9}	nano	n
10^{-12}	pico	p
10^{-15}	femto	f
10^{-18}	atto	a

Multiple	Prefix	Symbol
10	deka	da
10^2	hecto	h
10^3	kilo	k
10^6	mega	M
10^9	giga	G
10^{12}	tera	T
10^{15}	peta	P
10^{18}	exa	E

Recommended Values of Physical Constants

Physical constant	Symbol	Value
Avogadro constant	N_A	$6.022\ 05 \times 10^{23}\ mol^{-1}$
Boltzmann constant	k	$1.380\ 66 \times 10^{-23}\ J \cdot K^{-1}$
charge to mass ratio	e/m	$1.758\ 796 \times 10^{11}\ C \cdot kg^{-1}$
electronic charge	e	$1.602\ 19 \times 10^{-19}\ C$
Faraday constant	F	$9.648\ 46 \times 10^{4}\ C \cdot mol^{-1}$
gas constant	R	$8.314\ J\ K^{-1}\ mol^{-1}$
'ice point' temperature	T_{ice}	273.150 K (exactly)
molar volume of ideal gas (stp)	V_m	$2.241\ 38 \times 10^{-2}\ m^3 \cdot mol^{-1}$
permittivity of vacuum	ϵ_o	$8.854\ 188 \times 10^{-12}\ kg^{-1}\ m^{-3} \cdot s^4 \cdot A^2\ (F \cdot m^{-1})$
Planck constant	h	$6.626\ 2 \times 10^{-34}\ J \cdot s$
standard atmosphere pressure	p	$101\ 325\ N \cdot m^{-2}$ (exactly)
atomic mass unit	m_u	$1.660\ 566 \times 10^{-27}\ kg$
speed of light in vacuum	c	$2.997\ 925 \times 10^{8}\ m \cdot s^{-1}$

BL-114A
(5-90)

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11. ABSTRACT (A 200-WORD OR LESS FACTUAL SUMMARY OF MOST SIGNIFICANT INFORMATION. IF DOCUMENT INCLUDES A SIGNIFICANT BIBLIOGRAPHY OR LITERATURE SURVEY, MENTION IT HERE.)

This Special Publication contains infrared and mass spectra for a wide range of chloro-fluoro-bromo ethanes and ethylenes that are relevant to research on alternative refrigerants. Alternative refrigerants are working fluids that are thought not to contribute significantly to atmospheric ozone depletion. In addition to the spectroscopic data, some physical property and safety information is included for each fluid as well. Not all of the compounds covered in this publication can be used as refrigerants. Indeed, some of them are in fact solids under ambient conditions, and others are fully halogenated, thus making them unfavorable from an ozone depletion standpoint. The study of all of these materials is important, however, since many will be found as impurities or reaction/decomposition products of refrigerant fluids. This publication provides a signal source for some particularly useful analytical information needed in the identification of these compounds.

12. KEY WORDS (6 TO 12 ENTRIES; ALPHABETICAL ORDER; CAPITALIZE ONLY PROPER NAMES; AND SEPARATE KEY WORDS BY SEMICOLONS)

alternative refrigerants; chemical analysis; infrared spectrophotometry; mass spectrometry; safety

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