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Basic Tables for Chemical Analysis

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NBS technical note

Basic Tables for Chemical Analysis

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BASIC TABLES FOR CHEMICAL ANALYSIS

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Tables of important data for use in the analytical chemistry laboratory are provided. These tables contain information for use in gas chromatography, liquid chromatography, infrared and ultraviolet spectrophotometry, mass spectrometry, and wet chemical techniques. Tables relating to safe practice in the analytical laboratory are also included.

Key words: chemical analysis; instrumental analysis.

Introduction

This set of tables is intended to serve as a handy reference for both the practicing chemist and student. Included are data which are not easily obtainable elsewhere, collected in a source which is intended to reduce the need for consulting a bookshelf of reference works in the daily practice of analytical chemistry.

This technical note grew out of a booklet of tables which accompanied a series of lectures on analytical chemistry presented by one of the authors (T.J.B) for the professional staff and students working at the National Bureau of Standards Boulder Laboratories. That booklet has now been expanded and augmented by the authors in this volume. The primary purpose of these tables is to support the teaching and research activities of the authors, and it is offered to the scientific community as a low-cost source of useful information for the practicing scientist.

The topics covered in this volume include gas chromatography, liquid chromatography, thin layer chromatography, infrared and ultraviolet spectrophotometry, mass spectrometry , and "wet" chemical tests. Aspects of safety in the analytical laboratory are also considered. Topics such as atomic absorption, x-ray methods, and electroanalytical chemistry have not been included in the present volume but will be included in a future edition.

While the authors have endeavored to include data and information which they perceive to be most useful, there will undoubetdly be areas which have been slighted. We therefore ask you, the reader, to assist us in this regard and inform the corresponding author (T.J.B.) of any topics which should be included in future editions. The authors have made every effort to provide correct and up-to-date information in this volume. For the occasional mistake which may have crept into these pages, however, each author blames the other.

The authors would like to acknowledge the assistance of Juli Schroeder in the preparation of several of these tables. Terry Yenser, Barb Powers, and Marlene Deutsch are to be thanked for the excellent word processing services. The authors would like to acknowledge one of their teachers, Professor Charles

F. Hammer of Georgetwon University, who taught them much of what they know about spectroscopy. One of the authors (T.J.B.) gratefully acknowledges the financial support of the Gas Research Institute and the United States Department of Energy, Office of Basic Energy Sciences.

DISCLAIMER

Note

Occasional use is made of non-SI units in order to conform to standard and accepted practice in modern analytical chemistry.

I. Tables for Gas Chromatography

Mesh Sizes and Particle Diameters

The following tables give the relationship between particle size diameter (in μm) and several standard sieve sizes. The standards are as follows:

United States Standard Sieve Series, ASTM E-11-61

Canadian Standard Sieve Series, 8-GP-16

British Standards Institution, London, BS-410-62

Japanese Standard Specification, JI S-Z-8801

French Standard, AFNOR X-11-501

German Standard, DIN-4188

Particle Size, μm	U.S. Sieve Size	Tyler Mesh Size	British Sieve Size	Japanese Sieve Size	Canadian Sieve Size
4000	5	--	--	--	--
2000	10	9	8	9.2	8
1680	12	10	--	--	--
1420	14	12	--	--	--
1190	16	14	--	--	--
1000	18	16	--	--	--
841	20	20	18	20	18
707	25	24	--	--	--
595	30	28	25	28	25
500	35	32	--	--	--
420	40	35	36	36	36
354	45	42	--	--	--
297	50	48	52	52	52
250	60	60	60	55	60
210	70	65	72	65	72
177	80	80	85	80	85
149	100	100	100	100	100
125	120	115	120	120	120
105	140	150	150	145	150
88	170	170	170	170	170
74	200	200	200	200	200
63	230	250	240	250	240
53	270	--	300	280	300
44	325	--	350	325	350
37	400	--	--	--	--

French and German
Sieve Sizes

Particle size, μm	Sieve size
2000	34
800	30
500	28
400	27
315	26
250	25
200	24
160	23
125	22
100	21
80	20
63	19
50	18
40	17

Gas Chromatographic Support Materials

The following table lists the more common solid supports used in packed column gas chromatography, along with relevant properties [1-4]. The performance of several of these materials can be improved significantly by acid washing and treatment with DMCS (dimethyldichlorosilane) to further deactivate the surface. Most of the materials are available in several particle size ranges. The use of standard sieves will help insure reproducible packings from one column to the next.

REFERENCES:

[1] Poole, C.F., Schuette, S.A., Contemporary Practice of Chromatography, Elsevier, Amsterdam, 1984.

[2] Gordon, A.J., Ford, R.A., The Chemist's Companion, John Wiley and Sons, New York, 1972.

[3] Heftmann, E., ed., Chromatography: A Laboratory Handbook of Chromatographic and Electrophoretic Methods, 3rd ed., Van Nostrand Reinhold, New York, 1975.

[4] Grant, D.W., Gas Liquid Chromatography, Van Nostrand Reinhold, London, 1971.

Support name	Support type	Density (free fall) g/mL	Density (packed) g/mL	pH	Surface area m^2/g	Maximum liquid loading	Color	Notes
Chromosorb A	diatomite	0.40	0.48	7.1	2.7	25%	pink	most useful for preparative gas chromatography; high strength; high liquid phase capacity; low surface activity.
Chromosorb G	diatomite	0.47	0.58	8.5	0.5	5%	oyster white	high mechanical strength; low surface activity; high density.
Chromosorb P	diatomite firebrick	0.38	0.47	6.5	4.0	30%	pink	high mechanical strength; high liquid capacity; moderate surface activity; for separations of moderately polar compounds.
Chromosorb W	diatomite	0.18	0.24	8.5	1.0	15%	white	lower mechanical strength than pink supports; very low surface activity; for polar compound separation.
Chromosorb T	PTFE*	0.42	0.49		7.5	5%	white	maximum temperature of 250°C; handling is difficult due to static charge; tends to deform when compressed; useful for analysis of high polarity compounds.

*PTFE - polytetrafluoroethyrene

Support name	Support type	Density (free fall) g/mL	Density (packed) g/mL	pH	Surface area m^2/g	Maximum liquid loading	Color	Notes
Chromosorb A	diatomite	0.40	0.48	7.1	2.7	25%	pink	most useful for preparative gas chromatography; high strength; high liquid phase capacity; low surface activity.
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Chromosorb P	diatomite firebrick	0.38	0.47	6.5	4.0	30%	pink	high mechanical strength; high liquid capacity; moderate surface activity; for separations of moderately polar compounds.
Chromosorb W	diatomite	0.18	0.24	8.5	1.0	15%	white	lower mechanical strength than pink supports; very low surface activity; for polar compound separation.
Chromosorb T	PTFE*	0.42	0.49		7.5	5%	white	maximum temperature of 250 °C; handling is difficult due to static charge; tends to deform when compressed; useful for analysis of high polarity compounds.

*PTFE - polytetrafluoroethyrene

Carrier Gas Properties

The following table gives the properties of common gas chromatographic carrier gases. These properties are those used most often in designing separation and optimizing detector performance. The density values are determined at 0°C and 0.101 MPa (760 Torr) [1]. The thermal conductivity values are determined at 48.9°C (120°F) [1]. The viscosity values are determined at the temperatures listed, and at 0.101 MPa (760 Torr) [1]. The heat capacity (constant pressure) values are determined at 15°C and 0.101 MPa (760 Torr) [2].

REFERENCES:

[1] Weast, R. C., ed., Handbook of Chemistry and Physics, 63rd ed., CRC Press, Boca Raton, 1983.

[2] Dal Nogare, S., Juvet, R. S., Gas-Liquid Chromatography: Theory and Practice, John Wiley and Sons (Interscience), New York, 1962.

Carrier Gas	Density (kg/m^3)	Thermal Conductivity x 10^{-2} (W/m•K)	Thermal Conductivity Differences			Viscosity x10^{-5} (Pa•s)	Heat Capacity (J/kg•K)	Molecular Weight
			δλ (He)	δλ (N_2)	δλ (Ar)			
hydrogen	0.08988	19.71	3.97	16.96	17.81	0.876 (20.7°C) 1.086 (129.4°C) 1.381 (299.0°C)	14,112.7	2.016
helium	0.17847	15.74	--	12.99	13.84	1.941 (20.0°C) 2.281 (100.0°C) 2.672 (200.0°C)	5,330.6	4.003
methane	0.71680	3.74	-12.00	0.99	1.84	1.087 (20.0°C) 1.331 (100.0°C) 1.605 (200.5°C)	2,217.2	16.04
oxygen	1.42904	2.85	-12.89	0.10	0.95	2.018 (19.1°C) 2.568 (127.7°C) 3.017 (227.0°C)	915.3	32.00
nitrogen	1.25055	2.75	-12.99	--	0.85	1.781 (27.4°C) 2.191 (127.2°C) 2.559 (226.7°C)	1,030.5	28.016
carbon monoxide	1.25040	2.67	-13.07	-0.08	0.77	1.753 (21.7°C) 2.183 (126.7°C) 2.548 (227.0°C)	1,030.7	28.01

Carrier Gas	Density (kg/m³)	Thermal Conductivity x 10^{-2} (W/m•K)	Thermal Conductivity Differences			Viscosity x10^{-5} (Pa•s)	Heat Capacity (J/kg•K)	Molecular Weight
			δλ (He)	δλ (N_2)	δλ (Ar)			
ethane	1.35660	2.44	-13.30	-0.31	0.54	0.901 (17.2°C) 1.143 (100.4°C) 1.409 (200.3°C)	1,614.0	30.07
ethene	1.26040	2.30	-13.44	-0.45	0.40	1.008 (20.0°C) 1.257 (100.0°C) 1.541 (200.0°C)	--	28.05
propane	2.00960	2.03	-13.71	-0.72	0.13	0.795 (17.9°C) 1.009 (100.4°C) 1.253 (199.3°C)	--	44.09
argon	1.78370	1.90	-13.84	-0.85	--	2.217 (20.0°C) 2.695 (100.0°C) 3.223 (200.0°C)	523.7	39.94
carbon dioxide	1.97690	1.83	-13.91	-0.92	-0.07	1.480 (20.0°C) 1.861 (99.1°C) 2.221 (182.4°C)	836.6	44.01
n-butane	2.51900	1.82	-13.92	-0.93	-0.08	0.840 (14.7°C)	--	58.12
sulfur hexafluoride	6.50 (20°C)	1.63	-14.11	-1.12	-0.27	1.450 (21.1°C)	674.0	146.05

Properties of Some Liquid Phases

The following table lists some of the more common gas-chromatographic liquid phases, along with some relevant data and notes [1,2]. Most of these have been largely superseded by silicone phases used in capillary columns, but these liquid phases still find application in many instances. The minimum temperatures, where reported, indicate the point at which some of the phases approach solidification, or when the viscosity increases to the extent that performance is adversely effected. The maximum working temperatures are determined by vapor pressure (liquid phase bleeding) and chemical stability considerations. The liquid phases are listed by their most commonly used names. Where appropriate, chemical names or common generic names are provided in the notes.

The McReynolds constants tabulated here are based on the retention characteristics of the following test probe samples:

Constant	Test probe
X	benzene
Y	1-butanol
Z	3-pentanone
U	1-nitroporpane
S	pyridine

Compounds which are chemically similar to these probe solutes will show similar retention characteristics. Thus, benzene can be thought of as representing lower aromatic or olefinic compounds. Higher values of the McReynolds constant usually will indicate a longer retention time (higher retention volume) for a compound represented by that constant, for a given liquid (stationary) phase.

Properties of Some Liquid Phases (cont.)

Solvents:

Ace - acetone
Chlor - chloroform
Pent - pentane
DMP - dimethylpentane
MeCl - methylene chloride
Tol - toluene
MeOH - methanol
H_2O - water

Polarity:

N - nonpolar
P - polar
I - intermediate polarity
H.B. - hydrogen bonding
S - specific interaction

REFERENCES:

[1] McReynolds, W.O., J. Chromatogr. Sci, 8, 685, 1970.

[2] McNair, H. ., Bonelli, E.J., Basic Gas Chromatography, Varian Aerograph, Palo Alto, 1968.

Liquid Phase	T_{min}, °C	T_{max}, °C	Polarity	Solvents	McReynolds Const.					Notes
					X	Y	Z	U	S	
acetonyl acetone (2,5-hexanedione)	-4	25	I	Ace						
acetyl tributyl citrate	25	180	I	Ace	135	268	202	314	233	
adiponitrile	5	50	I	Chlor MeCl						1,4-dicyanobutane
Alka terge-T, amine surfactant	59	75	I	Chlor meCl MeOH						60% oxazoline, weakly cationic
Ammine 220	0	180	P	Chlor MeCl	117	380	181	293	133	2-(8-Heptadecenyl)-2-imidazoline-1-ethanol
Apiezon H	50	275	N	Chlor	59	56	81	151	129	low vapor pressure hydrocarbon oil
Apiezon J	50	300	N	Chlor MeCl	38	36	27	49	57	low vapor pressure hydrocarbon oil
Apiezon L	50	300	N	Chlor MeCl	32	22	15	32	42	low vapor pressure hydrocarbon oil
Apiezon M	50	275	N	Chlor MeCl	31	22	15	30	40	low vapor pressure hydrocarbon oil
Apiezon N	50	300	N	Chlor MeCl	38	40	28	52	58	low vapor pressure hydrocarbon oil
Apiezon K	50	300+	N	Chlor						low vapor pressure hydrocarbon oil
Apiezon W	50	275	N	Chlor	82	135	99	155	154	low vapor pressure hydrocarbon oil

Liquid Phase	T_{min}, °C	T_{max}, °C	Polarity	Solvents	McReynolds Const.					Notes
					X	Y	Z	U	S	
Apolane-87	30	280	N	Tol	21	10	3	12	35	24,24-diethyl-19,29-dioctadecyl heptatetracontane, C-87 hydrocarbon
Armeen SD		100	P,S HB	Chlor MeCl						primary aliphatic amine
Armeen 12D		100	P, HB	Chlor MeCl						
Armeen 2-C		125	P,HB	Tol						secondary aliphatic amine
Armeen 2HT		100	P,HB	Chlor						
Arneel DD		100	P	MeOH						aliphatic nitrile
Aroclor 1254		125	I	Chlor MeCl						chlorinated biphenyl
Asphalt		300	N	Chlor MeCl						complex mixture of aliphatic, aromatic and heterocyclic compounds
Atpet 80			I	Chlor						sorbitan partial fatty acid esters
p,p-azoxydiphenetol	130	140	I	Chlor						
Bentone-34	20	200	S	Tol						dimethyl dioctadecylammonium bentonite
benzyl cyanide		50	I	MeOH						phenyl acetonitrile
benzyl cyanide-$AgNO_3$		25	S	MeCl						
benzyl diphenyl		100	I	Ace						

Liquid Phase	T_{min}, °C	T_{max}, °C	Polarity	Solvents	McReynolds Const.					Notes
					X	Y	Z	U	S	
7,8-benzoquinoline		150	I	Chlor MeCl						
Benzyl Cellosolve		50	I	Chlor MeCl						ethylene glycol monobenzyl ether
benzyl ether		50	I	Chlor MeCl						dibenzyl ether
bis (2-butoxyethyl) phthalate		175	I	MeOH	151	282	227	338	267	
bis (2-ethoxylethyl) phthalate					214	375	305	446	364	
bis (2-ethoxyethyl) Sebacate					151	306	211	320	274	
N,N-bis (2-cyanoethyl formamide)	0	125	I	MeOH	690	991	853	110	000	
bis (2-ethoxyethyl) adipate	0	150	I	Ace						
bis (2-methoxyethyl) adipate	20	150	I	Ace Chlor						
bis (2-Ethylhexyl tetrachlorophthalate	0	150	I	Chlor MeCl	112	150	123	108	181	
butanediol adipate	60	225	I,P	Chlor MeCl						
butanediol 1,4-succinate		200	I,P	Chlor	370	571	488	651	611	

Liquid Phase	T_{min}, °C	T_{max}, °C	Polarity	Solvents	McReynolds Const. X	Y	Z	U	S	Notes
bis[2-(2-methoxy-ethoxy ethyl] ether		50	I	Chlor						tetraethylene glycol dimethylether
Carbowax 300	10	100	P	MeCl						polyethylene glycol, av. mol. wt. < 380
Carbowax 400	10	125	P	MeCl	333	653	405			polyethylene glycol, av. mol. wt. 380-420
Carbowax 400 mono-oleate	10	125	P	MeCl						
Carbowax 550	20	125	P	MeCl						
Carbowax 600	30	125	P	MeCl	323	583	382			polyethylene glycol, av. mol. wt. 570-630
Carbowax 600 monostearate		125	P	MeCl						
Carbowax 750	25	150	P	MeCl						methoxy polyethylene glycol, av. mol. wt. 715-785
Carbowax 1000	40	175	P	MeCl	347	607	418	626	589	polyethylene glycol av. mol. wt. 950-1050
Carbowax 1500 (or Carbowax 540)	40	200	P	MeCl						polyethylene glycol, av. mol. wt. 500-600
Carbowax 1540	40	200	P	MeCl	371	639	453	666	641	polyethylene glycol, av. mol. wt. 1300-1600
Carbowax 4000 (or 3350)	60	200	P	MeCl	317	545	378	578	521	polyethylene glycol, av. mol. wt. 3000-3700
Carbowax 4000 TPA		175	P	MeCl MeOH						terminated with terephthalic acid

Liquid Phase	T_{min}, °C	T_{max}, °C	Polarity	Solvents	McReynolds Const.					Notes
					X	Y	Z	U	S	
Carbowax 4000 monosterate	60	220	P	MeCl	282	496	331	517	467	
Carbowax 6000	60	200	P	MeCl	322	540	369	577	512	polyethylene glycol, av. mol. wt. 6000-7500
Carbowax 8000	60	120	P	Chlor	322	540	369	577	512	polyethylene glycol av. mol. wt. 7000-8500
Carbowax 20M	60	250	P	MeCl	322	536	368	572	510	polyethylene glycol, av. mol. wt. 15,000-20,000
Carbowax 20M-TPA	60	250	P	MeCl	321	537	367	573	520	terminated with terephthalic acid
Castorwax	90	200	P	MeCl	108	265	175	229	246	triglyceride of 12-hydroxysteric acid (hydrogenated castor oil)
Chlorowax 70		130	P	MeCl						chlorinated parafin, 70% (wt/wt) Cl
1-chloronapthalene		75	I	Tol						
cyanoethyl sucrose	20	175	P	Ace	647	919	043	976		vitrifies at -10°C
cyclohexane dimethanol succinate	100	250	I	Chlor	269	446	328	498	481	
n-decane		30	N	MeCl						
di(ethoxyethoxy-) ethyl) phthalate					233	408	317	470	389	

Liquid Phase	T_{min}, °C	T_{max}, °C	Polarity	Solvents	McReynolds Const.					Notes
					X	Y	Z	U	S	
di(butoxyethyl) adipate	-10	150	P	Ace	137	278	198	300	235	
di(butoxyethyl) phthalate	-30	200	P	Tol	157	292	233	348	272	
di-n-butyl maleate	0	50	I	Tol						
dibutyl phthalate	-20	100	I	Tol						
dibutyltetra-chloro phthalate	0	150	I	Tol						
didecyl phthalate	20	150	I	Tol	136	255	213	320	235	
dicyclohexyl phthalate					146	257	206	316	245	
diethylene glycol adipate	0	200	I	MeCl	378	603	460	665	658	
diethylene glycol glutarate		225	I	MeCl						
diethylene glycol sebacate	80	190	I	MeCl						
diethylene glycol succinate	20	190	P	MeCl	496	746	590	837	835	
diethylene glycol stearate					64	193	106	143	191	
di(2-ethylhexyl) phthalate	20	150	P	Tol	135	254	213	320	235	

Liquid Phase	T_{min}, °C	T_{max}, °C	Polarity	Solvents	McReynolds Const.					Notes
					X	Y	Z	U	S	
di(2-ethylhexyl) adipate	-30	250	P	Ace	76	181	121	197	134	dioctyl adipate
di(2-ethylhexyl) sebacate	-20	125	I	Tol	72	168	108	180	125	
diethyl-D-tartarate		125	P,S	MeCl						
diglycerol	20	120	H.B.	MeCl MeOH	371	826	560	676	854	
dilauryl phthalate		150	I	Tol	79	158	120	192	158	
diisodecyl adipate	-10	175	P	Ace	71	171	113	185	128	
diisooctyl adipate	90	150	P	Ace	78	187	126	204	140	
diisodecyl phthalate	0	150	I	Tol Ace	84	173	137	218	155	
diisoctyl sebacate		175	I	Ace						
2,4-dimethyl sulfolane	0	50	P	Chlor						
dimer acid		100	I	MeCl						C_{36} dicarboxylic acid
diisooctyl phthalate	0	175	I	Tol	94	193	154	243	202	
dimethyl formamide	-20	20	P	Anl						DMF
dimethyl sulfoxide	20	30	P	MeCl						DMSO
dinonyl phthalate	20	150	I	Tol	83	183	147	231	159	
dioctyl phthalate	-20	150	I	Tol	92	186	150	230	167	

Liquid Phase	T_{min}, °C	T_{max}, °C	Polarity	Solvents	McReynolds Const. X	Y	Z	U	S	Notes
dioctyl sebacate		100	I	MeCl	72	168	108	180	123	
diphenyl formamide	75	100	I	Tol						
di-n-propyl tetrachlorophthalate	10	75	I	Tol						
ditridecyl phthalate	-10	225	P	Tol	75	156	122	195	140	
Emulphor un-870	0	200	I	Chlor	202	395	251	395	344	aryloxy polyethylene oxyethanol
EPON 1001	60	225	P	MeCl hot	284	489	406	539	601	epichlorohydrin-bisphenol A resin, av. mol. wt = 900
Ethofat 60/25	50	125	I	MeCl hot	191	382	244	380	333	polyethylene oxyglycol stearate
Ethomeen		75	P	MeCl	186	395	242	370	339	polyethoxylated aliphatic amine
ethylene glycol adipate	100	225	IP	MeCl	372	576	453	655	617	
ethyleneglycol phthalate	100	200	IP	Tol	453	697	602	816	872	
ethylene glycol succinate	100	200	IP	Ace	537	787	643	903	889	
ethylene glycol glutarate		225	I,P	MeCl						
ethylene glycol sebacate		200	I,P	MeCl hot						

Liquid Phase	T_{min}, °C	T_{max}, °C	Polarity	Solvents	McReynolds Const. X	Y	Z	U	S	Notes
ethylene glycol tetrachlorophthalate	120	200	P	Tol	307	345	318	428	466	
ethylene glycol		30	HB	MeOH						
ethylene glycol silver nitrate		30	S	Ace						
eutectic		400		H_2O						27.3% $LiNO_3$, 18.2% N_aNO_3, 54.4% KNO_3
FFAP	50	250	P,S	Chlor	340	580	397	602	627	Carbowax 20M nitro terephthalic acid ester
formamide	20	50	I	MeOH						
glycerol	20	100	HB	MeOH						
Fluorad FC-431	40	200		EAC	281	423	297	509	360	Fluorocarbon surfactant
Hallcomid M-18	40	150	I	MeCl	79	580	397	602	627	dimethylsteramide
Hallcomid M-18-OL	8	150	I	MeCl	89	280	143	239	165	dimethyloleamide
Halocarbon 10-25	20	100	I	Chlor	47	70	108	113	111	
Halocarbon K 352	0	250	I		47	70	73	238	146	
Halocarbon W9X(600)	50	150		Ace	55	71	116	143	123	
Halocarbon-1321	0	100		Ace						
Halocarbon-11-14	0	100		Ace						
HMPA	20	35	P	Chlor						hexamethylphosphoramide
Hi-Eff-1 AP	20	210	I,P	Chlor	378	603	460	665	658	diethyleneglycol adipate

Liquid Phase	T_{min}, °C	T_{max}, °C	Polarity	Solvents	McReynolds Const.					Notes
					X	Y	Z	U	S	
Hi-Eff-2 AP	100	210	I,P	Chlor	372	576	453	655	617	
Hi-Eff-8 BB	100	250	I,P	Chlor	271	444	333	498	463	cyclohexane dimethanol succinate
Hi-Eff-1 BP	20	200	I,P	Chlor	499	751	593	840		diethylene glycol succinate
Hi-Eff-2 BP	100	200	I,P	Chlor	537	787	643	903	889	ethylene glycol succinate
Hi-Eff-3 AP	50	230	I,P	Chlor						neopentyl glycol adipate
Hi-Eff-8 AP	100	250	I,P	Chlor						cyclohexane dimethanol adipate
Hi-Eff-9 AP	100	250	I,P	Chlor						tetramethyl cyclobutanediol adipate
Hi-Eff-3 BP			I,P							neopentyl glycol succinate
Hi-Eff-4 BP	50	230	I,P	Chlor						butane-1,4-diol succinate
Hi-Eff-10 BP	20	230	I,P	Chlor						phenyl diethanolamine succinate
Hi-Eff-2 CP	100	200	I,P	Chlor						ethylene glycol sebacate
Hi-Eff-3 CP	50	230	I,P	Chlor						neopentyl glycol sebacate
Hi-Eff-2 EP	100	210	I,P	Chlor						ethylene glycol isophthalate
Hi-Eff-26 P	100	210	I,P	Chlor						ethylene glycol phthalate
Hyprose-SP-80		225	P	MeOH	336	742	492	639	727	octakis (2-hydroxy propyl) sucrose

Liquid Phase	T_{min}, °C	T_{max}, °C	Polarity	Solvents	McReynolds Const.					Notes
					X	Y	Z	U	S	
1,2,3,4,5,6 hexakis-(2-cyanoethoxy-cyclo hexane)	125	150	I,P	Tol	567	825	713	978	901	
Hercoflex 600		150	P	MeCl	112	234	168	261	194	high boiling ester of pentaerythritol and a saturated aliphatic acid
n-hexadecane	20	50	N	Pent						
hexadecene	20	50	N	Pent						
n-hexadecanol		35	I	MeOH						
hexatricontane	80	150	N	MeCl	12	2	-3	1	11	$C_{36} H_{74}$
IGEPAL CO-880	100	200	I	MeCl hot	259	461	311	482	426	nonyl phenoxypolyethyleneoxy ethanol n = 30
IGEPAL CO-990	100	200	I	MeCl hot	298	508	345	540	475	nonylphenoxypoly (ethylene-oxyethanol) n = 100
IGEPAL CO-630	100	200	I	MeCl hot	192	381	253	382	344	nonylphenoxy poly (ethylene oxyethanol) n = 9
IGEPAL CO-730					224	418	279	428	379	
IGEPAL CO-710					205	397	266	401	361	
IGEPAL CO-710	100	200	I		205	397	266	401	361	
β,β-iminodipropionitrile		110	I	MeOH						
isoquinoline		50	I,P	MeCl						

Liquid Phase	T_{min}, °C	T_{max}, °C	Polarity	Solvents	McReynolds Const.					Notes
					X	Y	Z	U	S	
Lexan	220	270	P	DMP hot						polycarbonate resin
mannitol	170	200	HB	H_2O						
neopentylglycol adipate	50	240	I	MeCl	234	425	312	402	438	
neopentylglycol isophthalate	50	240	I	MeCl						
neopentylglycol sebacate	50	225	I	MeCl	172	327	225	344	326	
neopentylglycol succinate	50	225	I	MeCl	272	469	366	539	474	
Nujol		100	N	Pent	9	5	2	6	11	paraffin oil
n-octadecane	30	55	N	Pent						
Oronite NIW		170			180	370	242	370	327	complex mixture of petroleum liquids
phenyl diethanolamine succinate		225	P	Ace	386	555	472	674	654	
polyethylene imine	0	250	P	MeOH	322	800	-	573	524	
poly-m-phenylxylene	125	375	I	Tol	257	355	348	433	-	PPE-20
poly-m-phenyl ether		250	I	Tol						5 rings
poly-m-phenyl ether	0	300	I	Ace, Tol	182	233	228	313	293	6 rings
poly-m-phenyl ether	50	400	I	Tol						high polymer

Liquid Phase	T_{min}, °C	T_{max}, °C	Polarity	Solvents	McReynolds Const.					Notes
					X	Y	Z	U	S	
poly-m-phenyl ether squalane	50	100	I	MeCl						6 rings
polypropylene glycol	0	150	HB	MeOH	128	294	173	264	226	av. mol. wt. = 2000
polypropylene glycol sebacate	20	225	I	Chlor	196	345	251	381	328	
polypropylene glycol silver nitrate	20	75	S	MeCl						
polypropylene imine	0	200	I,P	Chlor	122	425	168	263	224	
propylene carbonate	0	60	P	MeCl						1,2 propanediol cyclic carbonate
polysulfone	0	315	I	Ace						
polyvinyl pyrrolidone	80	225	HB	MeOH						
Quadrol	0	150	HB	Chlor	214	571	357	472	489	N,N,N',N'-tetrakis (2-hydroxypropyl) ethylenediamine
Reoplex 400	0	200	I	MeCl	364	619	449	647	671	poly(propylene glycol adipate)
Reoplex 100	0	200	I	MeCl						poly (propylene glycol sebacate)
sebaconitrile		150	P							
squalane	20	100	N	Pent	0	0	0	0	0	
squalene	0	100	N,I	Pent	152	341	238	329	344	

Liquid Phase	T_{min}, °C	T_{max}, °C	Polarity	Solvents	McReynolds Const. X	Y	Z	U	S	Notes
sorbitol	15	150		Chlor	232	582	313			hexahydric alcohol, $C_6H_6(OH)_6$
STAP	100	255	P	Chlor	345	586	400	610	627	steroid analysis phase
Siponate-DS-10	20	210	I,P	MeOH						sodium dodecylbenzene sulfonate
sorbitan monooleate	20	150	P	Chlor	97	266	170	216	268	SPAN-80
sorbitol hexaacetate					335	553	449	652	543	
sucrose acetate isobutyrate	0	200	I,P	MeCl	172	330	251	378	295	
sucrose octaacetate	90	250	I,P	Ace	344	570	461	671	569	
Tergitol Nonionic NP-35	10	175	P	Chlor	197	380	258	389	351	Surfactant mixture
TCEPE	30	175	P,S	MeCl	526	782	677	920	837	tetracyano-ethylatedpentaerythritol
terephthalic acid	100	250	P,I	Tol						
tetraethylene glycol		70	P	MeCl						
tetraethylenepent-amine		150	HB	MeOH						
1,2,3,4-tetrakis-(2-cyanoethyl) butane	110	200	I,P	Chlor	617	860	773	048	941	
THEED	0	125	HB	Chlor	463	942	626	801	893	tetrahydroxyethylenediamine

Liquid Phase	T_{min}, °C	T_{max}, °C	Polarity	Solvents	McReynolds Const.					Notes
					X	Y	Z	U	S	
β,β'-thiodipropionitrile		100	P	MeOH						
triacetin		60	P	MeOH	glyc	ryl	riac	tate		
tributyl phosphate	20	125	I	Ace						
tricresyl phosphate	20	125	I	MeOH	176	321	250	374	299	tritolyl phosphate
triethanolamine		100	HB	MeOH						
trimer acid	20	200	HB	MeOH	94	271	163	182	378	C_{54} tricarboxylic acid
1,2,3-tris (2-cyano-ethoxy) propane	30	150	P	MeOH	594	857	759	031	917	
tris (tetrahydrofurfuryl) phosphate	20	125	I	Ace						
tris (2-cyanoethyl) nitromethane	20	140	I,P	Chlor						
Triton X-100	20	190	P	MeCl	203	399	268	402	362	octylphenoxypolyethyl ethanol
Triton X-305	20	250	P	Ace	262	467	314	488	430	octylphenoxypolyethyl ethanol
trixylol phosphate	20	250	I,P	Ace						
TWEEN 20	20	150	P	MeOH						polyethoxysorbitan monolaurate
TWEEN 80	20	160	P	MeOH	227	430	283	438	396	polyethoxysorbitan monooleate
UCON LB-550-X	0	200	P	Chlor	118	271	158	243	206	10% polyethylene glycol, 90% propylene glycol

Liquid Phase	T_{min}, °C	T_{max}, °C	Polarity	Solvents	McReynolds Const.					Notes
					X	Y	Z	U	S	
UCON 50-HB-280-X	0	200	P	Chlor	177	362	227	351	302	30% polyethylene glycol, 70% propylene glycol
UCON 50-HB-2000	0	200	P	Chlor	202	394	253	392	341	40% polyethylene glycol, 60% propylene glycol
UCON 50-HB-5100	20	200	P	MeCl	214	418	278	421	375	50% polyethylene glycol, 50% propylene glycol
UCON LB-1715	20	200	I	MeCl	132	297	180	275	235	
Versamide 900	190	250	P	MeCl						polyamide resin
Versamide 940	115	200	P	MeCl	109	314	145	212	209	polyamide resin
xylenyl phosphate		175	I	MeCl						
Zonyl E7		200	I	MeCl	223	359	468	549	465	fluoroalkyl ester
Zonyl E91		200	I	MeCl	130	250	320	377	293	fluoroalcohol camphorate
zinc stearate	135	175	I	Ace (warm)	61	231	59	98	544	
UCON 75-H-90,000	20	200	P	MeCl	255	452	299	470	406	80% polyethylene glycol, 10% propylene glycol
Versamide 930	115	150	P	MeCl	109	313	144	211	209	polyamide resin

Stationary Phases for Packed Column Gas Chromatography

The following stationary phases have been shown to be useful in separating the following classes of compounds, using coated packed columns. The resolution obtained will probably be lower than that obtainable with capillary columns. Alternative stationary phases are to be found in the previous table.

Compounds	Suggested Stationary Phase
- Alcohols	
C_1 - C_5	Hallcomid M-18 OL, Carbowax 600 - Carbowax 1540
C_1 - C_{18}*	FFAP, Carbowax 20M
Di-Poly	FFAP, QF-1, Porapak Q, Porapak QS
- Aldehydes	
C_1 - C_5	Ethofat
C_5 - C_{18}*	Carbowax 20M
- Alkaloids*	QF-1, SE-30
- Amides	Versamid 900, FFAP, Ethofat or Carbowax 600 (on Chromosorb T)
- Amino Acid Derivatives	DEGS/EGSS-X
- Amines	Dowfax 9N9/KOH, Pennwalt 213, Chromosorb 103
- Boranes	Apiezon L, Hexadecane, Octadecane, Squalane
- Essential Oils * **	FFAP, Carbowax 20M
- Esters	DNP, Porapak Q
- Ethers	Carbowax 1500 - 20M
- Glycols	Porapak-Q, QF-1
- Halogen Compounds	Carbowax 1500-20M, QF-1, FS-1265, FFAP Porapak (for freons)

* - consider a capillary column

** - consider HPLC

Stationary Phases for Packed Column Gas Chromatography (cont.)

Compounds	Suggested Stationary Phase
- Hydrocarbons	
C_1 - C_5	Carbowax 400 - Carbowax 1500, Proplyene Carbonate, Tributylophosphate, Didecylphalate
C_5 - C_{12}*	Carbowax 20M, SE-30, Squalane
Aromatics	Tetracyanoethylatedpentaerythritol, DNP, Liquid Crystalline Phases (such as Cyanobiphenyls, Cholesterics)
- Ketones	Lexan, FFAP, Carbowax 20M
- Nitriles	FFAP, XF-1150
- Organometallics**	FFAP, SE-30 (lower temperatures)
- Phosphorous Compounds	SE-30, STAP
- Silanes	SF-96, STAP
- Sulfur Compounds	Carbowax 20M, FFAP, DNP, Solid Absorbents

* - consider a capillary column

** - consider HPLC

Silicone Liquid Phases

The following table lists the chromatographic properties of some of the more popular polysiloxane based liquid phases [1-8]. The polysiloxanes are the most widely used stationary phases in gas chromatography, and are especially applicable to capillary columns. The listing provided here is far from exhaustive. Since it is impractical to present the structures of all polysiloxane-based phases, the OV phases have been chosen as representatives since their properties are among the most well characterized. The phases which are listed in the notes as "similar phases" have thermal and chromatographic properties which are similar to the phase described.

The McReynolds constants are indices with respect to the following test probe compounds:

McReynolds Constant	Test Probe
1	benzene
2	1-butanol
3	2-pentanone
4	1-nitropropane
5	pyridine
6	2-methyl-2-pentanol
7	1-iodobutane
8	2-octyne
9	1,4-dioxane
10	cis-hydrindane

The use of these constants is described in the previous table.

Solvents:

Ace - acetone

Chlor - chloroform

Tol - toluene

Note: ϕ denotes a phenyl group in a structure.

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[4] Trash, C.R., J. Chromatogr. Sci., 11, 196, 1973.

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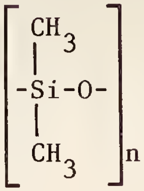
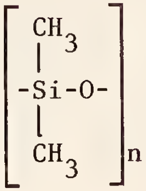
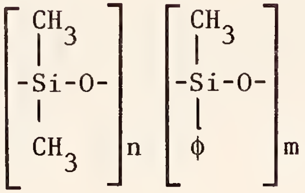
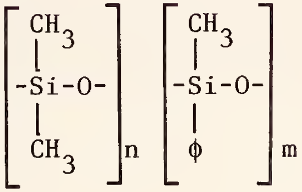
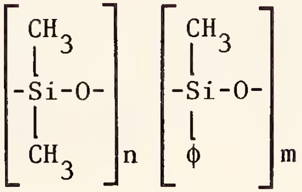
[6] Heftmann, E., Chromatography: A Laboratory Handbook of Chromatographic and Electrophoretic Methods, 3rd ed., Van Nostrand Reinhold, New York, 1975.

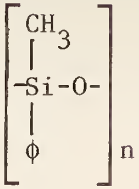
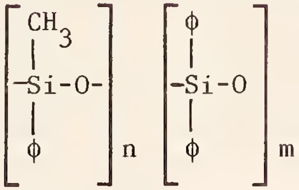
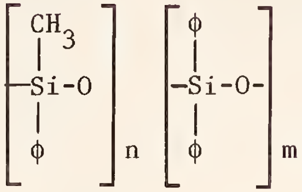
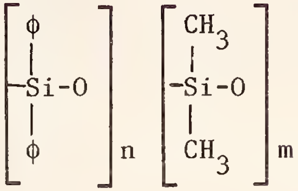
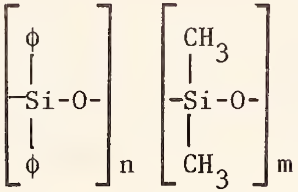
[7] Grant, D.W., Gas Liquid Chromatography, Van Nostrand Reinhold, London, 1971.

[8] Coleman, A.E., J. Chromatogr. Sci., 11, 198, 1973.

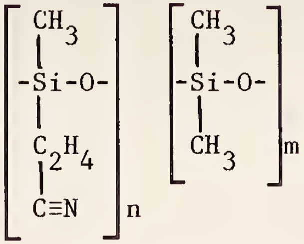
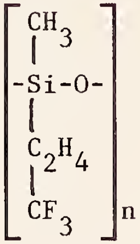
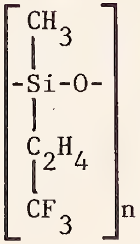
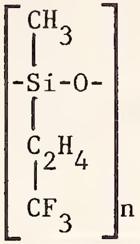
Liquid Phase	Tmin °C	Tmax °C	Polarity	Solvent	McReynolds Constants 1	2	3	4	5	6	7	8	9	10
OV-1, dimethylsilicone gum	100	350	N	Tol	16	55	44	65	42	32	4	23	45	-1
OV-101 dimethylsilicone fluid	20	350	N	Tol	17	57	45	67	43	33	4	23	46	-2
OV-3, phenylmethyl-dimethylsilicone	20	350	I	Ace	44	86	81	124	88	55	39	46	84	17
OV-7 phenylmethyl-dimethylsilicone	20	350	I	Ace	69	113	111	171	128	77	68	66	120	35
OV-11 phenylmethyl-dimethylsilicone	0	350	I	Ace	102	142	145	219	178	100	103	92	164	59

Liquid Phase	Wt. Av. Mol. Wt.	Viscosity (cSt)	Structure	Notes
OV-1 dimethylsilicone gum	> 10^6	gum	 $\left[\begin{array}{c} CH_3 \\ \mid \\ -Si-O- \\ \mid \\ CH_3 \end{array}\right]_n$	100% methyl, low selectivity, boiling point separations; similar phases: UCC-L45, UCC-W-98, SE-30
OV-101 dimethylsilicone fluid	3×10^4	1500	 $\left[\begin{array}{c} CH_3 \\ \mid \\ -Si-O- \\ \mid \\ CH_3 \end{array}\right]_n$	100% methyl; low selectivity, boiling point separations; similar phases: DC-11 DC-200, DC-550, SF-96, SP 2100, STAP
OV-3, phenylmethyl- dimethyl silicone	2×10^4	500	 $\left[\begin{array}{c} CH_3 \\ \mid \\ -Si-O- \\ \mid \\ CH_3 \end{array}\right]_n \left[\begin{array}{c} CH_3 \\ \mid \\ -Si-O- \\ \mid \\ \phi \end{array}\right]_m$	10% phenylmethyl similar to SE-52
OV-7 phenylmethyl- dimethylsilicone	1×10^4	500	 $\left[\begin{array}{c} CH_3 \\ \mid \\ -Si-O- \\ \mid \\ CH_3 \end{array}\right]_n \left[\begin{array}{c} CH_3 \\ \mid \\ -Si-O- \\ \mid \\ \phi \end{array}\right]_m$	20% phenylmethyl
OV-11 phenylmethyl- dimethylsilicone	7×10^3	500	 $\left[\begin{array}{c} CH_3 \\ \mid \\ -Si-O- \\ \mid \\ CH_3 \end{array}\right]_n \left[\begin{array}{c} CH_3 \\ \mid \\ -Si-O- \\ \mid \\ \phi \end{array}\right]_m$	35% phenylmethyl similar phases: DC-710

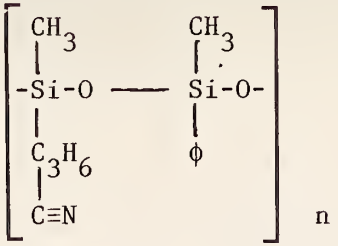
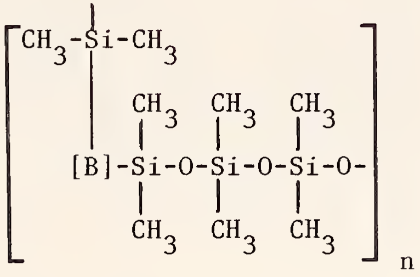
Liquid Phase	Tmin °C	Tmax °C	Polarity	Solvent	McReynolds Constants									
					1	2	3	4	5	6	7	8	9	10
OV-17 phenylmethyl silicone	20	350	I	Ace	119	158	162	243	202	112	119	105	184	69
OV-22 phenylmethyl diphenyl silicone	20	350	I	Ace	160	188	191	283	253	133	152	132	228	99
OV-25 phenylmethyl diphenyl silicone	20	350	I	Ace	178	204	208	305	280	144	169	147	215	113
OV-61 diphenyldimethyl silicone	20	350	I	Tol	101	143	142	213	174	99	-	86	-	-
OV-73 diphenyldimethyl silicone gum	20	350	I	Tol	40	86	76	114	85	57	-	39	-	-

Liquid Phase	Wt. Av. Mol. Wt.	Viscosity (cSt)	Structure	Notes
OV-17 phenylmethylsilicone	4×10^3	1300	 $\left[-\overset{CH_3}{\underset{\phi}{Si}}-O-\right]_n$	50% methyl similar phases: SP-2250
OV-22 phenylmethyl diphenyl silicone	8×10^3	> 50,000	 $\left[-\overset{CH_3}{\underset{\phi}{Si}}-O-\right]_n \left[-\overset{\phi}{\underset{\phi}{Si}}-O\right]_m$	65% phenyl
OV-25 phenylmethyl-diphenyl silicone	1×10^4	100,000	 $\left[-\overset{CH_3}{\underset{\phi}{Si}}-O\right]_n \left[-\overset{\phi}{\underset{\phi}{Si}}-O-\right]_m$	75% phenyl
OV-61 diphenyldimethyl silicone	4×10^4	> 50,000	 $\left[-\overset{\phi}{\underset{\phi}{Si}}-O\right]_n \left[-\overset{CH_3}{\underset{CH_3}{Si}}-O\right]_m$	33% phenyl
OV-73 diphenyldimethyl silicone gum	8×10^5	gum	 $\left[-\overset{\phi}{\underset{\phi}{Si}}-O-\right]_n \left[-\overset{CH_3}{\underset{CH_3}{Si}}-O-\right]_m$	5.5% phenyl similar phases: SE-52, SE-54

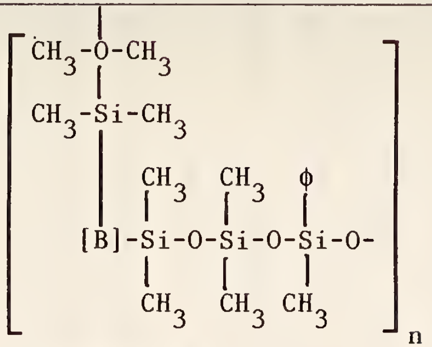
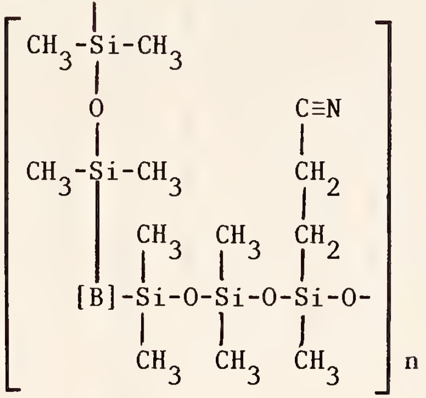
Liquid Phase	Tmin °C	Tmax °C	Polarity	Solvent	McReynolds Constants 1	2	3	4	5	6	7	8	9	10
OV-105 cyano propylmethyl-dimethyl silicone	20	250	N,I	Ace	36	108	93	139	86	74	-	29	-	-
OV-202 trifluoropropyl-methyl silicone	0	275	I,P	Chlor	146	238	358	468	310	202	139	56	283	60
OV-210 trifluoropropyl-methyl silicone	20	275	I,P	Chlor	146	238	358	468	310	206	139	56	283	60
OV-215 trifluoropropyl-methyl silicone gum			I,P		149	240	363	478	315	208	-	56	-	-

Liquid Phase	Wt. Av. Mol. Wt.	Viscosity (cSt)	Structure	Notes
OV-105 cyano propylmethyl-dimethyl silicone		1,500	 $\left[\begin{array}{c} \mathrm{CH_3} \\ \vert \\ \mathrm{-Si-O-} \\ \vert \\ \mathrm{C_2H_4} \\ \vert \\ \mathrm{C{\equiv}N} \end{array}\right]_n \left[\begin{array}{c} \mathrm{CH_3} \\ \vert \\ \mathrm{-Si-O-} \\ \vert \\ \mathrm{CH_3} \end{array}\right]_m$	
OV-202 trifluoropropyl-methyl silicone	1×10^4	500	 $\left[\begin{array}{c} \mathrm{CH_3} \\ \vert \\ \mathrm{-Si-O-} \\ \vert \\ \mathrm{C_2H_4} \\ \vert \\ \mathrm{CF_3} \end{array}\right]_n$	50% trifluoropropyl fluid; similar phases: SP-2401
OV-210 trifluoropropyl-methyl silicone	2×10^5	10,000	 $\left[\begin{array}{c} \mathrm{CH_3} \\ \vert \\ \mathrm{-Si-O-} \\ \vert \\ \mathrm{C_2H_4} \\ \vert \\ \mathrm{CF_3} \end{array}\right]_n$	50% trifluoropropyl similar phases: QF-1, FS-1265, SD-2401
OV-215 trifluoropropyl-methyl silicone gum		gum	 $\left[\begin{array}{c} \mathrm{CH_3} \\ \vert \\ \mathrm{-Si-O-} \\ \vert \\ \mathrm{C_2H_4} \\ \vert \\ \mathrm{CF_3} \end{array}\right]_n$	50% trifluoropropyl

Liquid Phase	Tmin °C	Tmax °C	Polarity	Solvent	McReynolds Constants									
					1	2	3	4	5	6	7	8	9	10
OV-225 cyanopropyl-methylphenyl methylsilicone	20	275	I,P	Ace	228	369	338	492	386	282	226	150	342	117
OV-275 dicyanoallyl silicone	20	275	P	Ace	781	1006	885	1177	1089	-	-	-	-	-
Dexsil 300	50	450	I	Chlor	47	80	103	148	96	-	-	-	-	-

Liquid Phase	Wt. Av. Mol. Wt.	Viscosity (cSt)	Structure	Notes
OV-225 cyanopropyl-methylphenyl methyl silicone	8×10^3	9,000		25% phenyl, 25% cyanopropylmethyl; similar phases: EX-60, AN-600
OV-275 dicyanoallyl silicone	5×10^3	20,000		
Dexsil 300 copolymer;	16,000-20,000	waxy solid	 [B] = $CB_{10}H_{10}C$, meta-carborane	carborane-methyl silicone siloxane to carborane ratio, 4:1

Liquid Phase	Tmin °C	Tmax °C	Polarity	Solvent	McReynolds Constants 1	2	3	4	5	6	7	8	9	10
Dexsil 400	20	375	I	Chlor	60	115	140	188	174	-	-	-	-	-
Dexsil 410	20	375	I	Chlor	85	165	170	240	180	-	-	-	-	-

Liquid Phase	Wt. Av. Mol. Wt.	Viscosity (cSt)	Structure	Notes
Dexsil 400	12,000- 16,000		 [B] = $CB_{10}H_{10}C$ meta - carborane	carborane methyl phenyl silicone copolymer; siloxane to carborane ratio, 5:1
Dexsil 410	9,000- 12,000		 [B] = $CB_{10}H_{10}C$ meta-carborane	carborane methyl- β -silicone cyanoethyl copolymer; siloxane to carborane ratio, 5:1

Adsorbents for Gas-Solid Chromatography

The following table lists the more common adsorbents used in gas-solid chromatography, along with relevant information on separation and technique [1-3]. They are used chiefly for the analysis of gaseous mixtures. The maximum temperatures listed represent the point of severe resolution loss. The materials are chemically stable to much higher temperatures. The 60-100 mesh sizes are most useful for chromatographic applications. All of these materials must be activated before being used, and the degree of activation will influence the retention behavior. Due to surface adsorption of solutes, some experimentation with temperature may be necessary to prevent tailing or to avoid statistical correlation (or a propagating error) among replicate analyses [4].

REFERENCES:

[1] Jeffery, P.G., Kipping, P.J., Gas Analysis by Gas Chromatography, Pergamon Press, Oxford, 1972.

[2] Cowper, C.J., DeRose, A.J., The Analysis of Gases by Chromatography, Pergamon Press, Oxford, 1983.

[3] Breck, D.W., Zeolite Molecular Sieves, John Wiley and Sons, New York, 1973.

[4] Bruno, T.J., J. Res. Nat. Bur. Stds. (U.S.), 90(2), 1127, 1985.

Packing Name	Maximum Temperature °C	Separation Effected	Notes
silica gel	300	H_2, Air, CO, C_1 to C_4 normal hydrocarbons, alkenes and alkynes	used often as a second column (with a molecular sieve); very hydrophilic; requires activation; can be unpredictable; largely replaced by porous polymers.
porous silica	300	Same as silica gel	higher surface area than silica gel; often used with a humidified carrier gas; can be coated with a conventional liquid; Spherosil and Porasil are examples.
alumina	300	light hydrocarbons at ambient temperature (C_1 to C_5) H_2 and light hydrocarbons at subambient temperature	often useful with controlled water-preadsorption after activation; can be coated with a conventional liquid phase.
activated carbon	300	H_2, CO, CO_2, C_1 to C_3 alkanes, alkenes and alkynes	requires oxygen-free carrier gas; largely replaced by porous polymers.
graphite	300	light hydrocarbons, H_2S, SO_2, CH_3SH, sour gas	often modified with small quantities (1.5-5%) of conventional liquid phases; requires oxygen-free carrier.
carbon molecular sieve	300	H_2 (O_2, N_2 co-elute), CO, CH_4, H_2O, CO_2, C_1 to C_3 alkanes, alkenes, alkynes	high affinity for hydrocarbons; requires oxygen-free carrier.
molecular sieve, 5A	225	air and light gas analysis; H_2, O_2, N_2, (CH_4, CO, NO, SF_6 co-elute)	synthetic calcium alumino-silicate (zeolite) having an effective pore diameter of 5A; CO_2 is adsorbed strongly; 5A usually gives the best results of all synthetic zeolites; should be activated before use, and used above critical adsorption temperature; 21.6% (wt/wt) water capacity.

Packing Name	Maximum Temperature °C	Separation Effected	Notes
molecular sieve, 13X	200	same as 5A, but with C_1 to C_4 alkanes, alkenes, and alkynes being separated as well	sodium alumino-silicate (zeolite), having a larger pore size than 5A, thus producing lower retention times and less resolution; 28.6% (wt/wt) water capacity.
molecular sieve, 3A	200	light permanent gases	potassium alumino-silicate (zeolite); 20% (wt/wt) water capacity, smaller pore size than 5A, thus different retention characteristics.
molecular sieve, 4A	200	light permanent gases	sodium alumino-silicate (zeolite); 22% (wt/wt) water capacity; retention characteristics differ from 5A due to smaller pore size.

Porous Polymer Phases

Porous polymer phases, first reported by Hollis [1], are of great value for a wide variety of separations. They are usually white in color, but may darken during use at higher temperatures. This darkening does not effect their performance. High temperature conditioning is required to drive off solvent and residual monomer. The polymers may either swell or shrink with heating; thus flow rate changes must be anticipated. The retention indices (c) reported here are from the work of Dave [2]:

Index	Test Probe
W	Benzene
X	t-butanol
Y	2-butanone
Z	acetonitrile

The physical property data were taken from the work of Poole and Schuette [3].

References:

[1] Hollis, O.L., Anal. Chem., 38, 309, 1966.

[2] Dave, S., J. Chromatogr. Sci., 7, 389, 1969.

[3] Poole, C.F., Schuette, S.A., Contemporary Practice of Chromatography, Elsevier, Amsterdam, 1984.

Packing Name	Maximum Temperature °C	Material Type	Free Fall Density g/cm^3	Surface Area m^2/g	Pore Diameter Av., μm
Chromosorb 101	275	styrene-divinylbenzene copolymer	0.30	<50	0.3-0.4
Chromosorb 102	250	styrene-divinylbenzene copolymer	0.29	300-500	0.0085
Chromosorb 103	275	polystyrene, cross-linked	0.32	15-25	0.3-0.4
Chromosorb 104	250	acrylonitrile divinylbenzene copolymer	0.32	100-200	0.06-0.08
Chromosorb 105	250	acrylic ester (polyaromatic)	0.34	600-700	0.04-0.06

Packing Name	Retention Indices W	 X	 Y	 Z	Separation effected	Notes
Chromosorb 101	745	565	645	580	free fatty acids, glycols, alcohols alkanes, esters, aldehydes, ketones, ethers	hydrophobic, condition at 250°C; not recommended for amines or anilines, lower retention times than obtained with Chromosorb 102
Chromosorb 102	650	525	570	460	subambient temperature: H_2, O_2, N_2, Ar, NO, CO; Ambient temperature: H_2, (Air + Ar + NO + CO), CH_4, CO_2, H_2O, N_2O, C_2H_6; Above ambient temperature: C_1-C_4 hydrocarbons, H_2S, COS, SO_2, esters, ethers, alcohols, ketones, aldehydes, glycols	may entrain some species; hydrophobic; condition at 225°C; not recommended for amines or nitriles; little tailing of water or oxygenated hydrocarbons
Chromosorb 103	720	575	640	565	ammonia, light amines, light amides, alcohols, aldehydes, hydrazines	hydrophobic; high affinity for basic species; not recommended for acidic species, glycols, nitriles, nitro alkanes
Chromosorb 104	845	735	860	885	sulfur gases, ammonia, nitrogen oxides, nitriles, nitroalkanes, xylenols, water in benzene	hydrophobic; condition at 225°C; not recommended for glycols and amines; moderately polar
Chromosorb 105	635	545	580	480	permanent and light hydrocarbon gases; aqueous solutions of light organics such as formalin	hydrophobic; less polar than Chromosorb 104; condition at 225°C; not recommended for acidic species, glycols, amines and amides

Packing Name	Maximum Temperature °C	Material Type	Free Fall Density g/cm^3	Surface Area m^2/g	Pore Diameter Av., μm
Chromosorb 106	250	polystyrene, cross-linked	0.28	700-800	0.05
Chromosorb 107	250	acrylic ester, cross-linked	0.30	400-500	0.8
Chromosorb 108	250	acrylic ester, cross-linked	0.30	100-200	0.25
Porapak-Q	250	ethylvinylbenzene-divinyl benzene copolymer	0.35	500-700	0.0075
Porapak-P	250	styrene-divinyl benzene copolymer	0.28	100-200	
Porapak-N	200	vinylpyrolidone	0.39	225-350	
Porapak-R	250	vinylpyrolidone	0.33	300-450	0.0076

Packing Name	Retention Indices W	 X	 Y	 Z	Separation effected	Notes
Chromosorb 106	605	505	540	405	fatty acids from fatty alcohols, up to C_5; benzene from nonpolar organic compounds	hydrophobic, not recommended for glycols and amines
Chromosorb 107	660	620	650	550	aqueous solutions of formaldehyde; alkynes from alkanes	hydrophobic; moderately polar; not recommended for glycols and amines
Chromosorb 108	710	645	675	605	polar materials such as water, alcohols, aldehydes, glycols	hydrophobic; condition at 250°C
Porapak-Q	630	538	580	450	similar to Chromosorb 102	similar to Chromosorb 102; condition at 250°C
Porapak-P	765	560	650	590	similar to Porapak-Q	hydrophobic; low polarity; larger pore size than Porapak-Q, thus lower retention times are observed; not recommended for amines or anilines; condition at 250°C
Porapak-N	735	605	705	595	similar to Chromosorb 105; high water retention; CO_2, NH_3, H_2O, C_2H_2, from light hydrocarbons	condition at 175°; not recommended for glycols, amines, or acidic species
Porapak-R	645	545	580	455	ethers, esters, H_2O from chlorine gases (HCl, Cl_2) nitriles and nitroalkanes	moderately polar; condition at 250°C; not recommended for glycols and amines

Packing Name	Maximum Temperature °C	Material Type	Free Fall Density g/cm^3	Surface Area m^2/g	Pore Diameter Av., μm
Porapak-S	250	vinyl pyridine	0.35	300-450	0.0076
Porapak-T	200	ethylene glycol-dimethacrylate	0.44	250-300	0.009
Porapak-QS	250	ethylvinylbenzene-divinylbenzene copolymer	-	-	-
Porapak-PS	250	styrene-divinylbenzene copolymer	-	-	-
Tenax	375	p-2,6 diphenylphenylene oxide polymer	0.37	18.6	-

Packing Name	Retention Indices W	 X	 Y	 Z	Separation effected	Notes
Porapak-S	645	550	575	465	normal and branched alcohols, aldehydes, ketones, halocarbons	high polarity; not recommended for acidic species and amines, condition at 250°C
Porapak-T	-	675	700	635	water in formalin (and other aqueous organic mixtures), retention characteristics similar to Chromosorb 107	condition at 180°C; highest polarity of Porapak series; not recommended for glycols and amines
Porapak-QS	625	525	565	445	similar to Porapak-Q	silanized Porapak-Q, reduces tailing of high polarity compounds; condition at 250°C
Porapak-PS	-	-	-	-	similar to Porapak-P	silanized Porapak-P, condition at 250°C
Tenax	-	-	-	-	similar to Porapak-Q	highest thermal stability of all porous polymers

Cryogens for Subambient Temperature Gas Chromatography

The following table lists properties of common cryogenic fluids used to produce subambient temperatures for gas chromatographic columns [1-4]. These properties are of value in designing low temperature chromatographic experiments efficiently and safely. Due to the potential dangers in handling extremely low temperatures and high pressures, appropriate precautions must be observed.

REFERENCES:

[1] Zabetakis, M. G., Safety with Cryogenic Fluids, Plenum Press, New York, 1967.

[2] Cook, G. A., ed., Argon, Helium and the Rare Gases, John Wiley & Sons (Interscience) New York, 1961.

[3] Brettell, T. A., Grob, R. L., Am. Laboratory, 17 (10), 19, 1985.

[4] Cowper, C. J., DeRose, A. J., The Analysis of Gases by Chromatography, Pergamon Press Oxford, 1983.

Cryogen Name	Boiling Point, °C	Vapor Pressure (MPa)	Thermal Conductivity w/m•K	Viscosity Pa•s x10^{-5}	Heat Capacity,Cp J/kg•K	Heat Capacity,Cv J/kg•K	Critical Temperature °C	Liquid/Gas expansion ratio
Carbon Dioxide CO_2	-78.5	5.72 (21 °C)	0.0147 (0°C)	1.48 (21 °C)	831.78 (15.6°C)	638.06 (15.6°C)	31.1	790 from solid
Methane[1] CH_4	-161.61	*		1.20 (21 °C)	2205.39 (15.6°C)	1686.99 (15.6°C)	-82.1	650
Oxygen O_2	-183.0	*	0.0246 (0°C)	2.06 (20°C)	910.86 (15°C)	650.19	-118.4	875
Argon Ar	-185.7	*	0.0161 (0°C)	2.21 (21 °C)	523.84 (21 °C)	313.80 (15.6°C)	-122.46	860
Nitrogen N_2	-195.81	*	0.0253 (21 °C)	1.744 (15°C)	103.64 (21 °C)	738.48 (21 °C)	-147.15	710
Helium He	-268.92	*	0.1418 (0°C)	1.96 (21 °C)	5221.63 (21 °C)	3146.37 (15.6°C)	-267.9	780

[1] Flamability limits:
Air: 5-15 percent vol/vol
Oxygen: 5-61 percent vol/vol

*Fluid is supercritical at ambient temperature

Some Useful Fluids for Supercritical Fluid Chromatography

The following table lists some useful carrier fluids for supercritical fluid chromatography, along with relevant critical properties [1]. These fluids have either been used or proposed for use in supercritical fluid chromatography or supercritical extraction.

Fluid	T_c(°C)	ρ_c (g/mL)	P_c (MPa)
Carbon Dioxide	31.3	0.460	7.4
Ammonia	132.3	0.235	11.3
Nitrous Oxide	36.5	0.450	7.2
Sulfur Dioxide	157.5	0.520	7.9
Water	374.4	0.40	23.0
Methanol	240.5	0.272	8.0
Isopropanol	235.3	0.273	4.8
n-Pentane	196.6	0.232	3.4
n-Hexane	234.2	0.234	3.0
Dichlorofluoromethane	178.5	0.522	5.2
Trichlorofluoromethane	196.6	0.554	4.2
Chlorotrifluoromethane	28.8	0.578	4.0
dichlorotetrafluoroethane	146.1	0.582	3.6
dichlorodifluoromethane	111.7	0.558	4.0
Benzene	288.9	0.304	4.9
Xenon	16.6	1.155	5.9
Toluene	320.8	0.29	4.2

[1] Bruno, T.J., Proc. 2nd Symp. Energy Engineering Sciences, 81, 1984.

II. Tables for Liquid Chromatography

Solvents for Liquid Chromatography

The following table provides the important physical properties for the selection of solvent systems for high performance liquid chromatography (HPLC) [1-5]. These properties are required for proper detector selection, and the prediction of expected column pressure gradients. The values of dielectric constant aid in estimating the relative solubilities of solutes and other solvents.

REFERENCES:

[1] Willard, H.H., Merritt, L.L., Dean, J.A., Settle, F.A., Instrumental Methods of Analysis, 6th ed., Wadsworth Publishing Co., Belmont, 1981.

[2] Snyder, L.R., Kirkland, J.J., Introduction to Modern Liquid Chromatography, 2nd ed., John Wiley and Sons (Interscience), New York, 1979.

[3] Dreisbach, R.R., Physical Properties of Chemical Compounds, Number 22 of the Advances in Chemistry Series, American Chemical Society, Washington D.C., 1959.

[4] Krstulovic, A.M., Brown, P.R., Reverse Phase High Performance Liquid Chromatography, John Wiley and Sons (Interscience), New York, 1982.

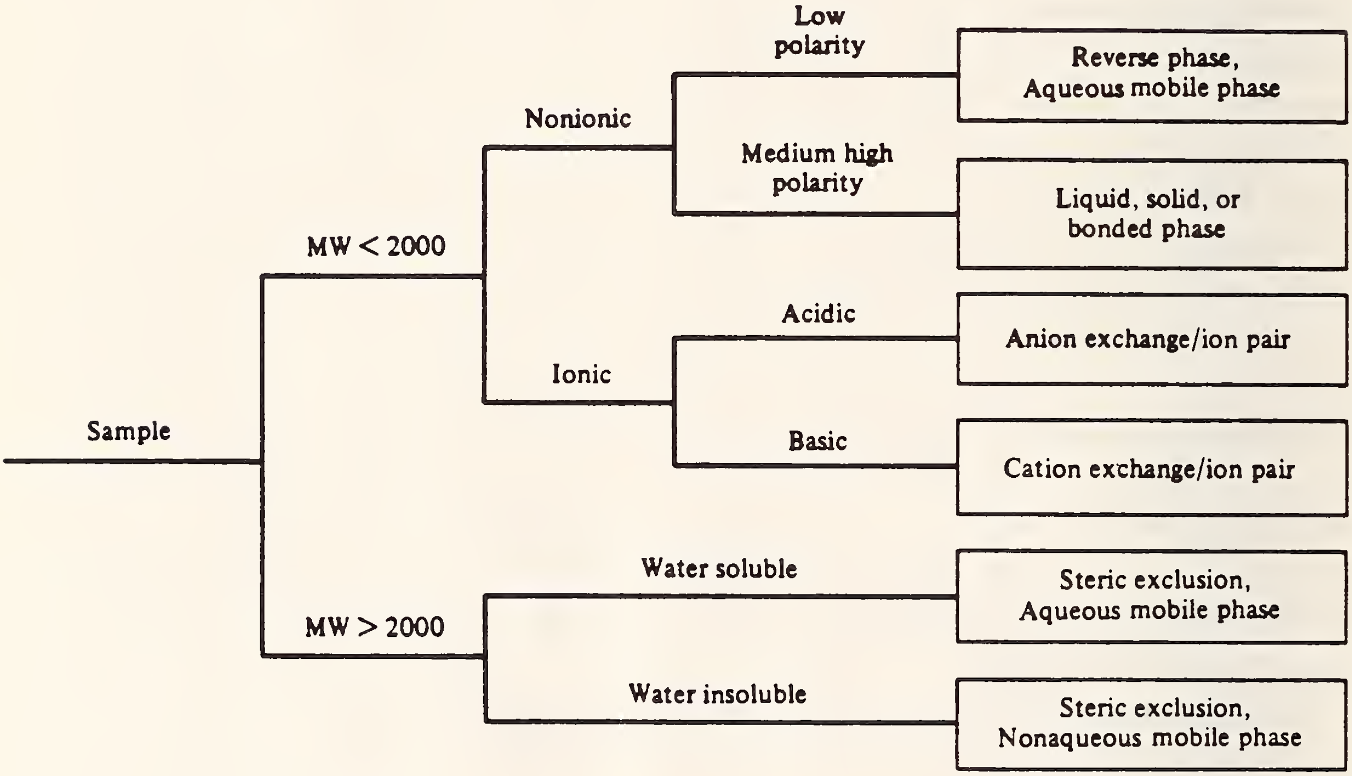
[5] Weast R.C., Handbook of Chemistry and Physics, 63rd ed., CRC Press, Boca Raton, 1983.

Solvent	Viscosity mN•sec/m² (20°C)	UV Cutoff nm	Refractive Index 20°C	Boiling Point °C	Dielectric Constant (20°C)
acetic acid	1.31(15)		1.372	117.9	6.2
acetone	0.30(25)	330	1.359	56.3	20.7 (25)
acetonitrile	0.34(25)	190	1.344	81.6	37.5
benzene	0.65	278	1.501	80.1	2.284
1-butanol	2.95	215	1.399	117.7	17.8
2-butanol	4.21	260	1.397	99.6	15.8 (25)
n-butyl acetate	0.73	254	1.394	126.1	
butylchloride	0.47(15)	220	1.402	78.4	
carbon tetrachloride	0.97	263	1.460	76.8	2.238
chlorobenzene	0.80	287	1.525	131.7	2.708
chloroform	0.58	245	1.446	61.2	4.806
cyclohexane	0.98	200	1.426	80.7	2.023
cyclopentane	0.44	200	1.406	49.3	1.965
o-dichlorobenzene	1.32(25)	295	1.551	180.5	9.93 (25)
n,n-dimethylacetamide	2.14	268	1.438	166.1	37.8
dimethylformamide	0.92	268	1.430	153.0	36.7
dimethyl sulfoxide	2.20	286	1.478	189.0	4.7
dioxane	1.44(15)	215	1.422	101.3	2.209 (25)
2-ethoxyethanol	2.05	210	1.408	135.6	
ethyl acetate	0.46	256	1.372	77.1	6.02 (25)
ethyl ether	0.24	218	1.352	34.6	4.335
glyme (ethylene glycol dimethyl ether)	0.46(25)	220	1.380	93.0	
heptane	0.42	200	1.388	98.4	1.92
hexadecane	3.34	200	1.434	287.0	
hexane	0.31	200	1.375	68.7	1.890
isobutyl alcohol	4.70(15)	220	1.396	107.7	15.8 (25)
methanol	0.55	205	1.328	64.7	32.63 (25)
2-methoxyethanol	1.72	210	1.402	124.6	16.9
2-methoxyethyl acetate		254	1.402	144.5	

Solvent	Viscosity $mN \cdot sec/m^2$ (20°C)	UV Cutoff nm	Refractive Index 20°C	Boiling Point °C	Dielectric Constant (20°C)
methylene chloride	0.45(15)	233	1.424	39.8	9.08
methylethylketone	0.42(15)	329	1.379	79.6	18.5
methylisocimylketone		330	1.406	-144.0	
methylisobutylketone	0.54(25)	334	1.396	116.5	
N-methyl-2-pyrrolidone	1.67(25)	285	1.488	202.0	32.0
nonane	0.72	200	1.405	150.8	1.972
pentane	0.24	200	1.357	36.1	1.84
petroleum ether	0.30	226		30-60	
β-phenethylamine		285	1.529(25)	197-198	
1-propanol	2.26	210	1.386	97.2	20.1 (25)
2-propanol	2.86(15)	205	1.377	82.3	18.3 (25)
propylene carbonate			1.419	240.0	
pyridine	0.95	330	1.510	115.3	12.3 (25)
tetrachloroethylene	0.93(15)	295	1.506	121.2	
tetrahydrofuran	0.55	212	1.407	66.0	7.6
tetramethyl urea		265	1.449(25)	175.2	23.0
toluene	0.59	284	1.497	110.6	2.379 (25)
trichloroethylene	0.57	273	1.477	87.2	3.4 (16)
1,2,2-trichloro-1,2,2-trifluoroethane	0.71	231	1.356(25)	47.6	
2,2,4-trimethylpentane	0.50	215	1.391	99.2	
water	1.00	<190	1.333	100.0	80.0
o-xylene	0.81	288	1.505	144.4	2.568
p-xylene		290	1.5004	138.5	2.270

Modes of Liquid Chromatography

The following flow chart provides a rough guide among the various liquid chromatographic techniques, based on sample properties [1].



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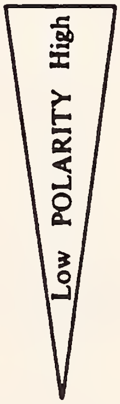
[1] Courtesy of Millipore Corporation, Waters Chromatography Division.

Reverse Phase Materials and Solvents

The following chart provides a rough guide to basic solvent systems for bonded reverse phase packings [1]. These packings are the most widely used in high performance liquid chromatography.

Sample	Column packing	Mobile phase
Low/moderate polarity (soluble in aliphatic hydrocarbons)	Bonded C-18	Methanol/water
Moderate polarity (soluble in methyl ethyl ketone)	Bonded C-8	Acetonitrile/water
High polarity (soluble in lower alcohols)	Bonded C-2	1,4-Dioxane/water



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[1] Reprinted with permission from: Willard, H.H., Merritt, L.L., Dean, J.A., Settle, F.A., *Instrumental Methods of Analysis*, 6th ed., Wadsworth Publishing Co., Belmont, 1981.

HPLC Column Packings

The following table provides a summary of the general characteristics of the more popular stationary phases used in modern high performance liquid chromatography [1-3]. The most commonly used phases are the bonded reverse phase materials, in which separation control is a function of the mobile (liquid) phase. The selection of a particular phase and solvent system is an empirical procedure involving survey analyses. The references provided below will assist the reader in this procedure.

REFERENCES:

[1] Snyder, L.R., Kirkland, J.J., Introduction to Modern Liquid Chromatography, 2nd ed., John Wiley and Sons, New York, 1979.

[2] Poole, C.F., Schuette, S.A., Contemporary Practice of Chromatography, Elsevier, Amsterdam, 1984.

[3] Krstulovic, A.M., Brown, P.R., Reverse-Phase High Performance Liquid Chromatography, John Wiley and Sons (Interscience), New York, 1982.

Phase Type	Bond Type	Functional Group	Separation Mode	Notes and Applications
Silica (pure)	SiO_2	--	Adsorption	Usually used with nonpolar mobile phase; selectivity is based on differences in number and location of polar groups; results can be unpredictable due to changes in the surface due to adsorption; water or acetic acid is often added (in low concentrations) to the mobile phase to better control surface characteristics.
Alumina (pure)	Al_2O_3	--	Adsorption - normal phase	Similar in characteristics and application to silica.
Bonded amine	Si-O-Si-C or Si-C	$-NH_2$	Polar bonded phase	Selectivity is modified with respect to silica, although highly polar; useful for sugar and carbohydrate separations; not recommended for samples which contain aldehydes and ketones.
Bonded nitrile	Si-C	-CN	Polar bonded phase	Highly polar phase, but with selectivity modified with respect to Silica; less sensitive to mobile phase impurities than Silica.
Bonded diol	Si-O-Si-C	-OH	Polar bonded phase	Useful in size-exclusion chromatography.
Bonded nitro	Si-C	$-NO_2$	Polar bonded phase	
ODS	Si-C	Octadecyl, $n-C_{18}$ hydrocarbon chain	Bonded, reverse phase	Octadecylsilane Most common material used in HPLC; high resolution possible; pH must be maintained between 2 and 7. between 2 and 7.

Phase Type	Bond Type	Functional Group	Separation Mode	Notes and Applications
OS	Si-C	Octyl, n-C_8 hydrocarbon chain	Bonded, reverse phase	Octylsilane Lower resolution than the octadecyl bonded phase; useful when separations involve species of greatly different polarity.
TMS	Si-C	Methyl, CH_3	Bonded, reverse phase	Tetramethylsilane Lowest resolution of reverse-phase packings; useful for "survey" separations and for large molecules.
Phenyl	Si-C	$-\Phi$	Normal or reverse phase	Lower efficiency than other bonded phases; more polar than ODS, OS and TMS phases; used with both normal and reverse phase solvent systems.
Ion exchange	Varies, usually Si-O-Si	Sulfonic Acid	Cation exchange	Separates cations, with divalent ions more strongly retained than monovalent ions; phosphate buffer systems are often used, sometimes with low concentrations of polar non-aqueous modifiers added.
Ion exchange	Varies	Quarternary ammonium	Anion exchange	Separates anions; separation and retention of organic ions is due to both ionic and reverse phase effects.
Ion exchange	Varies	$-N(CH_3)_2$	Anion exchange	Similar to the quarternary ammonium phase, with different retention and selectivity.

Note: Φ denotes a phenyl group

III. Tables for Ultraviolet Spectrophotometry

Solvents for Ultraviolet Spectrophotometry

The following table lists some useful solvents for ultraviolet spectrophotometry, along with their wavelength cutoffs and dielectric constants [1-4].

REFERENCES:

[1] Willard, H.H., Merritt, L.L., Dean, J.A., Settle, F.A., Instrumental Methods of Analysis, 6th ed., Wadsworth Publishing Co., Belmont, 1981.

[2] Weast, R.C., ed., Handbook of Chemistry and Physics, 63rd ed., CRC Press, Boca Raton, 1983.

[3] Dreisbach, R.R., Physical Properties of Chemical Compounds, Advances in Chemistry Series, No. 15, American Chemical Society, Washington, D.C., 1955.

[4] Dreisbach, R.R., Physical Properties of Chemical Compounds, Advances in Chemistry Series, No. 22, American Chemical Society, Washington, D.C., 1959.

Solvent	Wavelength Cutoff nm	Dielectric Constant (20°C)	
acetic acid	260	6.15	
acetone	330	20.7	(25°C)
acetonitrile	190		
benzene	280	2.284	
2-butanol	260	15.8	(25°C)
n-butyl acetate	254		
carbon disulfide	380	2.641	
carbon tetrachloride	265	2.238	
1-chlorobutane	220	7.39	(25°C)
chloroform [1]	245	4.806	
cyclohexane	210	2.023	
1,2-dichloroethane	226	10.19	(25°C)

1 - Stabilized with ethanol to avoid phosgene formation

Solvent	Wavelength Cutoff nm	Dielectric Constant (20°C)	
1,2-dimethoxyethane	240		
N,N-dimethylacetamide	268	59	(83°C)
N,N-dimethylformamide	270		
dimethylsulfoxide	265		
1,4-dioxane	215	2.209	(25°C)
diethyl ether	218	4.335	
ethanol	210	24.30	(25°C)
2-ethoxyethanol	210		
ethyl acetate	255	6.02	(25°C)
ethylene chloride	228		
glycerol	207	42.5	(25°C)
n-hexadecane	200	2.06	(25°C)
n-hexane	210	1.890	
methanol	210	32.63	(25°C)
2-methoxyethanol	210		
methyl cyclohexane	210	2.02	(25°C)
methyl ethyl ketone	330	18.5	
methyl isobutyl ketone	335		
2-methyl-1-propanol	230	1	
n-methylpyrrolidone	285		
pentane	210	1.844	
pentyl acetate	212		
1-propanol	210	20.1	(25°C)
2-propanol	210	18.3	(25°C)
pyridine	330	12.3	(25°C)

Solvent	Wavelength Cutoff nm	Dielectric Constant (20°C)
tetrachloroethylene [2]	290	
tetrahydrofuran	220	
toluene	286	2.379 (25°C)
1,1,2-trichloro-1,2,2-trifluoroethane	231	
2,2,4-trimethylpentane	215	1.936 (25°C)
o-xylene	290	2.568
p-xylene	290	2.270
m-xylene	290	2.374
water		78.54 (25°C)

2 - Stabilized with thymol (isopropyl meta-cresol)

Transmittance - Absorbance Conversion

The following is a conversion table for absorbance and transmittance. Included for each pair is the percent error propagated into a measured concentration (using the Beer-Lambert Law), assuming an uncertainty in transmittance of ± 0.005 [1]. The value of transmittance which will give the lowest percent error in concentration is 0.368. Where possible, analyses should be designed for the low error area.

REFERENCE:

[1] Kennedy, J. H., Analytical Chemistry Principles, Harcourt, Brace and Jovanovich, San Diego, 1984.

Transmittance	Absorbance	Percent Error
0.990	0.004	50.227
0.980	0.009	25.242
0.970	0.013	16.915
0.960	0.018	12.752
0.950	0.022	10.256
0.940	0.027	8.592
0.930	0.032	7.405
0.920	0.036	6.515
0.910	0.041	5.823
0.900	0.046	5.270
0.890	0.051	4.818
0.880	0.056	4.442
0.870	0.060	4.125
0.860	0.065	3.853
0.850	0.071	3.618
0.840	0.076	3.412
0.830	0.081	3.231

Transmittance	Absorbance	Percent Error
0.820	0.086	3.071
0.810	0.091	2.928
0.800	0.097	2.799
0.790	0.102	2.684
0.780	0.108	2.579
0.770	0.113	2.483
0.760	0.119	2.396
0.750	0.125	2.316
0.740	0.131	2.243
0.730	0.137	2.175
0.720	0.143	2.113
0.710	0.149	2.055
0.700	0.155	2.002
0.690	0.161	1.952
0.680	0.167	1.906
0.670	0.174	1.863
0.660	0.180	1.822
0.650	0.187	1.785
0.640	0.194	1.750
0.630	0.201	1.717
0.620	0.208	1.686
0.610	0.215	1.657
0.600	0.222	1.631
0.590	0.229	1.605
0.580	0.237	1.582
0.570	0.244	1.560
0.560	0.252	1.539
0.550	0.260	1.520
0.540	0.268	1.502
0.530	0.276	1.485
0.520	0.284	1.470
0.510	0.292	1.455
0.500	0.301	1.442
0.490	0.310	1.430

Transmittance	Absorbance	Percent Error
0.480	0.319	1.419
0.470	0.328	1.408
0.460	0.337	1.399
0.450	0.347	1.391
0.440	0.356	1.383
0.430	0.366	1.377
0.420	0.377	1.372
0.410	0.387	1.367
0.400	0.398	1.364
0.390	0.409	1.361
0.380	0.420	1.359
0.370	0.432	1.358
0.360	0.444	1.359
0.350	0.456	1.360
0.340	0.468	1.362
0.330	0.481	1.366
0.320	0.495	1.371
0.310	0.509	1.376
0.300	0.523	1.384
0.290	0.538	1.392
0.280	0.553	1.402
0.270	0.569	1.414
0.260	0.585	1.427
0.250	0.602	1.442
0.240	0.620	1.459
0.230	0.638	1.478
0.220	0.657	1.500
0.210	0.678	1.525
0.200	0.699	1.553
0.190	0.721	1.584
0.180	0.745	1.619
0.170	0.769	1.659
0.160	0.796	1.704
0.150	0.824	1.756

Transmittance	Absorbance	Percent Error
0.140	0.854	1.816
0.130	0.886	1.884
0.120	0.921	1.964
0.110	0.958	2.058
0.100	1.000	2.170
0.090	1.046	2.306
0.080	1.097	2.473
0.070	1.155	2.685
0.060	1.222	2.961
0.050	1.301	3.336
0.040	1.398	3.881
0.030	1.523	4.751
0.020	1.699	6.387
0.010	2.000	10.852

Correlation Table for Ultraviolet Active Functionalities

Chromophore	System	λ_{Max}	ε_{Max}	λ_{Max}	ε_{Max}	λ_{Max}	ε_{Max}
Ether	-O-	185	1000				
Thioether	-S-	194	4600	215	1600		
Amine	$-NH_2-$	195	2800				
Thiol	-SH	195	1400				
Disulfide	-S-S-	194	5500	255	400		
Bromide	-Br	208	300				
Iodide	-I	260	400				
Nitrile	-C≡N	160					
Acetylide	-C≡C-	175-180	6000				
Sulfone	$-SO_2-$	180					
Oxime	-NOH	190	5000				
Azido	>C=N-	190	5000				
Ethylene	-C=C-	190	8000				
Ketone	>C=O	195	1000	270-285	18-30		
Thioketone	>C=S	205	strong				
Esters	-COOR	205	50				
Aldehyde	-CHO	210	strong	280-300	11-18		
Carboxyl	-COOH	200-210	50-70				

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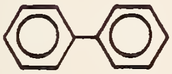
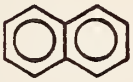
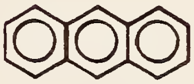
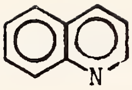
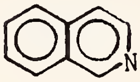
Chromophore	System	λMax	εMax	λMax	εMax	λMax	εMax
Sulfoxide	$>S\rightarrow O$	210	1500				
Nitro	$-NO_2$	210	strong				
Nitrite	$-ONO$	220-230	1000-2000	300-4000	10		
Azo	$-N=N-$	285-400	3-25				
Nitroso	$-N=O$	302	100				
Nitrate	$-ONO_2$	270 (shoulder)	12				
Conjugated Systems	$-(C=C)_2-$ (acyclic)	210-230	21,000				
	$-(C=C)_3-$	260	35,000				
	$-(C=C)_4-$	300	52,000				
	$-(C=C)_5-$	330	118,000				
	$-(C=C)_2-$ (alicyclic)	230-260	3000-8000				
	$C=C-C\equiv C$	219	6500				
	$C=C-C=N$	220	23,000				
	$C=C-C=O$	210-250	10,000-20,000			300-350	weak
	$C=C-NO_2$	229	9500				
Benzene	Φ	184	46,700	202	6900	255	170
Diphenyl				246	20,000		
Naphthalene		220	112,000	275	5600	312	175
Anthracene		252	199,000	375	7900		
Pyridine		174	80,000	195	6000	251	1700

Quinoline		227	37,000	270	3600	314	2750
Isoquinoline		218	80,000	266	4000	317	3500

Note: Φ denotes a phenyl group.

IV. Tables for Infrared Spectrophotometry

Infrared Optics Materials

The following table lists the more common materials used for optical components (windows, prisms, etc.) in the infrared region of the electromagnetic spectrum. The properties listed are needed to choose the materials with optimal transmission characteristics [1,2]. The thermal properties are useful when designing experiments for operation at elevated temperatures [3,5]. This listing is far from being exhaustive, but these are the most popular materials used in instrumentation laboratories.

REFERENCES:

[1] Gordon, A. J., The Chemist's Companion, John Wiley and Sons, New York, 1972.

[2] Willard, H. H., Merritt, L. L., Dean, J. A., Settle, F. A., Instrumental Methods of Analysis 6th ed., Van Nostrand, New York, 1985.

[3] Touloukien, Y. S., Powell, R. W., Ho, C. Y., Klemens, P. G., Thermophysical Properties of Matter: Thermal Conductivity of Nonmetallic Solids Vol. 2, IF - Plenum Data Corp., New York, 1970.

[4] Touloukien, Y. S., Kirby, R. K. Taylor, R. E., Lee, T., Thermophysical Properties of matter: Thermal Expansion of Nonmetallic Solids, Vol. 13, IF - Plenum Data Corp. New York, 1977.

[5] Weast, R.C., ed. Handbook of Chemistry and Physics, 63rd. ed., CRC Press, Boca Raton, 1983.

Material	Wavelength range, µm	Wave number range, cm^{-1}	Refractive Index at 2µm)	Thermal Conductivity $W/m{\cdot}K(X10^2)$	Thermal Expansion $\Delta L/L$., percent	Notes
sodium chloride $NaCl$	0.25-16	40,000-625	1.52	7.61 (273K) 6.61 (300K) 4.85 (400K)	0.448 (400K) 0.896 (500K)	Most common material, absorbs water; for aqueous solutions, use saturated NaCl solution as the solvent
potassium bromide KBr	0.25-25	40,000-4000	1.53	5.00 (275K) 4.87 (301.5K) 4.80 (372.2K)	0.028 (400K) 0.429 (500K) 0.846 (600K)	Useful for the study of to be C-Br stretch region, useful for solid sample pellets.
silver chloride $AgCl$	0.4-23	25,000-435	2.0	1.19 (269.8K) 1.10 (313.0K) 1.05 (372.5K)	0.356 (400K) 0.729 (500K) 1.183 (600K)	Not good for amines or liquids with basic nitrogen, light sensitive
silver bromide $AgBr$	0.50-35	20,000-286	2.2	0.90 (308.2K) 0.79 (353.2K) 0.71 (413.2K)	0.024 (300K) 0.109 (325K) 0.196 (350K)	Not good for amines or liquids with basic nitrogen, light sensitive
calcium fluoride CaF_2	0.15-9	6670-1110	1.40	10.40 (237K) 9.60 (309K) 4.14 (402K)	0.214 (400K) 0.431 (500K) 0.670 (500K)	Useful for obtaining high resolution for. OH, NH and CH stretching frequencies

Material	Wavelength range, μm	Wave number range, cm^{-1}	Refractive Index at 2μm)	Thermal Conductivity W/m•K(X10^2)	Thermal Expansion $\Delta L/L$., percent	Notes
barium fluoride BaF_2	0.20-11.5	50,000-870	1.46	11.7 (284K) 10.9 (305K) 10.5 (370K)	0.233 (400K) 0.461 (500K) 0.698 (600K)	Shock sensitive, should be handled with care
cesium bromide CsBr	1-37	10,000-270	1.67	9.24 (269.4K) 8.00 (337.5K) 7.76 (367.5K)	0.526 (400K) 1.063 (500K) 1.645 (600K)	Useful for C-Br stretching frequencies
cesium iodide CsI	1-50	10,000-200	1.74	1.15 (277.7K) 1.05 (296.0K) 9.50 (360.7K)		Useful for C-Br stretching frequencies
thalium bromide thalium iodide Tl Br-TlI (KRS-5)	0.5-35	20,000-286	2.37		0.464 (373K) 1.026 (473K)	Highly toxic, handle with care; 42% TlBr, 58% TlI
zinc selenide ZnSe	1-18	10,000-550	2.4		0.086 (400K) 0.175 (500K) 0.272 (600K)	Vacuum deposited
germanium Ge	0.5-11.5	20,000-870	4.0			
silicon Si	0.20-6.2	50,000-1613	3.5		0.033 (400K) 0.066 (500K) 0.102 (600K)	

Material	Wavelength range, µm	Wave number range, cm^{-1}	Refractive Index at 2µm)	Thermal Conductivity W/m•K(X10^2)	Thermal Expansion ΔL/L., percent	Notes
aluminum oxide (Sapphire) Al_2O_3	0.20-6.5	50,000-1538	1.76	25.1 (293.2K) 21.3 (323K) 14.2 (432.2K)	0.075 (400K) 0.148 (500K) 0.225 (600K)	
polyethylene	16-300	625-33	1.54			not useful for many organic compounds
mica	200-425	50-23.5				

WAVELENGTH-WAVENUMBER CONVERSION TABLE

Wavelength (µm)	Wavenumber (cm^{-1}) 0	1	2	3	4	5	6	7	8	9
2.0	5000	4975	4950	4926	4902	4878	4854	4831	4808	4785
2.1	4762	4739	4717	4695	4673	4651	4630	4608	4587	4566
2.2	4545	4525	4505	4484	4464	4444	4425	4405	4386	4367
2.3	4348	4329	4310	4292	4274	4255	4237	4219	4202	4184
2.4	4167	4149	4232	4115	4098	4082	4065	4049	4032	4016
2.5	4000	3984	3968	4953	3937	3922	3006	3891	3876	3861
2.6	3846	3831	3817	3802	3788	3774	3759	3745	3731	3717
2.7	3704	3690	3676	3663	3650	3636	3623	3610	3597	3584
2.8	3571	3559	3546	3534	3521	3509	3497	3484	3472	3460
2.9	3448	3436	3425	3413	3401	3390	3378	3367	3356	3344
3.0	3333	3322	3311	3300	3289	3279	3268	3257	3247	3236
3.1	3226	3215	3205	3195	3185	3175	3165	3155	3145	3135
3.2	3125	3115	3106	3096	3086	3077	3067	3058	3049	3040
3.3	3030	3021	3012	3003	2994	2985	2976	2967	2959	2950
3.4	2941	2933	2924	2915	2907	2899	2890	2882	2874	2865
3.5	2857	2849	2841	2833	2825	2817	2809	2801	2793	2786
3.6	2778	2770	2762	2755	2747	2740	2732	2725	2717	2710
3.7	2703	2695	2688	2681	2674	2667	2660	2653	2646	2639
3.8	2632	2625	2618	2611	2604	2597	2591	2584	2577	2571
3.9	2654	2558	2551	2545	2538	2532	2525	2519	2513	2506
4.0	2500	2494	2488	2481	2475	2469	2463	2457	2451	2445
4.1	2439	2433	2427	2421	2415	2410	2404	2398	2387	2387
4.2	2381	2375	2370	2364	2358	2353	2347	2342	2336	2331
4.3	2326	2320	2315	2309	2304	2299	2294	2288	2283	2278
4.4	2273	2268	2262	2257	2252	2247	2242	2237	2232	2227
4.5	2222	2217	2212	2208	2203	2198	2193	2188	2183	2179
4.6	2174	2169	2165	2160	2155	2151	2146	2141	2137	2132
4.7	2128	2123	2119	2114	2110	2105	2101	2096	2092	2088
4.8	2083	2079	2075	2070	2066	2062	2058	2053	2049	2045
4.9	2041	2037	2033	2028	2024	2020	2016	2012	2008	2004
5.0	2000	1996	1992	1988	1984	1980	1976	1972	1969	1965
5.1	1961	1957	1953	1949	1946	1942	1938	1934	1931	1927
5.2	1923	1919	1916	1912	1908	1905	1901	1898	1894	1890
5.3	1887	1883	1880	1876	1873	1869	1866	1862	1859	1855
5.4	1852	1848	1845	1842	1838	1835	1832	1828	1825	1821
5.5	1818	1815	1812	1808	1805	1802	1799	1795	1792	1788
5.6	1786	1783	1779	1776	1773	1770	1767	1764	1761	1757
5.7	1754	1751	1748	1745	1742	1739	1736	1733	1730	1727
5.8	1724	1721	1718	1715	1712	1709	1706	1704	1701	1698
5.9	1695	1692	1689	1686	1684	1681	1678	1675	1672	1669
6.0	1667	1664	1661	1568	1656	1653	1650	1647	1645	1642
6.1	1639	1637	1634	1631	1629	1626	1623	1621	1618	1616
6.2	1613	1610	1608	1605	1603	1600	1597	1595	1592	1590
6.3	1587	1585	1582	1580	1577	1575	1572	1570	1567	1565

WAVELENGTH-WAVENUMBER CONVERSION TABLE

	Wavenumber (cm^{-1})									
Wavelength (µm)	0	1	2	3	4	5	6	7	8	9
6.4	1563	1560	1558	1555	1553	1550	1548	1546	1543	1541
6.5	1538	1536	1534	1531	1529	1527	1524	1522	1520	1517
6.6	1515	1513	1511	1508	1506	1504	1502	1499	1497	1495
6.7	1493	1490	1488	1486	1484	1481	1479	1477	1475	1473
6.8	1471	1468	1466	1464	1462	1460	1458	1456	1453	1451
6.9	1449	1447	1445	1443	1441	1439	1437	1435	1433	1431
7.0	1429	1427	1425	1422	1420	1418	1416	1414	1412	1410
7.1	1408	1406	1404	1403	1401	1399	1397	1395	1393	1391
7.2	1389	1387	1385	1383	1381	1379	1377	1376	1374	1372
7.3	1370	1368	1366	1364	1362	1361	1359	1357	1355	1353
7.4	1351	1350	1348	1346	1344	1342	1340	1339	1337	1335
7.5	1333	1332	1330	1328	1326	1325	1323	1321	1319	1318
7.6	1316	1314	1312	1311	1309	1307	1305	1304	1302	1300
7.7	1299	1297	1295	1294	1292	1290	1289	1287	1285	1284
7.8	1282	1280	1279	1277	1276	1274	1272	1271	1269	1267
7.9	1266	1264	1263	1261	1259	1258	1256	1255	1253	1252
8.0	1250	1248	1247	1245	1244	1242	1241	1239	1238	1236
8.1	1235	1233	1232	1230	1229	1227	1225	1224	1222	1221
8.2	1220	1218	1217	1215	1214	1212	1211	1209	1208	1206
8.3	1205	1203	1202	1200	1199	1198	1196	1195	1193	1192
8.4	1190	1189	1188	1186	1185	1183	1182	1181	1179	1178
8.5	1176	1175	1174	1172	1171	1170	1168	1167	1166	1164
8.6	1163	1161	1160	1159	1157	1156	1155	1153	1152	1151
8.7	1149	1148	1147	1145	1144	1143	1142	1140	1139	1138
8.8	1136	1135	1134	1133	1131	1130	1129	1127	1126	1125
8.9	1124	1122	1121	1120	1119	1117	1116	1115	1114	1112
9.0	1111	1110	1109	1107	1106	1105	1104	1103	1101	1100
9.1	1099	1098	1096	1095	1094	1093	1092	1091	1089	1088
9.2	1087	1086	1085	1083	1082	1081	1080	1079	1078	1076
9.3	1075	1074	1073	1072	1071	1070	1068	1067	1066	1065
9.4	1064	1063	1062	1060	1059	1058	1057	1056	1055	1054
9.5	1053	1052	1050	1049	1048	1047	1046	1045	1044	1043
9.6	1042	1041	1040	1038	1037	1036	1035	1034	1033	1032
9.7	1031	1030	1029	1028	1027	1026	1025	1024	1022	1021
9.8	1020	1019	1018	1017	1016	1015	1014	1013	1012	1011
9.9	1010	1009	1008	1007	1006	1005	1004	1003	1002	1001
10.0	1000	999	998	997	996	995	994	993	992	991
10.1	990	989	988	987	986	985	984	983	982	081
10.2	980	979	978	978	977	976	975	974	973	972
10.3	971	970	969	968	967	966	965	964	963	962
10.4	962	961	960	959	958	957	956	955	954	953
10.5	952	951	951	950	949	948	947	946	945	944
10.6	943	943	942	041	940	939	938	937	936	935

WAVELENGTH-WAVENUMBER CONVERSION TABLE

Wavenumber (cm^{-1})

Wavelength (μm)	0	1	2	3	4	5	6	7	8	9
10.7	935	934	933	932	931	930	929	929	928	927
10.8	926	925	924	923	923	922	921	920	919	918
10.9	917	917	916	915	914	913	912	912	911	910
11.0	909	908	907	907	906	905	904	903	903	902
11.1	901	900	899	898	898	897	896	895	894	894
11.2	893	892	891	890	890	889	888	887	887	886
11.3	885	884	883	883	882	881	880	880	879	878
11.4	877	876	876	875	874	873	873	872	871	870
11.5	870	869	868	867	867	866	865	864	864	863
11.6	862	861	861	860	859	858	858	857	856	855
11.7	855	854	853	853	852	851	850	850	849	848
11.8	847	847	846	845	845	844	843	842	842	841
11.9	840	840	839	838	838	837	836	835	835	834
12.0	833	833	832	831	831	830	829	829	828	827
12.1	826	826	825	824	824	823	822	822	821	820
12.2	820	819	818	818	817	816	816	815	814	814
12.3	813	812	812	811	810	810	809	808	808	807
12.4	806	806	805	805	804	803	803	802	801	801
12.5	800	799	799	798	797	797	796	796	795	794
12.6	794	793	792	792	791	791	790	789	789	788
12.7	787	787	786	786	785	784	784	783	782	782
12.8	781	781	780	779	779	778	778	777	776	776
12.9	775	775	774	773	773	772	772	771	770	770
13.0	769	769	768	767	767	766	766	765	765	764
13.1	763	763	762	762	761	760	760	759	759	758
13.2	758	757	756	756	755	755	754	754	753	752
13.3	752	751	751	750	750	749	749	748	747	747
13.4	746	746	745	745	744	743	743	742	742	741
13.5	741	740	740	739	739	738	737	737	736	736
13.6	735	735	734	734	733	733	732	732	731	730
13.7	730	729	729	728	728	727	727	726	726	725
13.8	725	724	724	723	723	722	722	721	720	720
13.9	719	719	718	718	717	717	716	716	715	715
14.0	714	714	713	713	712	712	711	711	710	710
14.1	709	709	708	708	707	707	706	706	705	705
14.2	704	704	703	703	702	702	702	701	701	700
14.3	699	699	698	698	697	697	696	696	695	695
14.4	694	694	693	693	693	692	692	691	691	690
14.5	690	689	689	688	688	687	687	686	686	685
14.6	685	684	684	684	683	683	682	682	681	681
14.7	680	680	679	679	678	678	678	677	677	676
14.8	676	675	675	674	674	673	673	672	672	672
14.9	671	671	670	670	669	669	668	668	668	667

Useful Solvents for Infrared Spectrophotometry

The following tables provide the infrared absorption spectra of several useful solvents. The spectra were measured using a double beam spectrophotometer using a neat sample against an air reference. The physical properties listed are those needed most often in designing spectrophotometric experiments [1-4]. The refractive indices are values measured with the sodium-D line. The Chemical Abstract Service registry numbers are alos provided for each solvent.

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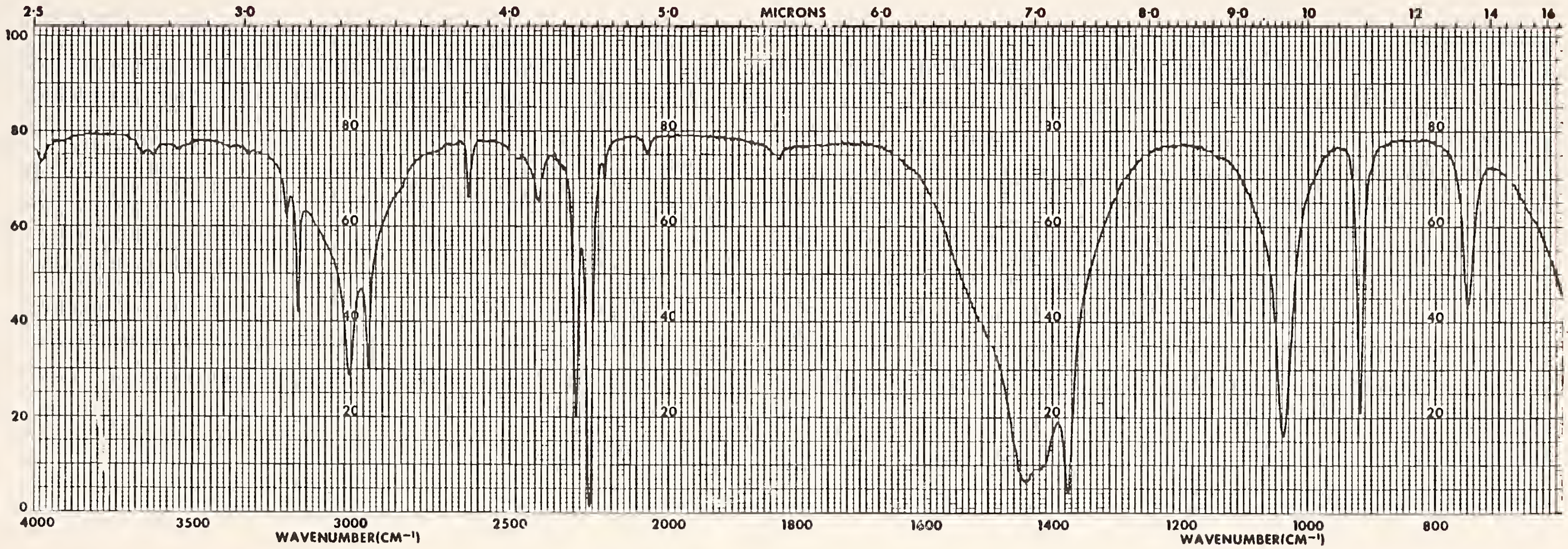
Acetonitrile CH_3CN

Physical Properties	
melting point	-45.7°C
boiling point	81.6°C
refractive index	1.34423 (20°C)
specific gravity	0.7857 (20°C)
thermal conductivity	0.1762 W/m•K
CAS	75-05-8

Notes

Highly polar solvent; soluble in water; flammable; highly toxic with an allowable limit of 40 ppm in air.

methyl cyanide, acetic acid nitrile



Benzene C_6H_6

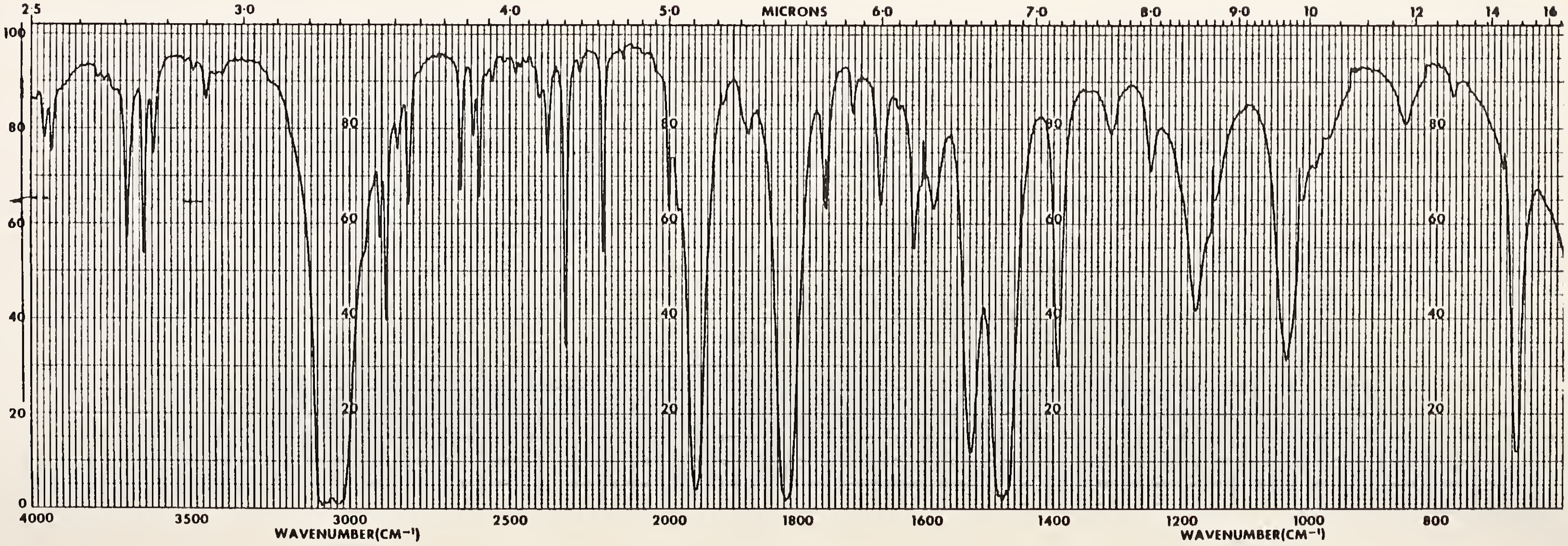
Physical Properties	
melting point	5.5°C
boiling point	80.1°C
vapor pressure	0.0097 MPa (25°C)
refractive index	1.50110 (20°C)
specific gravity	0.8790 (4°C)
thermal conductivity	0.1424 W/m•K (25°C)
dielectric constant	2.284 (20°C)
CAS	71-43-2

Notes

Non polar, aromatic solvent; very flammable and toxic; confirmed human carcinogen; soluble in alcohols, ether, chloroform, carbon tetrachloride, carbon disulfide, slightly soluble in water

cyclohexatriene

CONFIRMED HUMAN CARCINOGEN



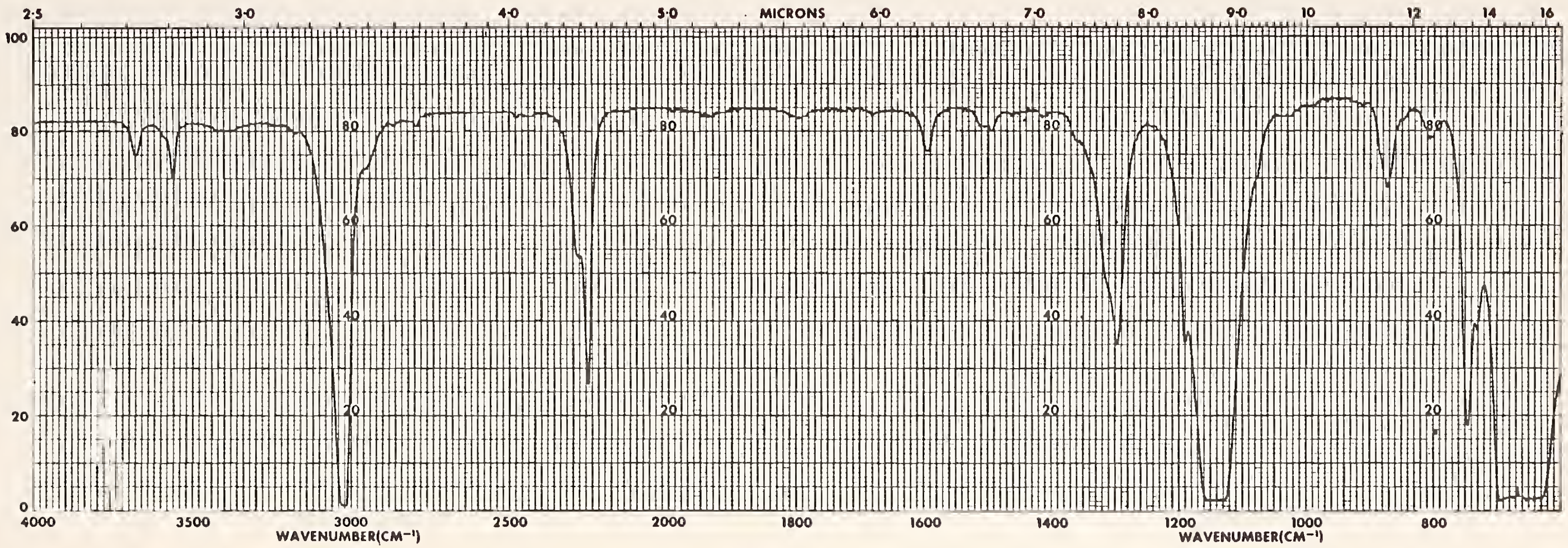
Bromoform $CHBr_3$

Physical Properties	
melting point	8.3°C
boiling point	149.5°C
vapor pressure	0.0008 MPa (25°C)
refractive index	1.6005 (20°C)
specific gravity	2.887 (20/4°C)
thermal conductivity	0.0961 W/m•K
dielectric constant	4.39 (20°C)
CAS	75-25-2

Notes

Moderately polar, weakly hydrogen bonding solvent; nonflammable; highly toxic (tolerance 0.5 ppm); soluble in alcohols, chloroform, hydrocarbons, benzene and many oils.

tribromomethane, methenyl tribromide



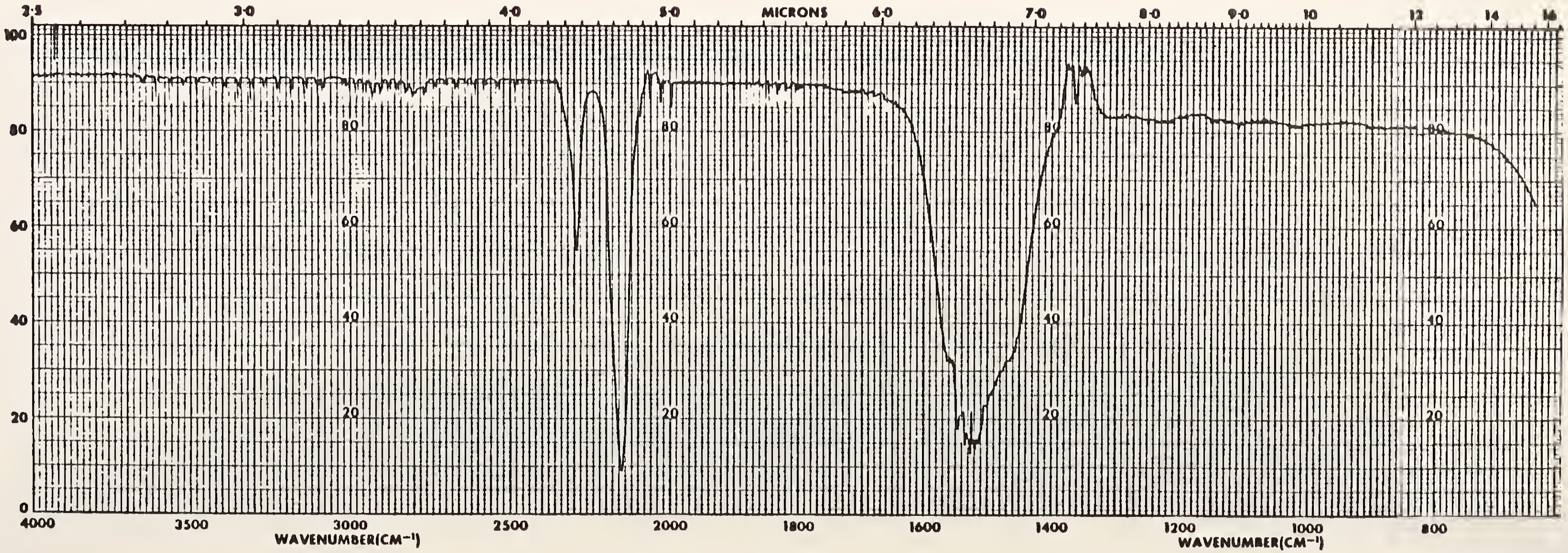
Carbon Disulfide CS_2

Physical Properties	
melting point	-111°C
boiling point	46.3°C
vapor pressure	0.0448 MPa (25°C)
refractive index	1.6232 (25°C)
specific gravity	1.260 (25/25°C)
dielectric constant	2.641 (20°C)
CAS	75-15-0

Notes

Moderately polar solvent, soluble in alcohols, benzene and ethers, slightly soluble in water; very flammable (explosive limits of between 1 and 50 percent); highly toxic (tolerance in air, 20 ppm).

carbon bisulfide



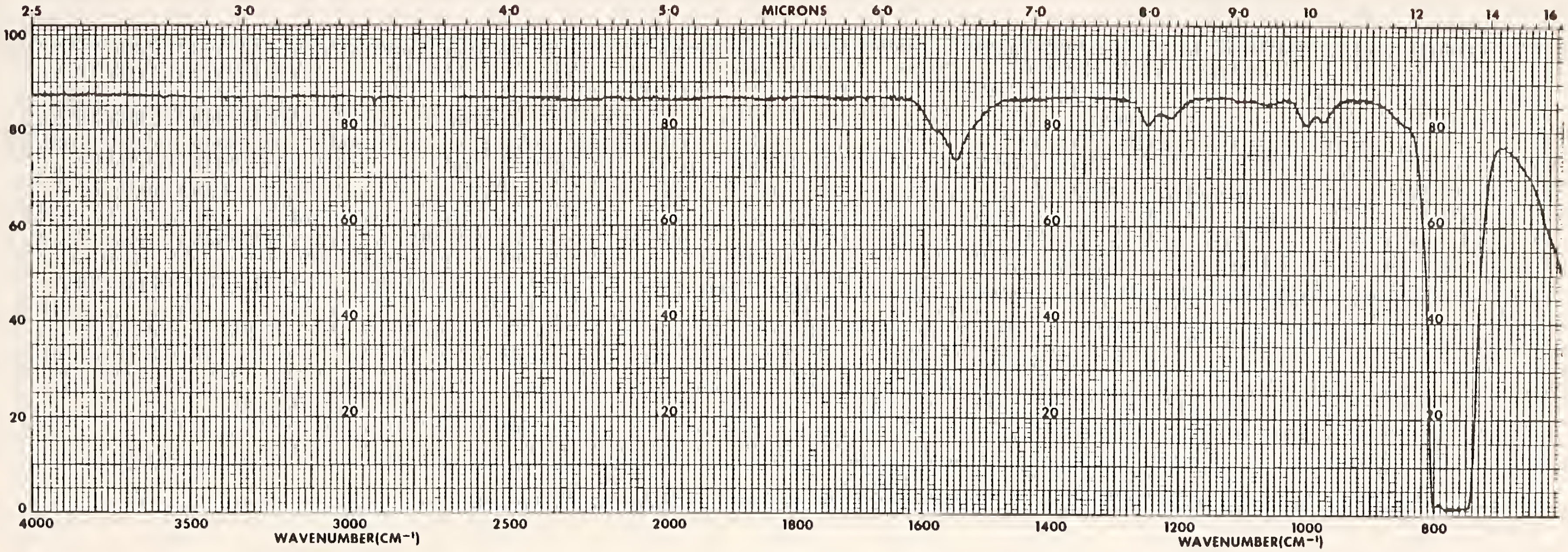
Carbon Tetrachloride CCl_4

Physical Properties	
melting point	-23.0°C
boiling point	76.74°C
vapor pressure	0.0122 MPa (25°C)
refractive index	1.4607 (20°C)
specific gravity	1.585
thermal conductivity	0.1070 W/m·K (20°C)
dielectric constant	2.238 (20°C)
CAS	56-23-5

Notes

Non polar solvent; soluble in alcohols, ethers, chloroform, benzene and most oils, insoluble in water; non-flammable; extremely toxic; carcinogenic

tetrachloromethane, perchloromethane



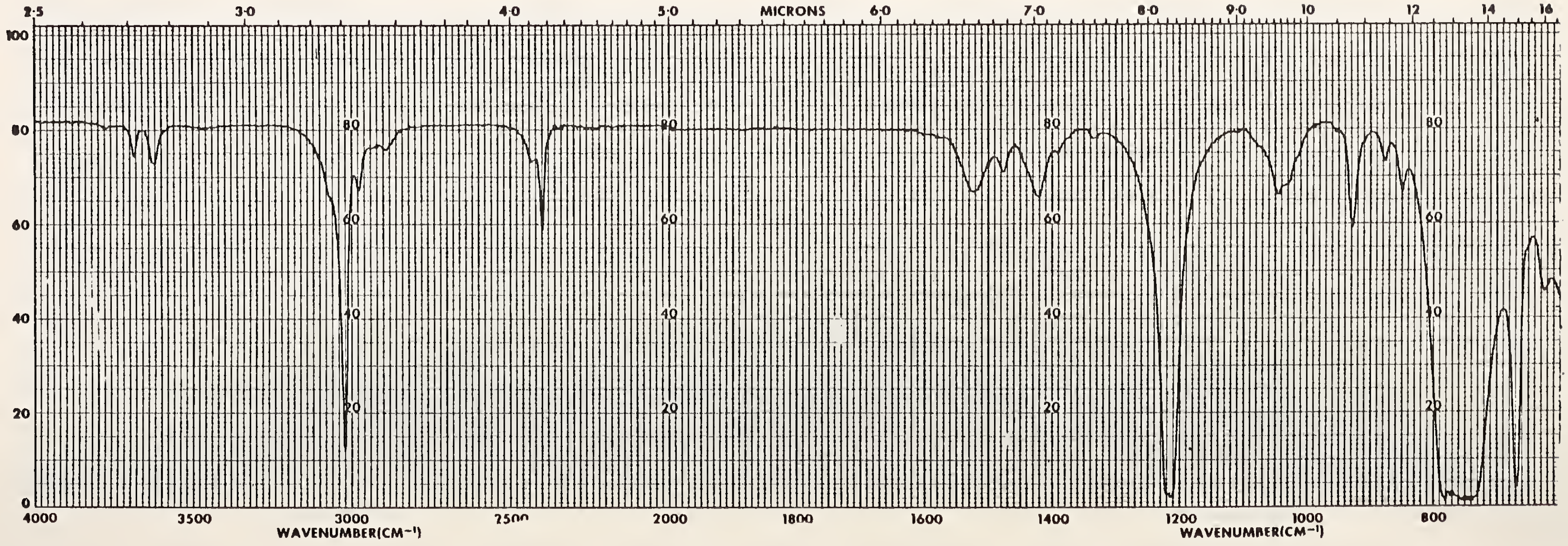
Chloroform $CHCl_3$

Physical Properties	
melting point	-63.5°C
boiling point	61.2°C
vapor pressure	0.0263 MPa (25°C)
refractive index	1.4422 (25°C)
specific gravity	1.485 (20/20°C)
thermal conductivity	0.1164 W/m·K (20°C)
dielectric constant	4.806 (20°C)
CAS	67-66-3

Notes

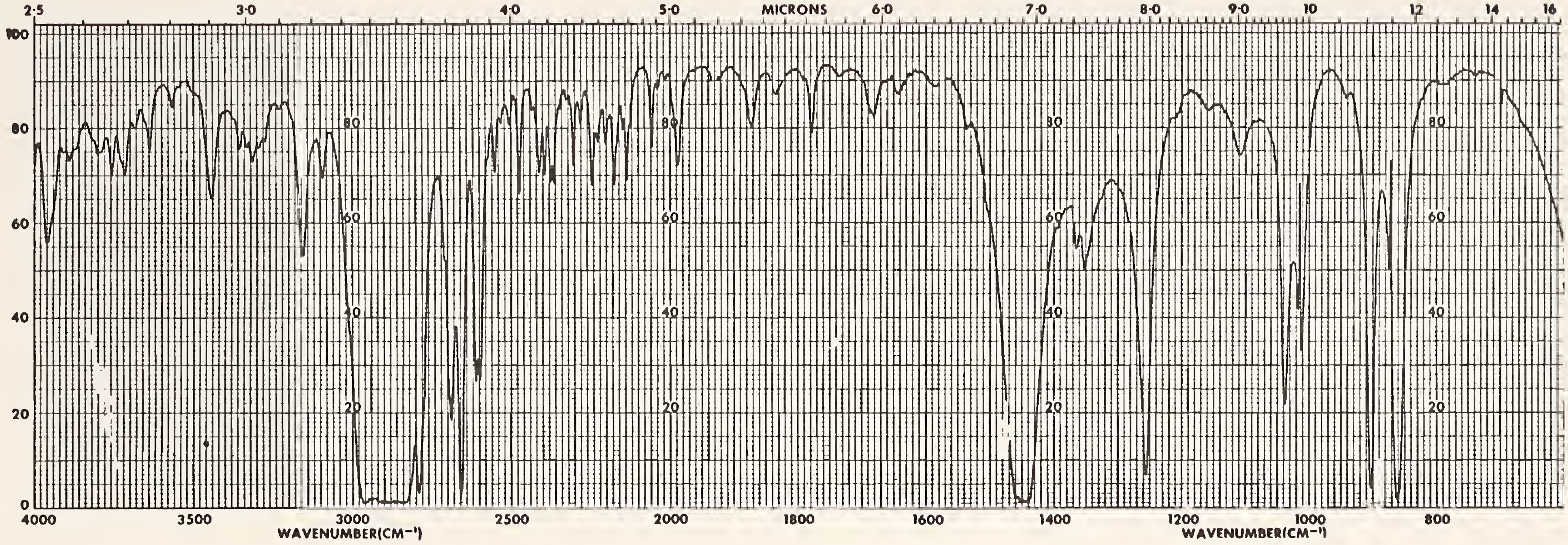
Polar solvent; soluble in alcohols, ether, benzene and most oils; usually stabilized with methanol to prevent phosgene formation; flammable and highly toxic (tolerance in air, 50 ppm); carcinogenic

trichloromethane



Cyclohexane C_6H_{12}

Physical Properties		Notes
melting point	6.3°C	Non polar hydrocarbon solvent; soluble in alcohols, acetone benzene; flammable; moderately toxic (tolerance in air, 300 ppm)
boiling point	80.7°C	
vapor pressure	0.0111 MPa (25°C)	
refractive index	1.4263 (20°C)	
specific gravity	0.779 (20/4°C)	hexamethylene, hexanaphthene, hexahydrobenzene
thermal conductivity	0.122 W/m•K (20°C)	
dielectric constant	2.023 (20°C)	
CAS	110-82-7	



Dimethyl Sulfoxide $(CH_3)_2SO$

Physical Properties		Notes
melting point	18.5°C	Powerful aprotic solvent; soluble in water; combustible; readily penetrates the skin.
boiling point	189°C	
specific gravity	1.01 (20°C)	
CAS	67-68-5	DMSO

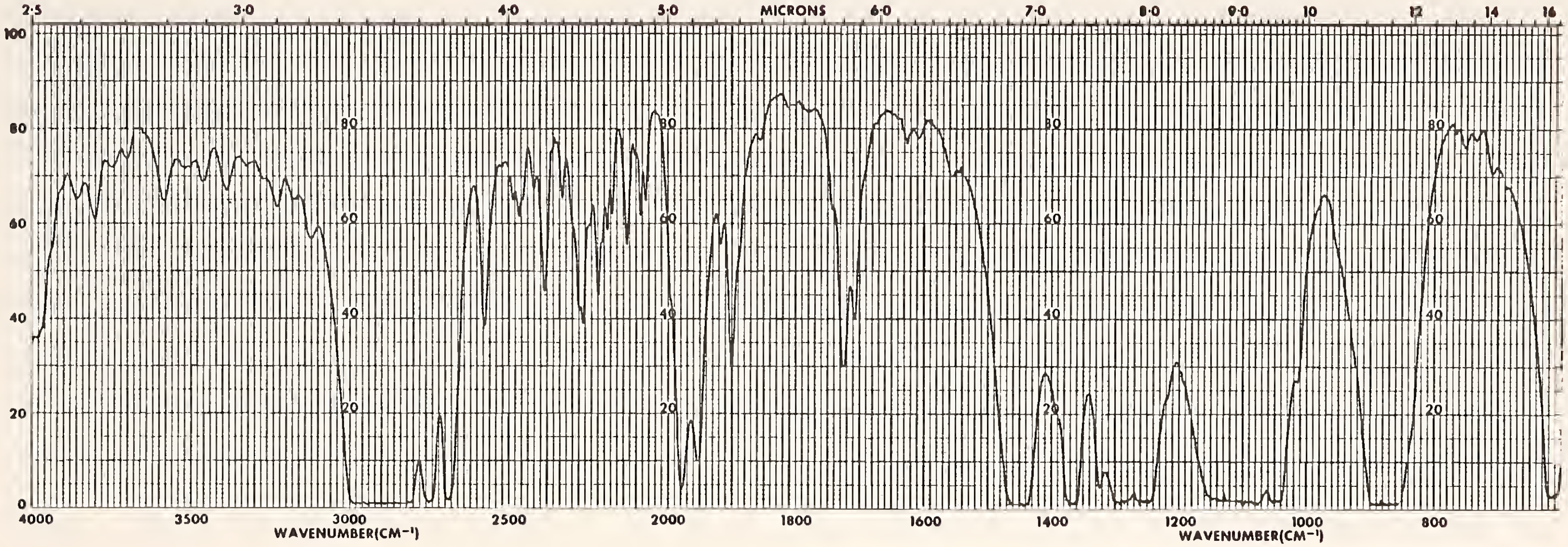
1,4-Dioxane $OCH_2CH_2OCH_2CH_2$

Physical Properties	
melting point	11°C
boiling point	101.3°C
vapor pressure	0.0053 MPa (25°C)
refractive index	1.4221 (20°C)
specific gravity	1.0356 (20/20°C)
dielectric constant	2.209 (20°C)
CAS	123-91-1

Notes

Moderately polar solvent; soluble in water and most organic solvents; flammable; highly toxic by ingestion and inhalation; absorbed through the skin (tolerance in air, 100 ppm).

diethylene ether, 1,4-diethylene dioxide, diethlene dioxide, dioxyethylene ether



Ethyl Acetate $CH_3COOC_2H_5$

Physical Properties	
melting point	-83.58°C
boiling point	77.06°C
vapor pressure	0.0097 MPa (20°C)
refractive index	1.3723 (20°C)
specific gravity	0.9003 (20/4°C)
dielectric constant	6.02 (25°C)
CAS	141-78-6

Notes

Polar solvent; soluble in water, alcohols, ether, and many oils; flammable (limits in air: 2.2 to 9 percent); moderately toxic by inhalation and skin absorption (tolerance in air 400 ppm).

acetic ether, acetic ester, vinegar naphtha
acetic acid ethyl ester

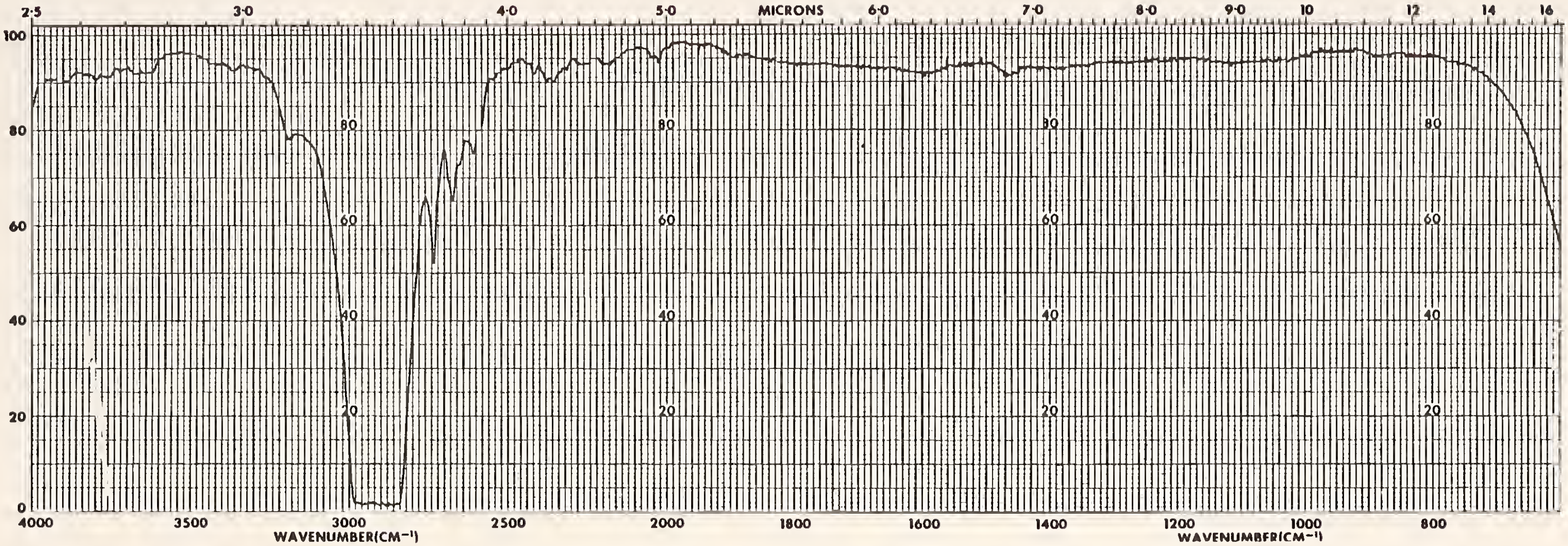
n-Hexane $CH_3(CH_2)_4CH_3$

Physical Properties	
melting point	-95 °C
boiling point	68.742 °C
vapor pressure	0.0222 MPa (25 °C)
refractive index	1.37486 (20 °C)
specific gravity	0.65937 (20/4 °C)
thermal conductivity	0.1217 W/m·K (20 °C)
dielectric constant	1.890 (20 °C)
CAS	110-54-3

Notes

Non polar solvent; soluble in alcohols, acetone and ethers, insoluble in water; flammable; moderately toxic by inhalation and ingestion (tolerance in air, 500 ppm).

hexane



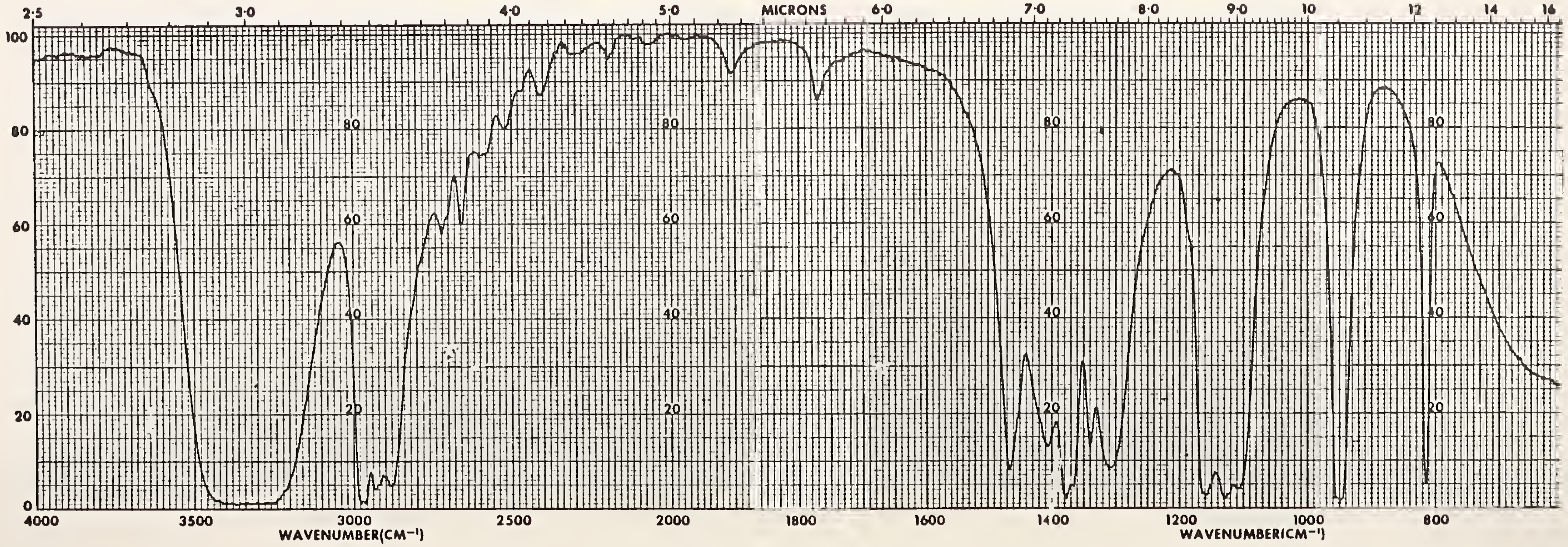
Isopropanol $(CH_3)_2CHOH$

Physical Properties	
melting point	-86°C
boiling point	82.4°C
vapor pressure	0.0044 MPa
refractive index	1.3756
specific gravity	0.7863 (20/20°C)
dielectric constant	18.3 (25°C)
CAS	67-63-0

Notes

Polar solvent; soluble in water, alcohols, ethers, many hydrocarbons and oils; flammable and moderately toxic by ingestion and inhalation (tolerance in air, 400 ppm).

dimethyl carbinol, sec-propyl alcohol, 2-propanol



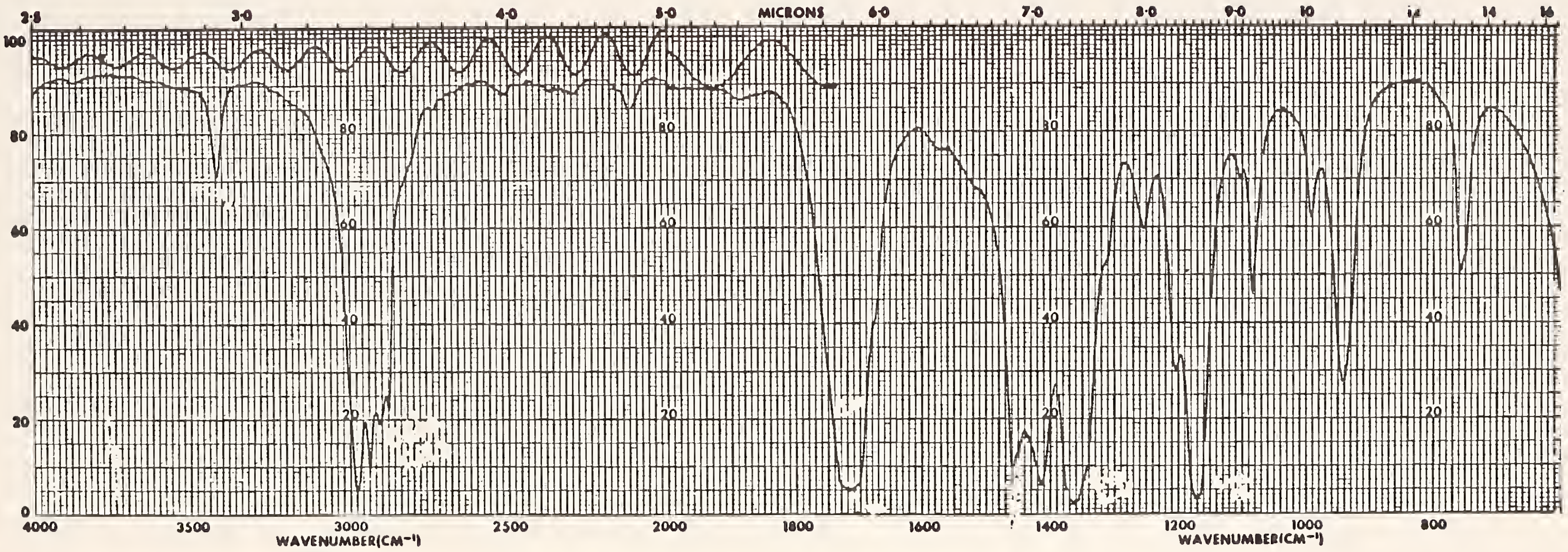
Methyl Ethyl Ketone $CH_3COC_2H_5$

Physical Properties	
melting point	-86.4°C
boiling point	79.6°C
vapor pressure	0.0129 MPa (25°C)
refractive index	1.379 (20°C)
specific gravity	0.8255 (4°C)
thermal conductivity	0.1465 W/m•K
dielectric constant	18.5 (20°C)
CAS	78-93-3

Notes

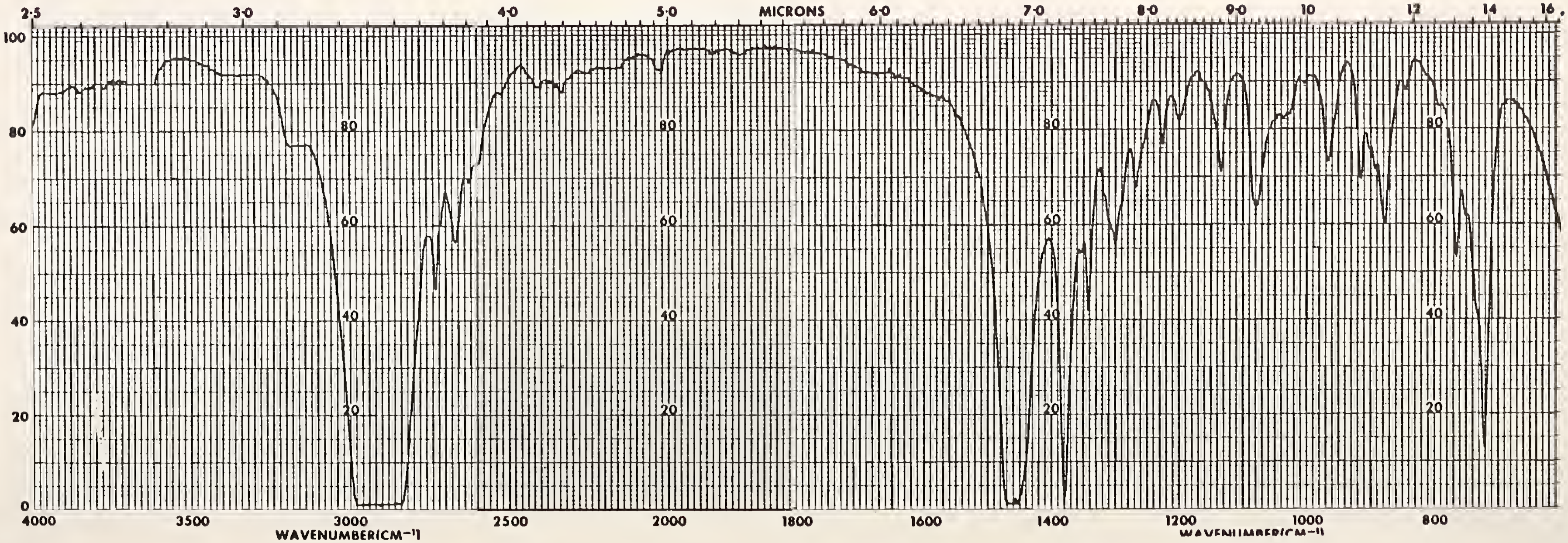
Polar solvent; soluble in water, alcohols, ether and many oils; highly flammable (explosive limits in air, 2 to 10 percent); narcotic by inhalation (tolerance in air, 200 ppm).

ethyl methyl ketone, 2-butanone



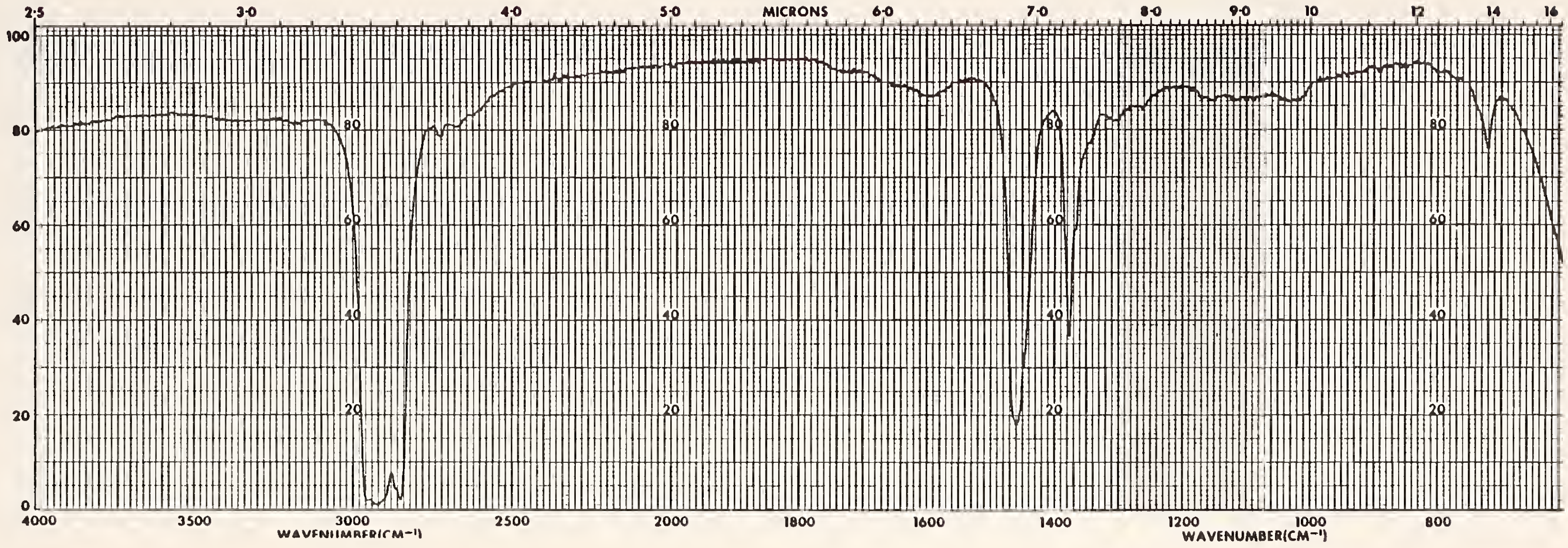
n-Octane $CH_3(CH_2)_6CH_3$

Physical Properties		Notes
melting point	-56.798°C	Non polar solvent; soluble in alcohol, acetone and hydrocarbons, insoluble in water; flammable; (tolerance in air, 400 ppm).
boiling point	125.667°C	
vapor pressure	0.0023 MPa (25°C)	
refractive index	1.39745 (20°C)	
specific gravity	0.7026 (20/4°C)	octane
dielectric constant	1.948 (20°C)	
CAS	111-65-9	



Paraffin oil

Physical Properties	Notes
properties depend on grades and viscosity	Viscous, combustible liquid used for mull preparation; slightly combustible; nontoxic.
	Nujol, mineral oil



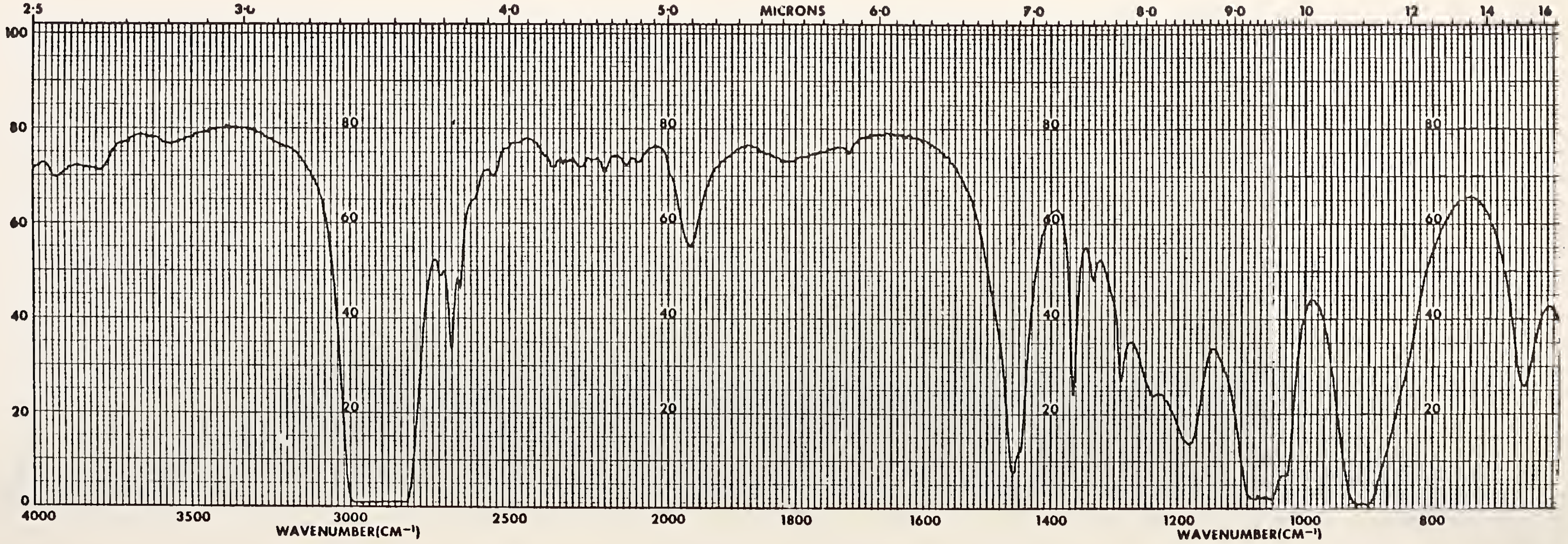
Tetrahydrofuran $\underbrace{CH_2(CH_2)_2CH_2O}$

Physical Properties	
melting point	-65°C
boiling point	66°C
refractive index	1.4070 (20°C}
specific gravity	0.888 (20/20°C)
CAS	109-99-9

Notes

Moderately polar solvent; soluble in water and most organic solvents; flammable; (explosive limits in air, 2 to 11.8 percent); highly toxic (tolerance in air, 200 ppm).

THF



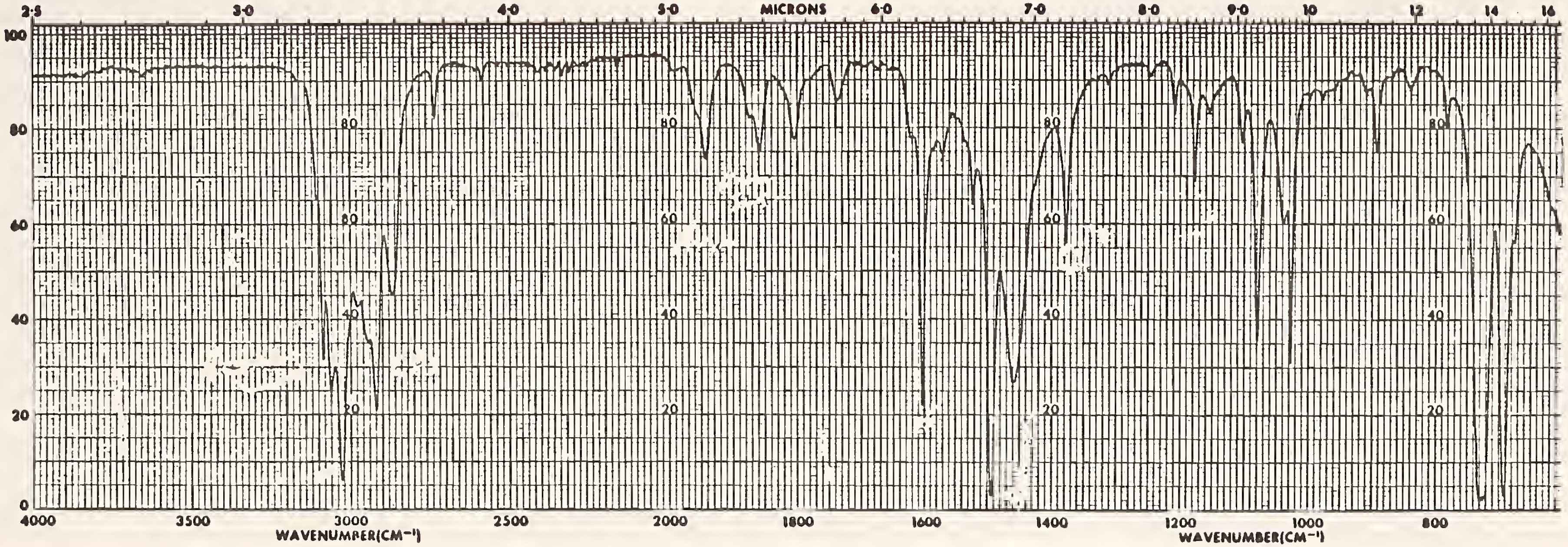
Toluene $CH_3C_6H_5$

Physical Properties	
melting point	-94.5°C
boiling point	110.7°C
vapor pressure	0.0036 MPa (25°C)
refractive index	1.497 (20°C)
specific gravity	0.866 (20/4°C)
thermal conductivity	0.1348 W/m·K (20°C)
dielectric constant	2.379 (25°C)
CAS	108-88-3

Notes

Aromatic solvent; soluble in benzene, alcohols, ethers, insoluble in water; highly flammable (explosion limits in air 1.27 to 7 percent); toxic by ingestion, inhalation and absorption through the skin (tolerance in air 200 ppm).

toluol, methylbenzene, phenylmethane

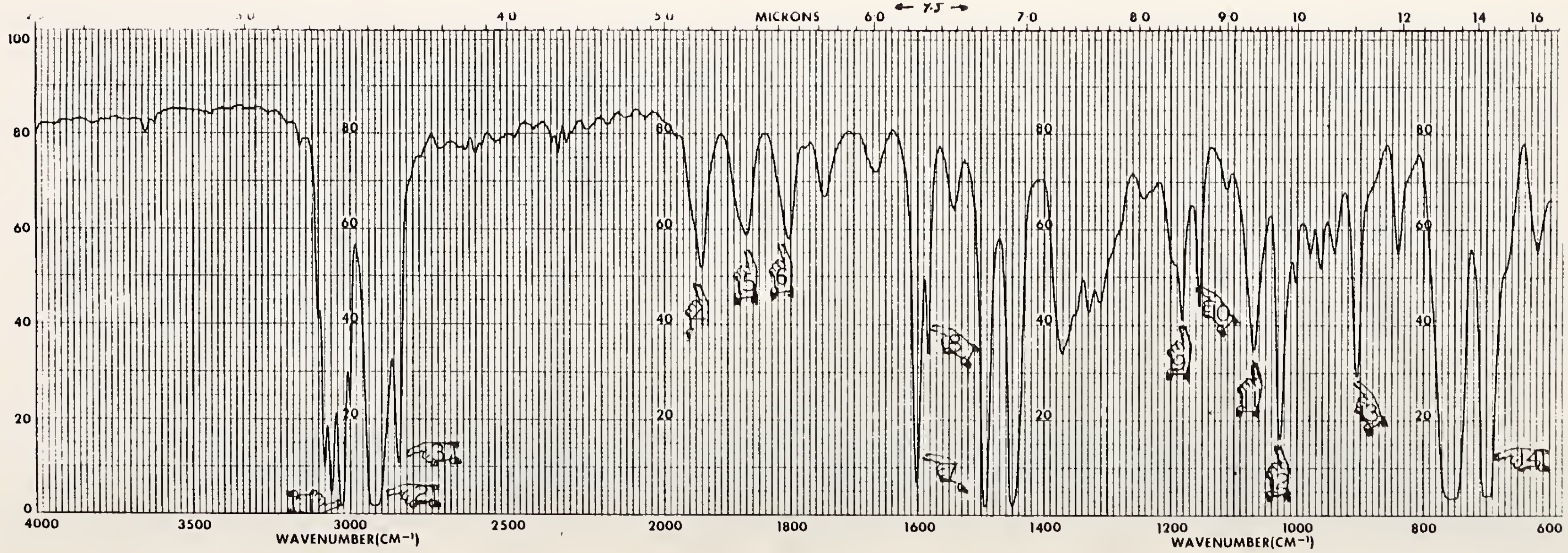


Polystyrene Wavenumber Calibration

The following are wavenumber readings assigned to the peaks on the spectrum:

1- 3027.1
2- 2924.0
3- 2850.7
4- 1944.0
5- 1871.0
6- 1801.6
7- 1601.4
8- 1583.1
9- 1181.4
10- 1154.3
11- 1069.1
12- 1028.0
13- 906.7
14- 698.9

Film Thickness - 50 µm
Molecular Weight - (104.15)η



IR CORRELATION CHART

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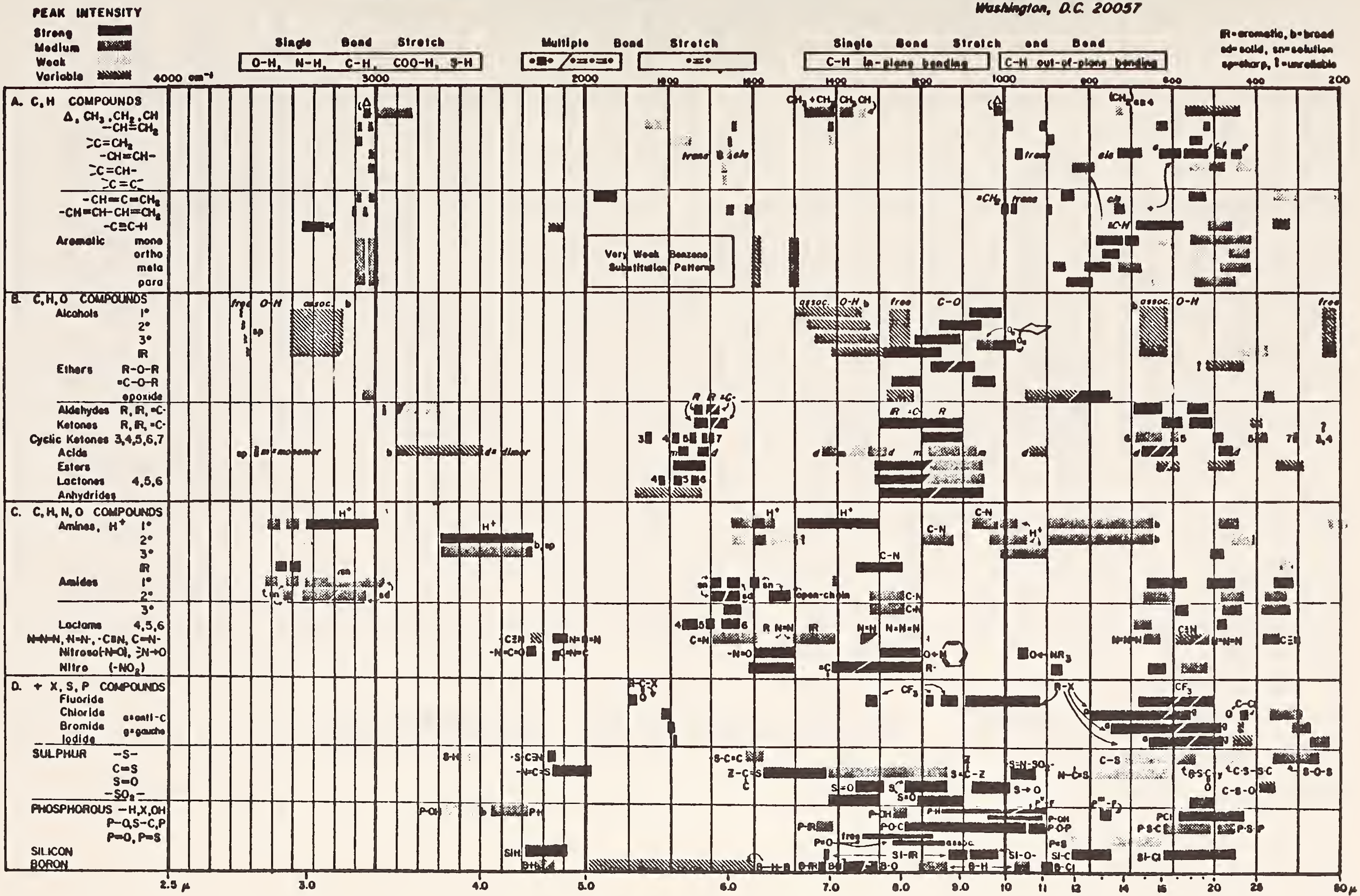

AROMATIC SUBSTITUTION BANDS

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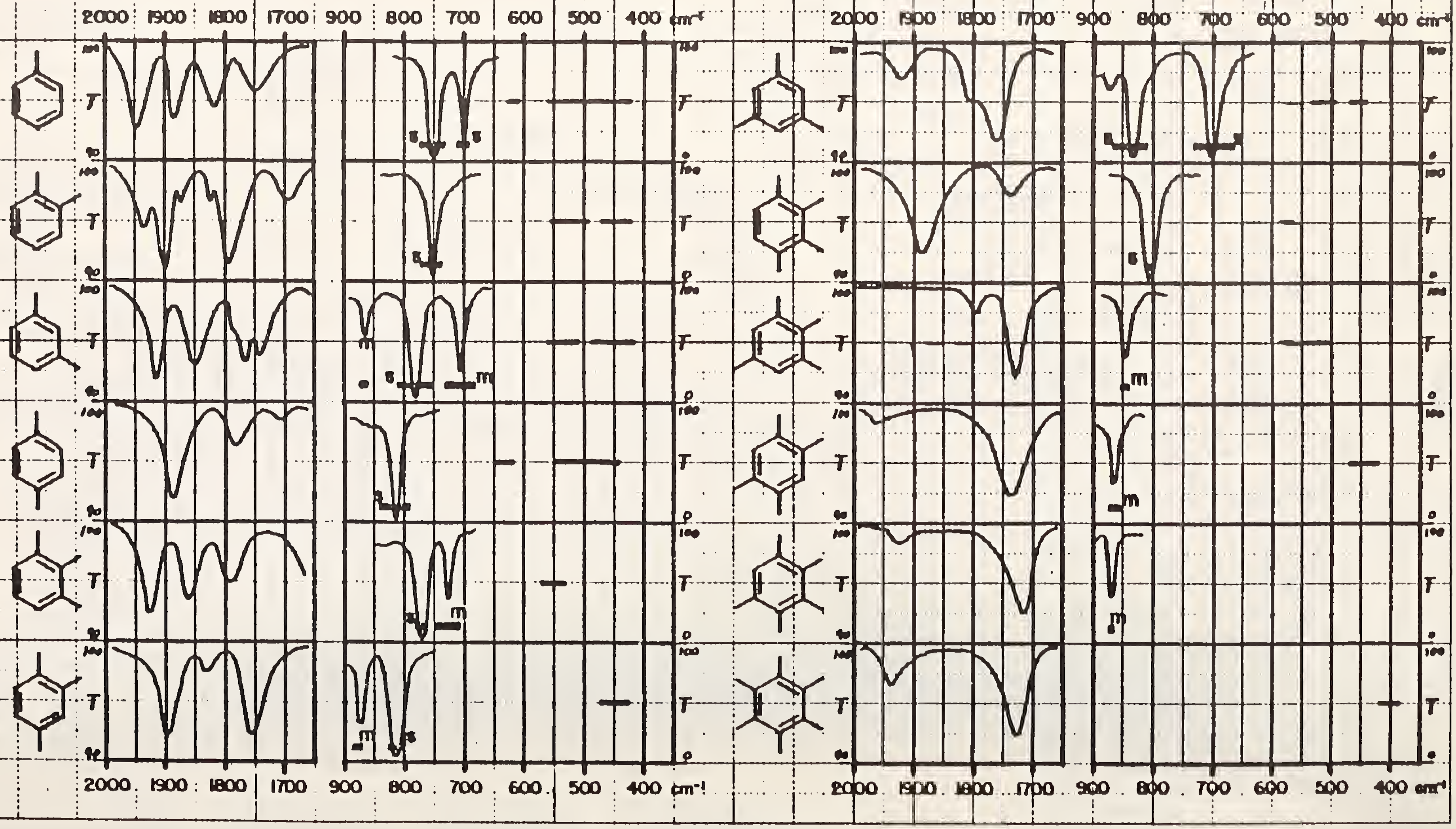

Infrared Absorptions of Major Chemical Families

The following tables provide expected IR absorptions of the major chemical families [1-13].

Abbreviations:

s	Strong
m	Medium
w	Weak
vs	Very strong
vw	Very weak
sym	Symmetrical
asym	Asymmetrical

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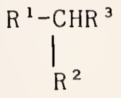
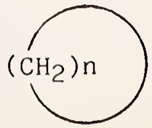
[12] Meyers, C.Y., Eighth Annual Report on Research, 1963, Sponsored by the Petroleum Research Fund, American Chemical Society, Washington, D.C., 1964.

[13] Meyers, C.Y., Estratto dalla Gazzetta Chimica Italiana, 93, 1206, 1963.

Hydrocarbon Compounds

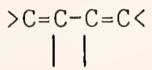
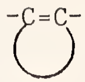
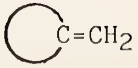
Wavenumbers (cm^{-1})

Family	General Formula	C-H stretch	C-H bend	C-C stretch	C-C bend
Alkanes, a) acyclic	C_nH_{2n+2}				
(i): straight chain	$CH_3(CH_2)_nCH_3$	3000-2840 (s/m) CH_3-, (asym): 3000-2960(s) CH_3-, (sym): 2880-2870(s) >CH_2, (asym): 2930-2920(s) >CH_2, (sym): 2860-2840(s)	Below 1500 (w/m/s) CH_3- (asym): 1460-1440(s) CH_3- (sym): 1380-1370(s) >CH_2 (scissoring): ~1465(s) >CH_2 (rocking): ~ 720(s) >CH_2 (twisting and wagging): 1350-1150(w).	1200-800 (w) (not of practical value).	Below 500 (not of practical value).
(ii): branched	 $R^1\text{-}\underset{R^2}{\underset{\vert}{C}}HR^3$	C-H (3°): ~2890(vw)	Gem dimethyl [$(CH_3)_2CH$-]: 1380, 1370 (m, symmetrical doublet) tert-butyl [$(CH_3)_3C$-]: 1390, 1370 (m, unsymmetrical doublet; latter more intense) CH_3- rocking: 930-920 w, not reliable.		
b) cyclic		Same as in acyclic alkanes; ring strain increases the frequencies up to 3100 cm^{-1}	>CH_2 (scissoring): lower than in acyclic alkanes (10-15 cm^{-1}).		

Hydrocarbon Compounds (Continued)

Family	General Formula	Wavenumbers (cm^{-1}) >C=C< stretch	>C=C-H stretch	>C=C-H bend (in plane)	>C=C-H bend (out-of-plane)	Notes
Alkenes (olefins) (I): Acyclic	C_nH_{2n}	1670-1600	above 3000			
(i): non-conjugated		1667-1640(m)				
(a) monosubstituted (vinyl)	$R^1CH=CH_2$	1658-1648(m)	3082-3000(m)	1420-1415(m) (scissoring)	~995(m) ~919(m)	
(b) disubstituted						
cis-	$\begin{matrix}R^1 & & R^2\\ & >C=C< & \\ H & & H\end{matrix}$	1662-1652(m)	3030-3015(m)	~1406(m)	715-675(s) (rocking)	C-H rocking not too dependable.
trans-	$\begin{matrix}R^1 & & H\\ & >C=C< & \\ H & & R_2\end{matrix}$	1678-1668(w)	3030-3020(m)	1325-1275(m) (deformation)	~965(s) (rocking)	
vinylidene	$\begin{matrix}R^1 & & H\\ & >C=C< & \\ R_2 & & H\end{matrix}$	1658-1648(m)	3090-3080(m) ~2980(m)	~1415(m)	~890(s) (rocking)	
c) trisubstituted	$\begin{matrix}R^1 & & H\\ & >C=C< & \\ R_2 & & R_3\end{matrix}$	1675-1665(w)	3090-3080(w)	~1415(w)	840-800(m) (deformation)	
d) tetrasubstituted	$\begin{matrix}R^1 & & R^3\\ & >C=C< & \\ R_2 & & R_4\end{matrix}$	~1670(vw)	---	---	---	>C=C< stretch may be absent.

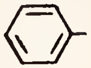
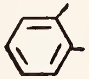
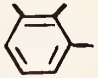
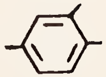
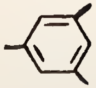
Hydrocarbon Compounds (Continued)

Family	General Formula	Wavenumbers (cm^{-1}) >C=C< stretch	>C=C-H stretch	>C=C-H bend (in plane)	>C=C-H bend (out-of-plane)	Notes
(ii): conjugated	 >C=C-C=C<	1610-1600(m) (frequently a doublet)	3050(vw)		~980 (rocking)	Conjugation of an olefinic >C=C< with an aromatic ring raises the frequency 20-25 cm^{-1}.
(iii): cumulated	>C=C=C<	2000-1900(m)	3300(m)	2000-1900(s) 1800-1700(w)	880-850(s)	
(II): Cyclic		1640-1560 (variable)			697-625(w) (wagging)	>C=C< stretch is coupled with C-C stretch of adjacent bonds. Alkyl substitution increases the >C=C< absorption frequency.
(III): External exocyclic		1781-1650	3080,2995(m)	~1300(w)		>C=C< frequency increases with decreasing ring size.

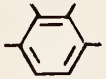
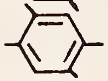
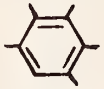
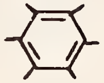
Hydrocarbon Compounds (Continued)

Family	General Formula	Wavenumbers (cm^{-1})			Notes
		-C≡C- stretch	-C≡C-H stretch	C-H bend	
Alkynes (i): non-conjugated	C_nH_{2n-2}				
(a) terminal	R^1-C≡C-H	2150-2100(m)	3310-3200(m) (sharp)	700-610(s) 1370-1220(w) (overtone)	-C≡C-H stretch peak is narrower than that of -OH or -NH stretch which are broader due to hydrogen bonding.
(b) non-terminal	R^1-C≡C-R^2	2260-2190(vw)	---	700-610(s) 1370-1220(w) (overtone)	
(ii): conjugated					
(a) terminal	R^1-C≡C-C≡C-H	2200,2040 (doublet)	3310-3200(m) (sharp)	700-610(s) 1370-1220(w) (overtone)	
(b) non-terminal	R^1-C≡C-C≡C-R^2	2200,2040 (doublet)	---	700-610(s) 1370-1220(w) (overtone)	

Hydrocarbon Compounds (Continued)

Family	General Formula	Wave Numbers (in cm^{-1})			Notes
		$>C=C\overset{H}{<}$ stretch	$>C=C<$ stretch	$>C-H$ bend (out-of-plane)	
Aromatic compounds					All show weak combination and overtone bands between 2000-16500 cm^{-1}. See aromatic substitution pattern chart.
(a) Monosubstituted		3100-3000	1600-1500	770-730(s) 710-690(s)	
(b) Disubstituted					
(i): 1,2-		3100-3000	1600-1500	770-735(s)	
(ii): 1,3-		3100-3000	1600-1500	810-750(s) 710-690(s)	
(iii): 1,4-		3100-3000	1600-1500	833-810(s)	
(c) Trisubstituted					
(i): 1,2,3-		3100-3000	1600-1500	780-760(s) 745-705(m)	
(ii): 1,2,4-		3100-3000	1600-1500	885-870(m) 825-805(s)	
(iii): 1,3,5-		3100-3000	1600-1500	865-810(s) 730-765(m)	

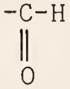
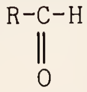
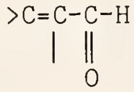
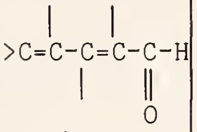
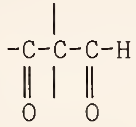
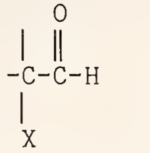
Hydrocarbon Compounds (Continued)

Family	General Formula	Wave Numbers (in cm^{-1}) $>C=C<^{H}$ stretch	$>C=C<$ stretch	$>C-H$ bend (out-of-plane)	Notes
(d) Tetrasubstituted					
(i): 1,2,3,4-		3100-3000	1600-1500	810-800	
(ii): 1,2,3,5-		3100-3000	1600-1500	850-840	
(iii): 1,2,4,5-		3100-3000	1600-1500	870-855	
(e) Pentasubstituted		3100-3000	1600-1500	~870	
(f) Hexasubstituted		3100-3000	1600-1500	below 500	

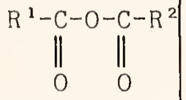
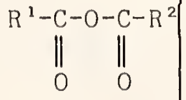
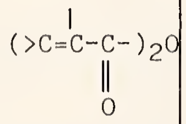
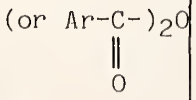
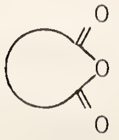
Organic Oxygen Compounds

Family	General Formula	Wavenumbers (cm^{-1})			Notes
		O-H stretch	>C-O stretch	-O-H bend	
Acetals	$R^1\text{-}\overset{\overset{\textstyle OR^2}{\vert}}{\underset{\underset{\textstyle OR^3}{\vert}}{C}}\text{-}H$		1195-1060(s) (three bands) 1055-1040(s) (sometimes obscured)		
Acyl halides	$R\text{-}\underset{\underset{\textstyle O}{\Vert}}{C}\text{-}X$ X=halogen				See Organic Halogen Compounds.
Alcohols	R-OH	3650-3584 (s,sharp)-for very dilute solutions or vapor phase spectra. 3550-3200 (s,broad)-for less dilute solutions where intermolecular hydrogen bonding is likely to occur. Intramolecular hydrogen bonding is responsible for a broad, shallow peak in the range of 3100-3050 cm^{-1}.		1420-1300(s)	α-unsaturation decrease >C-O stretch by 30 cm^{-1}. Liquid spectra of alcohols show a broad out-of-plane bending band (769-650,s).
(i): Primary	$R\text{-}CH_2OH$		~1050 cm^{-1}	~1420(m) and ~1330(m) (coupling of O-H in-plane bending and C-H wagging)	
(ii): Secondary	$R^1\text{-}\underset{\underset{\textstyle R^2}{\vert}}{C}HOH$		~1100 cm^{-1}	~1420(m) and ~1330(m) (coupling of O-H in-plane bending and C-H wagging)	
(iii): Tertiary	$R^1\text{-}\overset{\overset{\textstyle R^2}{\vert}}{\underset{\underset{\textstyle R^3}{\vert}}{C}}\text{-}OH$		~1150 cm^{-1}	only one band (1420-1330 cm^{-1}), position depending on the degree of hydrogen bonding)	

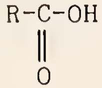
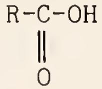
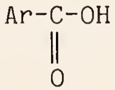
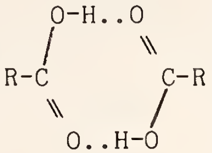
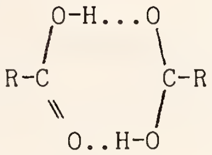
Organic Oxygen Compounds (Continued)

		Wavenumber (cm^{-1})		
Family	General Formula	>C=O stretch	 $-\underset{\underset{O}{\|}}{C}-H$ stretch	Notes
Aldehydes	 $R-\underset{\underset{O}{\|}}{C}-H$		~2820(m), ~2720(m) forms resonance between C-H stretch and first overtone of the aldehydic C-H bending	
(i): Saturated, aliphatic	R=alkyl	1720-1710(s)		
(ii): Aryl	R=aryl	1705-1695(s)	~2900(m), ~2750(m) (aromatic)	
(iii): α,β-unsaturated	 $>C=\underset{\|}{C}-\underset{\underset{O}{\|}}{C}-H$	1700-1680(s)		
(iv): α,β,γ,δ-unsaturated	 $>C=\overset{|}{C}-\underset{|}{C}=\overset{|}{C}-\underset{\underset{O}{\|}}{C}-H$	1680-1660(s)		
(v): β-keto-aldehyde	 $-\underset{\underset{O}{\|}}{C}-\underset{|}{\overset{|}{C}}-\underset{\underset{O}{\|}}{C}-H$	1670-1645(s) (lowering is possible due to intra-molecular hydrogen bonding in enol form).		
(vi): α-halo-	 $-\overset{|}{\underset{\underset{X}{|}}{C}}-\overset{\overset{O}{\|}}{C}-H$ X=halogen	~1740(s)		

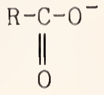
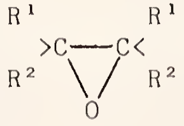
Organic Oxygen Compounds (Continued)

Family	General Formula	Wavenumbers (cm^{-1}) >C=O stretch	>C-O stretch	Notes
Amides				See Organic Nitrogen Compounds
Anhydrides	 $R^1-\underset{\underset{O}{\|}}{C}-O-\underset{\underset{O}{\|}}{C}-R^2$			
(i): Saturated acyclic	 $R^1-\underset{\underset{O}{\|}}{C}-O-\underset{\underset{O}{\|}}{C}-R^2$	~1820(s)(asym) ~1760(m/s)(sym)	1300-1050(s)(one or two bands)	
(ii): Conjugated acylic	 $(>C=\overset{\|}{C}-\underset{\underset{O}{\|}}{C}-)_2O$	1795-1775(s)(asym)	1300-1050(s)(one or two bands)	
	 $(\text{or } Ar-\underset{\underset{O}{\|}}{C}-)_2O$	1735-1715(m/s((sym)		
(iii): Cyclic		Ring strain raises band to higher frequencies (up to 1850 and 1790 cm^{-1}). Conjugation does not reduce the frequency considerably	1300-1175(s) 950-910(s)	

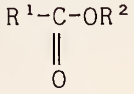
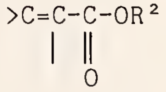
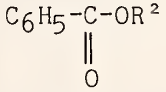
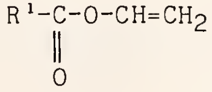
Organic Oxygen Compounds (Continue)

		Wavenumbers (cm^{-1})				
Family	General Formula	>C=O stretch	>C-O stretch	-O-H stretch	-O-H bend	Notes
Carboxylic acids	 $\mathrm{R{-}\underset{\underset{O}{\Vert}}{C}{-}OH}$	1760-1680(s)	1320-1210(m)	3300-2500(s)		Internal hydrogen bonding reduces the frequency of the >C=O (stretch) frequency (down to 1665 cm^{-1}). α- Halogen substituent increases the frequency by 10-20 cm^{-1}.
(i): monomer, saturated	 $\mathrm{R{-}\underset{\underset{O}{\Vert}}{C}{-}OH}$	~1760(s)	~1420	3550(s)	~1250(m/s)	
(ii): monomer, aromatic	 $\mathrm{Ar{-}\underset{\underset{O}{\Vert}}{C}{-}OH}$	1730-1710	~1400	3500(s)	~1250(m/s)	
(iii): dimer, saturated	 R=alkyl	1720-1706(s)	1315-1280(m) (sometimes doublet)	3300-2500(s, broad)	900-860(m, broad)(out-of-plane)	
(iv): dimer, α,β-unsaturated (or aromatic)	 R=alkenyl	1700-1680(s)	1315-1280(m) (sometimes doublet)	3300-2500(s, broad)	900-860(m, broad)(out-of-plane)	

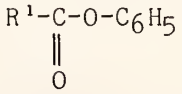
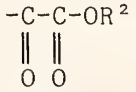
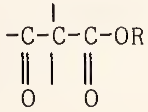
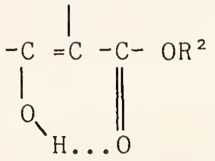
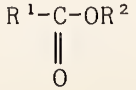
Organic Oxygen Compounds (Continued)

Family	General Formula	Wavenumbers (cm^{-1}) >C=O stretch	>C-O stretch	Notes
Carboxylic acids (cont.)				
(v): salt	 $R-\overset{\overset{\displaystyle O}{\|}}{C}-O^-$	1610-1550(s) asym. CO_2^- ~1400(s) sym. CO_2^-		
Cyanates	R-C≡N→O			See Organic Nitrogen Compounds.
Epoxides				~1250(s)(ring breathing, symm.) 950-810(s)(asym.) 840-810(s)(C-H bend) 3050-2990(m/s) (C-H stretch).

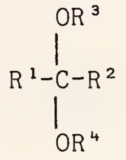
Organic Oxygen Compounds (Continued)

Family	General Formula	Wavenumbers (cm^{-1})		Notes
		$>C=O$ stretch	$>C-O$ stretch	
Esters	 $R^1\text{-}\underset{\underset{O}{\Vert}}{C}\text{-}OR^2$			
a) saturated, aliphatic	R^1,R^2=alkyl	1750-1735(s) α-halogen substitution results in an increase in frequency (up to 30 cm^{-1})	1210-1163(s) [acetates only: 1240(s)]	(O-C-C) 1064-1031(s)(1° alcohol) ~1100(s)(2° alcohol).
b) formates	R^1=H, R^2=alkyl	1730-1715(s)	~1180(s), ~1160(s)	
c) α,β-unsaturated	 $>C=\underset{\vert}{C}\text{-}\underset{\underset{O}{\Vert}}{C}\text{-}OR^2$ R^2=alkyl	1730-1715(s)	1300-1250(s) 1200-1050(s)	
d) benzoate	 $C_6H_5\text{-}\underset{\underset{O}{\Vert}}{C}\text{-}OR^2$ R^2=alkyl	1730-1715(s)	1310-1250(s) 1180-1100(s)	
e) vinyl	 $R^1\text{-}\underset{\underset{O}{\Vert}}{C}\text{-}O\text{-}CH=CH_2$ R^1=alkyl	1775-1755(s)	1300-1250(s) ~1210(vs)	

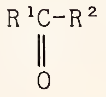
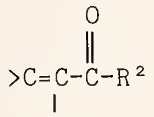
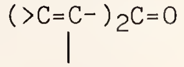
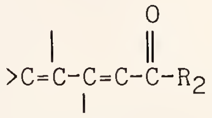
Organic Oxygen Compounds (Continued)

Family	General Formula	Wavenumbers (cm^{-1})		Notes
		>C=O stretch	>C-O stretch	
Esters (cont.)				
f) phenyl	 $R^1-\underset{\underset{O}{\|}}{C}-O-C_6H_5$ R^1=alkyl	~1770(s)	1300-1200(s) 1190-1140(s)	
g) α-keto	 $-\underset{\underset{O}{\|}}{C}-\underset{\underset{O}{\|}}{C}-OR^2$ R^2=alkyl	1775-1740(s)	1300-1050(s) (two peaks)	
h) β-ketoesters	 $-\underset{\underset{O}{\|}}{C}-\overset{\vert}{\underset{\vert}{C}}-\underset{\underset{O}{\|}}{C}-OR^2$ R^2=alkyl	~1735(s) ~1650(s) (due to enolization) 	1300-1050(s) (two peaks)	
i) aryl benzoates	 $R^1-\underset{\underset{O}{\|}}{C}-OR^2$ R^1,R^2=aryl	~1735(s)	1300-1050(s) (two peaks)	

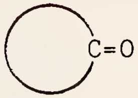
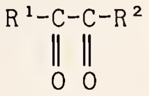
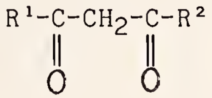
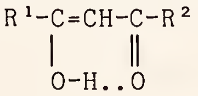
Organic Oxygen Compounds (Continued)

Family	General Formula	Wavenumbers (cm^{-1})		Notes
		>C-O-C< stretch asymmetrical	>C-O-C< stretch symmetrical	
Ethers	R^1-O-R^2			
a) aliphatic	R^1,R^2=alkyl	1150-1085(s) branching off on the carbons adjacent to oxygen creates splitting	very hard to trace	
b) aryl alkyl	R^1=alkyl R^2=aryl	1275-1200(s) (high due to resonance)	1075-1020(s)	
c) vinyl	R^1=vinyl R^2=aryl	1225-1200(s) (high due to resonance)	1075-1020(s)	1660-1610(m)(>C=CC) ~1000(m),909(m) (>C=C-H)(wagging).
Imides	$(R-C=O)_2N$			See Organic Nitrogen Compounds.
Isocyanates	R-N=C=O			See Organic Nitrogen Compounds.
Ketals	 $R^1-\underset{OR^4}{\overset{OR^3}{C}}-R^2$	1190-1160(s) 1195-1125(s) 1098-1063(s) 1055-1035(s)		
Ketenes	>C=C=O			~2150(s)(>C=C=O).

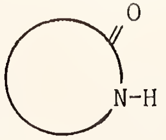
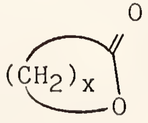
Organic Oxygen Compounds (Continued)

Family	General Formula	Wavenumbers (cm^{-1}) >C=O stretch	Wavenumbers (cm^{-1}) >C=C< stretch	Notes
Ketones	 $R^1\underset{\underset{O}{\|}}{C}-R^2$			>C=O overtone ~3400(w). Solid samples or solutions decrease >C=O stretch (10-20 cm^{-1}) α-Halogenation increases >C=O stretch (0-25 cm^{-1}) >C-H stretch is very weak (3100-2900 cm^{-1}).
a) aliphatic, saturated	R^1,R^2=alkyl	1720-1710(s)		
b) α,β-unsaturated	 $>C=\underset{|}{C}-\overset{\overset{O}{\|}}{C}-R^2$ R^2=alkyl	~1690(s)(s-cis) ~1675(s)(s-trans)	1650-1600(m)	
c) α,β-α¹,β¹-unsaturated	 $(>C=\underset{|}{C}-)_2C=O$	~1665(s)	~1640(m)	
d) α,β,γ,δ-unsaturated	 $>\overset{|}{C}=\underset{|}{C}-C=C-\overset{\overset{O}{\|}}{C}-R_2$ R_2=alkyl	~1665(s)	~1640(m)	
e) aryl	R^1=aryl R^2=alkyl	~1690(s)	~1600,1500(m/s) (aromatic)	
f) diaryl	R^1,R^2=aryl	~1665(s)	~1600,1500(m/s) (aromatic)	

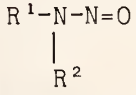
Organic Oxygen Compounds (Continued)

Family	General Formula	Wavenumbers (cm^{-1})		Notes
		>C=O stretch	>C=C< stretch	
Ketones (cont.)				
g) cyclic		3-membered: 1850(s) 4-membered: 1780(s) 5-membered: 1745(s) 6-membered: 1715(s) larger than 6-membered: 1705(s)		
h) α-keto (s-trans)	 $R^1-\underset{O}{\underset{\Vert}{C}}-\underset{O}{\underset{\Vert}{C}}-R^2$	~1720(s)(aliphatic) ~1680(s)(aromatic)		
i) β-keto	 $R^1-\underset{O}{\underset{\Vert}{C}}-CH_2-\underset{O}{\underset{\Vert}{C}}-R^2$	~1720(s) (two bands)	1640-1580(m,broad) due to enol from  $R^1-\underset{O-H}{\underset{\vert}{C}}=CH-\underset{..O}{\underset{\Vert}{C}}-R^2$	Show a shallow broad -OH band (enol form) at 3000-2700 cm^{-1})

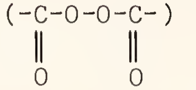
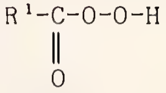
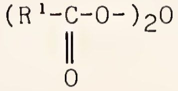
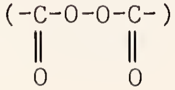
Organic Oxygen Compounds (Continued)

Family	General Formula	Wavenumbers (cm^{-1})			Notes
		>C=O stretch	>C=C< stretch	>C-O stretch	
Lactams					See Organic Nitrogen Compounds.
Lactones					
(i): saturated					
a) δ-	x = 4	~1735(s)		1300-1050(s,two peaks)	
b) γ-	x = 3	~1770(s)		1300-1050(s,two peaks)	
c) β-	x = 2	~1840(s)		1300-1050(s,two peaks)	
(ii): unsaturated, α- to the carbonyl (>C=O)	x = 4 x = 3	~1720(s) ~1750(s) (doublet 1785-1755 cm^{-1} when α-hydrogen present)		1300-1050(s,two peaks) 1300-1050(s,two peaks)	
(iii): unsaturated, α- to the oxygen	x = 4	~1760(s)	~1685(s)	1300-1050(s,two peaks)	
	x = 3	~1790(s)	~1660(s)	1300-1050(s,two peaks)	
(iv): unsaturated, α- to the carbonyl and α- to the oxygen	x = 4 (α-Pyrone; coumarin)	1775-1715(s,doublet)	1650-1620(s) 1570-1540(s)	1300-1050(s,two peaks)	

Organic Oxygen Compounds (Continued)

Family	General Formula	Wavenumbers (cm^{-1})			Notes
		>C=O stretch	>C=C< stretch	>C-O stretch	
Nitramines					See Organic Nitrogen Compounds.
Nitrates	$R-NO_3$				See Organic Nitrogen Compounds.
Nitro Compounds	$R-NO_2$				See Organic Nitrogen Compounds.
Nitrosamines					See Organic Nitrogen Compounds.
Nitrosocompounds	 $R^1-\underset{R^2}{\underset{\vert}{N}}-N=O$				See Organic Nitrogen Compounds.

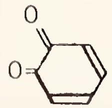
Organic Oxygen Compounds (Continued)

Family	General Formula	Wavenumbers (cm^{-1})				Notes
		>C-O stretch	-O-H stretch	>C=O stretch	-O-H bend	
Peroxides	$R^1\text{-O-O-}R^2$	-C-C-O-		 $(\text{-}\underset{\overset{\|}{O}}{C}\text{-O-O-}\underset{\overset{\|}{O}}{C}\text{-})$		
(i): aliphatic	R^1, R^2=alkyl	890-820(vw)				
(ii): aromatic	R^1, R^2=aryl	~1000(vw)				
(iii): acyl, aliphatic	R^1, R^2=acyl (aliphatic)	890-820(vw)		1820-1810(s) 1800-1780(s)		
(iv): acyl, aromatic	R^1, R^2=acyl (aromatic)	~1000(vw)		1805-1780(s) 1785-1755(s)		
Peroxyacids	 $R^1\text{-}\underset{\overset{\|}{O}}{C}\text{-O-O-H}$	~1260(s)	3300-3250(s, not as broad as in R-COOH)	1745-1735(s) (doublet)	~1400(m)	~850 cm^{-1}(m,-O-O- stretch).
Peroxyacids, anhydride	 $(R^1\text{-}\underset{\overset{\|}{O}}{C}\text{-O-})_2O$	 $(\text{-}\underset{\overset{\|}{O}}{C}\text{-O-O-}\underset{\overset{\|}{O}}{C}\text{-})$				
(i): alkyl	R^1=alkyl	1815(s), 1790(s)				
(ii): aryl	R^1=aryl	1790(s), 1770(s)				

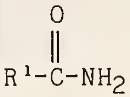
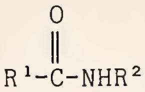
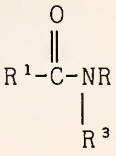
Organic Oxygen Compounds (Continued)

Family	General Formula	Wavenumbers (cm^{-1})			Notes
		>C-O stretch	-O-H stretch	-O-H bend	
Phenols	Ar-OH Ar=aryl	~1230(m)	~3610(m,sharp) (in $CHCl_3$ or CCl_4 solution) ~3100(m,broad) (in neat samples)	1410-1310(m, broad) (in-plane) ~650(m)(out-of-plane)	
Phosphates	$(R^1O)_3P=O$				See Organic Phosphorus Compounds.
Phosphinates	$(R^1O)P(=O)H_2$				See Organic Phosphorus Compounds.
Phosphine oxides	$R^1_2P=O$				See Organic Phosphorus Compounds.
Phosphonates	$(R^1O)_2P(=O)H$				See Organic Phosphorus Compounds.
Phosphorus acids	$R^1_2P(=O)OH$				See Organic Phosphorus Compounds.
Pyrophosphates	$(R^1-P=O)_2O$				See Organic Phosphorus Compounds.

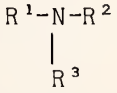
Organic Oxygen Compounds (Continued)

Family	General Formula	Wavenumbers (cm^{-1})		Notes
		$>C=O$ stretch	$>C=C<$ stretch	
Quinones				
a) 1,2-		~1675(s)	~1600(s)	
b) 1,4-		~1675(s)	~1600(s)	
Silicon compounds				See Organic Silicon Compounds
Sulfates				See Organic Sulfur Compounds
Sulfonamides				See Organic Sulfur Compounds
Sulfonates				See Organic Sulfur Compounds
Sulfones				See Organic Sulfur Compounds
Sulfonyl chlorides				See Organic Halogen Compounds
Sulfoxides				See Organic Sulfur Compounds

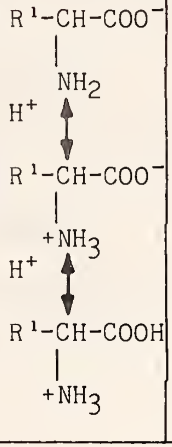
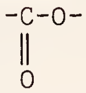
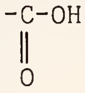
Organic Nitrogen Compounds

		Wavenumbers (cm^{-1})			
Family	General Formula	C-N	N-H	Others	Notes
Amides					
Primary	 $R^1\text{-}\overset{O}{\overset{\|}{C}}\text{-}NH_2$	1400(s)(stretch)	3520(m)(stretch) 3400(m)(stretch) 1655-1620(m)(bend) 860-666(m,broad) (wagging)	>C=O (1650)(s,solid state) (1690)(s, solution)	Lowering of N-H stretch occurs in solid samples due to hydrogen bonding; higher values arise in dilute samples.
Secondary	 $R^1\text{-}\overset{O}{\overset{\|}{C}}\text{-}NHR^2$	1400(s)(stretch)	3500-3400(w) (stretch) 1570-1515(w) (bend) 860-666(m, broad) (wagging)	>C=O (1700-1670)(s,solution) (1680-1630)(s,solid state) band due to interaction of N-H (bend) and (C-N)(stretch) (~1250)(m, broad)	Lowering of N-H stretch occurs in solid samples due to hydrogen bonding; higher values arise in dilute samples.
Tertiary	 $R^1\text{-}\overset{O}{\overset{\|}{C}}\text{-}\underset{R^3}{\underset{\|}{N}}R^2$	1400(s)(stretch)	---	>C=O (1680-1630)(s); higher values are obtained with electron attracting groups attached to the nitrogen	
Amines					
Primary	$R^1\text{-}NH_2$	1250-1020(m) (for non-conjugated amines) 1342-1266(s) (for aromatic amines)	3500(w)(stretch) 3400(w)(stretch) 1650-1580(m) (scissoring) 909-666(m) (wagging)		

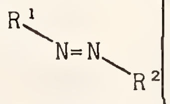
Organic Nitrogen Compounds (Continued)

Family	General Formula	Wavenumbers (cm^{-1})			Notes
		C-N	N-H	Others	
Amines (continued)					
Secondary	R^1-NHR^2	1250-1020(m) (for non-conjugated amines) 1342-1266(s) (for aromatic amines)	3350-3310(w) (stretch) 1515(vw) (scissoring) 909-666(m) (wagging)		
Tertiary	 $R^1-\underset{\displaystyle R^3}{\underset{\vert}{N}}-R^2$	1250-1020(m) (for non-conjugated amines) 1342-1266(s) (for aromatic amines)	---		
Amine salts					
Primary	$R\overset{+}{N}H_3X^-$		3000-2800(s) 2800-2200(m) (series of peaks) 1600-1575(m) 1550-1504(m)		

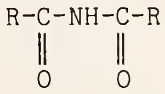
Organic Nitrogen Compounds (Continued)

Family	General Formula	Wavenumbers (cm^{-1})			Notes
		C-N	N-H	Others	
Amine salts (continued)					
Secondary	$R_2\overset{+}{N}H_2X^-$		3000-2700(s) 2700-2250(m) (series of peaks) 2000(w) 1620-1560(m)		
Tertiary	$R_3\overset{+}{N}HX^-$		2700-2250(s)		
Quaternary	$R_4\overset{+}{N}X^-$		---		
Amino acids (alpha)	 $\underset{NH_2}{\underset{\vert}{R^1\text{-CH-COO}^-}} \overset{H^+}{\updownarrow} \underset{{}^+NH_3}{\underset{\vert}{R^1\text{-CH-COO}^-}} \overset{H^+}{\updownarrow} \underset{{}^+NH_3}{\underset{\vert}{R^1\text{-CH-COOH}}}$		3100-2600(s, broad) 2222-2000(s, broad, overtone) 1610(w)(bend) 1550-1485(s) (bend)	 $-\underset{\underset{O}{\Vert}}{C}-O-$ (1600-1590)(s), (1400)(w)  $-\underset{\underset{O}{\Vert}}{C}-OH$ (1755-1730)(s)	

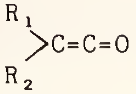
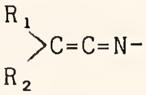
Organic Nitrogen Compounds (Continued)

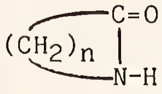
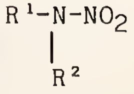
		Wavenumbers (cm^{-1})			
Family	General Formula	-N=N-	N-H	Others	>N-O stretch
Ammonium ion	NH_4^+		3300-3040(s) 2000-1709(m) 1429(s)		
Azides	$R-N_3$			2140(s)(asym stretch, N_3) 1295(s)(sym stretch, N_3)	
Azocompounds	 (trans)	forbidden in IR but allowed in Raman spectrum (1576)(w); peak is lowered down to 1429 cm^{-1} in unsymmetrical p-electron donating substituted azobenzenes			
Azoxy Compounds	$R-N=N\rightarrow O$				(1310-1250)(s)

Organic Nitrogen Compounds (Continued)

		Wavenumbers (cm^{-1})		
Family	General Formula	C-N multiple bond	Cumulated (-X=C=Y) double bond	Notes
Cyanocompounds (nitriles)	$R-C\equiv N$	2260-2240(w) (aliphatic) 2240-2220(m) (aromatic, conjugated)		electronegative elements α- to the $C\equiv N$ group reduce the intensity of the absorption
Diazonium salts	$R-\underset{+}{N}\equiv N$			2280 - 2240 (m) $(-\underset{+}{N}\equiv N)$
Imides	 $R-\underset{O}{\underset{\Vert}{C}}-NH-\underset{O}{\underset{\Vert}{C}}-R$			(1710,1700) (>C=O six-membered ring) (1770,1700) (>C=) five-membered ring)
Isocyanates	$R-N=C=O$		2273-2000(s)(broad)(asym.) 1400-1350(w)(sym.)	
Isocyanides (isonitriles)	$R-N\equiv C$	2400-2300(w) (aliphatic) 2300-2200(w) (aromatic)		
Isonitriles				See isocyanides
Isothiocyanates	$R-N=C=S$		2140-2000(s)(stretch)	

Organic Nitrogen Compounds (Continued)

Family	General Formula	Wavenumbers (cm^{-1}) C-N multiple bond	Cumulated (-X=C=Y) double bond	Notes
Ketene	 $R_1R_2>C=C=O$		2150(stretch); 1120	
Ketenimine	 $R_1R_2>C=C=N-$		2000(stretch)	

Family	General Formula	>C-N	>N-O (asymmetric)	>N-O (symmetric)	Others	Notes
Lactams					>C=O (s) (stretch) 1670 (six membered ring) 1700 (five membered ring) 1745 (four membered ring) N-H (out-of-plane wagging)(800-700)(broad)	Add ~15 cm^{-1} to every frequency in case of a >C=C< in conjugation; amide group is forced into the cis-conformation in rings of medium size.
Nitramines	 $R^1-N(R^2)-NO_2$			1620-1580(s) (asym) 1320-1290(s) (asym)		

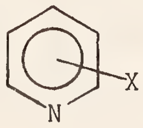
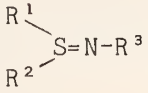
Organic Nitrogen Compounds (Continued)

Family	General Formula	>C-N	>N-O (asymmetric)	>N-O (symmetric)	Others	Notes
Nitrates	$RO-NO_2$				-N=O 1660-1625(s) (asym) 1300-1225(s) (asym) >N-O 870-833(s) (stretch) 763-690(s) (bend)	
Nitriles (cyano-compounds)	R-C≡N					See cyanocompounds
Nitrites	RO-N=O				-N=O stretch 1680-1650(vs)(trans) 1625-1610(vs)(cis) >N-O stretch 850-750(vs)	

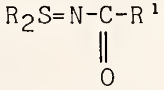
Organic Nitrogen Compounds (Continued)

Family	General Formula	>C-N	-N=O (stretch)	>N-O (stretch)	Others	Notes
Nitrocompounds	$R-NO_2$					
Aliphatic	R=alkyl	870	1615-1540(vs) (asym) 1390-1320(vs) (sym)	1390-1320(vs)	CNO bend:~610(m)	
Aromatic	R=aryl	(difficult to assign)	1548-1508(s) (asym) 1356-1340(s) (sym) (aromatics absorb at lower frequencies than aliphatics)	1356-1340(s)		
Nitrosamines	R_1 >N-N=O R_2				>N-O stretch (1520-1500)(s)(vapor) (1500-1480)(s)(neat) N-N(1150-925)(m)	

Organic Nitrogen Compounds (Continued)

Family	General Formula	Wavenumbers (cm^{-1})				Notes
		C-N	N-O (asymmetric)	N-O (symmetric)	Others	
Nitroso-compounds	R-N=O				N=O stretch 1585-1539(s)(3°, aliphatic) 1511-1495(s)(3°, aromatic)	1° and 2°C - nitroso-compounds are unstable and rearrange or dimerize.
Pyridines					N-H (3075,3030)(s) C-H (out-of-plane) (920-720)(s) (2000-1650)(overtone) C=C ring stretch (1600,1570,1500,1435)	Characteristic substitution pattern: α-substitution:(795-780), (755-745) β-substitution:(920-880), (840-770), 720.
Sulfilimines	 $R^1R^2S{=}N{-}R^3$					See Organic Sulfur Compounds.
Sulfonamides	R-SO_2NH_2					See Organic Sulfur Compounds.
Thiocyanates	R-SC≡N					See Organic Sulfur Compounds.

Organic Sulfur Compounds

		Wave Numbers (in cm^{-1})				
Family	General Formula	>S=0 (Asymmetric)	>S=0 (Symmetric)	>S=N-	Others	Comments
Disulfides	R^1-S-S-R^2				-S-S- (<500)(w)	
Mercaptans	R-S-H				-S-H (2600-2500)(w)	Only popular frequency around that region; lowering of 50-150 cm^{-1} due to hydrogen-bonding.
Sulfates	$(RO)_2S(=O)_2$	1415-1380(s)	1200-1185(s)			
Sulfides	R^1-S-R^2				R-S- (700-600)(w)	
Sulfilimines	R_2S=N-R^1					
(i) N-acyl	 $R_2S{=}N{-}\underset{\underset{O}{\parallel}}{C}{-}R^1$			800(s)	>C=0 (1625-1600)(s)	
(ii) N-alkyl	R_2S=N-R^1			987-935(s)		
(iii) N-sulfonyl	R_2S=N-SO_2R^1	1280-1200(s) 1095-1030(s)	1160-1135(s)	980-901(s)		

Organic Sulfur Compounds (Continued)

Family	General Formula	Wave Numbers (in cm^{-1}) >S=O (Asymmetric)	>S=O (Symmetric)	>S=N-	Others	Comments
Sulfonamides	$R-SO_2NH_2$	1370-1335(s)	1170-1155(s)		>N-H (1°) (3390-3330)(s) (3300-3247)(s) >N-H (2°) (3265)(s)	Solid phase spectra lower wave numbers by 10-20 cm^{-1}.
Sulfonates	$R^1-SO_2-OR^2$	1372-1335(s)	1195-1168(s)			Electron donating groups on the aryl group cause higher frequency absorption.
Sulfones	$R^1-SO_2-R^2$	1350-1300(s)	1160-1120(s)			Hydrogen bonding reduces the frequency absorption slightly.
Sulfonic acids (anhydrous)	$R-SO_3H$	1350-1342(s)	1165-1150(s)			Hydrated sulfonic acids show broad bands 1230-1150 cm^{-1}.
Sulfonic acids, salts	$R-SO_3^-$	ca. 1175(s)	ca. 1055(s)			
Sulfonyl chlorides	$R-SO_2Cl$	1410-1380(s)	1204-1177(s)			

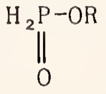
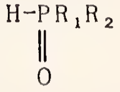
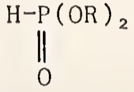
Organic Sulfur Compounds (Continued)

		Wave Numbers (in cm^{-1})				
Family	General Formula	>S=O (Asymmetric)	>S=O (Symmetric)	>S=N-	Others	Comments
Sulfoxides	$R_2S\rightarrow O$				$>S\rightarrow O$ (1070-1030)(s)	Hydrogen bonding reduces the frequency absorption slightly; electronegative substituents increase the $>S\rightarrow O$ frequency
Thiocarbonyls (not trimerized into cyclic sulfides)	$R^1-\underset{\overset{\|}{S}}{C}-R^2(H)$				$>C=S$ (1250-1020)(s)	
Thiocyanates	$R-S-C\equiv N$				$-C\equiv N$ (2175-2140)(s); higher values for aryl thiocyanates	
Thiol esters	$R^1-\underset{\overset{\|}{O}}{C}-SR^2$				$-\underset{O}{C}-$ (1690)(s) (S-alkyl thioester) (1710)(s) (S-aryl	The (+)mesomeric effect of sulfur is larger than its (-) Inductive effect
Thiols	R-SH					See Mercaptans
Thiophenols	Ar-SH				$-S-H$ (2600-2500)(w)	

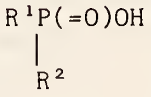
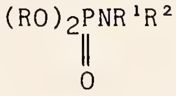
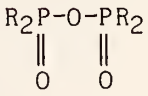
Organic Silicon Compounds

Family	General Formula	Wavenumbers (cm^{-1})					
		>Si-H stretch	>Si-H bend	>C-Si< stretch	>C-H bend	>Si-O- stretch	-OH stretch
Silanes	R_xSiH_y						
a) Monoalkyl	$R-SiH_3$	2130-2100(s)	890-860(s)	890-690(s)	~1260(s)(rocking)		
b) Dialkyl	R_2SiH_2	~2135(s)	890-860(s)	820-800(s)	~1260(s)(rocking)		
c) Trialkyl	R_3SiH	2360-2150(s)	890-860(s)	~840(s) ~755(s)	~1260(s)(rocking)		
d) Tetraalkyl	R_4Si			890-690(s)	~1260(s)(rocking)		
e) Alkoxy	$R^1_xSi(OR^2)_y$			890-690(s)	~1260(s)(rocking)	1090-1080(s) (doublet)	
Siloxanes	>Si-O-Si<						
a) disiloxanes						1110-1000(s) (Si-O-Si) ~1053(s)	
b) cyclic trimer						~1020(s)	
c) cyclic tetramer						~1082(s)	
Hydroxysilanes	$R_xSi(OH)_y$						~3680(s) (Confirmed by band at 870-820 cm^{-1})

Organic Phosphorus Compounds

		Wavenumbers (cm^{-1})				
Family	General Formula	→P=O stretch	>P-H stretch	>P-O-C< stretch	-OH stretch	Notes
Phosphates	$O{=}P(OR)_3$	1300-1100(s) (doublet)		~1050(s)(alkyl) 950-875(s)(aryl)		>P=O stretch can shift up to 65 cm^{-1} due to change in solvent.
a) alkyl		1285-1260(s) (doublet)				
b) aryl		1315-1290(s) (doublet)				
Phosphinates	 $\mathrm{H_2\underset{\underset{O}{\|}}{P}{-}OR}$	1220~1180(s)	~2380(m) ~2340(m) (sharp)	~1050(s)(alkyl) 950-875(s)(aryl)		
Phosphine oxides	 $\mathrm{H{-}\underset{\underset{O}{\|}}{P}R_1R_2}$					
a) alkyl		1185-1150(s)	2340-2280(m)			
b) aryl		1145-1095(s)	2340-2280(m)			
Phosphonates	 $\mathrm{H{-}\underset{\underset{O}{\|}}{P}(OR)_2}$	1265-1230(s)	2450-2420(m)	~1050(s)(alkyl) 950-875(s)(aryl)		

Organic Phosphorus Compounds (Continued)

Family	General Formula	Wavenumbers (cm^{-1}) →P=O stretch	>P-H stretch	>P-O-C stretch	-OH stretch	Notes
Phosphorus acids	 $\underset{R^2}{R^1P}(=O)OH$	1240-1180(vs)			2700-2200(s, broad)(assoc.)	
Phosphorus amides	 $(RO)_2\underset{\underset{O}{\|}}{P}NR^1R^2$	1275-1200(s)				
Pyrophosphates	 $R_2\underset{\underset{O}{\|}}{P}-O-\underset{\underset{O}{\|}}{P}R_2$	1310-1200(s) (single band)				

Organic Halogen Compounds

Family	General Formula	Wavenumbers (cm^{-1}) >C-X stretch	>CX_2 stretch	-CH_3 stretch	=C-X stretch
Fluorides	X = F	1120-1010	1350-1200(asym.) 1200-1080(sym.)	1350-1200(asym.) 1200-1080(sym.)	1230-1100
Chlorides	X = Cl	830-500 1510-1480 (overtone)	845-795(asym.) ~620(sym.)		
Bromides	X = Br	667-290			
Iodides	X = I	500-200			

V. Tables for Nuclear Magnetic Resonance Spectroscopy

Tables for Nuclear Magnetic Resonance Spectroscopy

The following tables provide valuable information on NMR spectroscopy. These tables are by no means meant to cover the whole field of nuclear magnetic resonance but should be more than adequate for the routine determination of organic compound identity or structure [1,8].

REFERENCES:

[1] Silverstein, R.M., Bassler, G.C., Morrill, T.C., Spectrometric Identification of Organic Chemistry, 4th edition, John Wiley, New York, 1981.

[2] Williams, D.H., Fleming, I., Spectroscopy Methods in Organic Chemistry, 3rd edition, McGraw-Hill, London, 1980.

[3] Lambert, J.B., Shurvell, H.F., Verbit, L., Cooks, R.G., Stout, G.H., Organic Structural Analysis, MacMillan Pub. Co., New York, 1976.

[4] Abraham, R.J., Loftus, P., Proton and Carbon-13 NMR Spectroscopy, Heyden, London, 1980.

[5] Bruno, T.J., Tables for Instrumental Methods of Chemical Analysis, Center for Chemical Engineering, Chemical Engineering Science Division, Boulder, 1985.

[6] Jackman, L.M., Sternell, S., Applications of NMR Spectroscopy in Organic Chemistry, 2nd edition, Pergamon Press, New York, 1969.

[7] Varian Associates, High Resolution NMR Spectra Catalogue, Vol. 1, 1962; Vol. 2, 1963.

[8] Bovey, F.A., NMR Spectrometry, Academic Press, New York, 1969.

[9] Tsujihara, R., Furukawa, N., Oae, S., Bull. of Chem. Soc. Japan, 43, 2153, 1970.

Magnetic Properties of Some Nuclei [1,2]

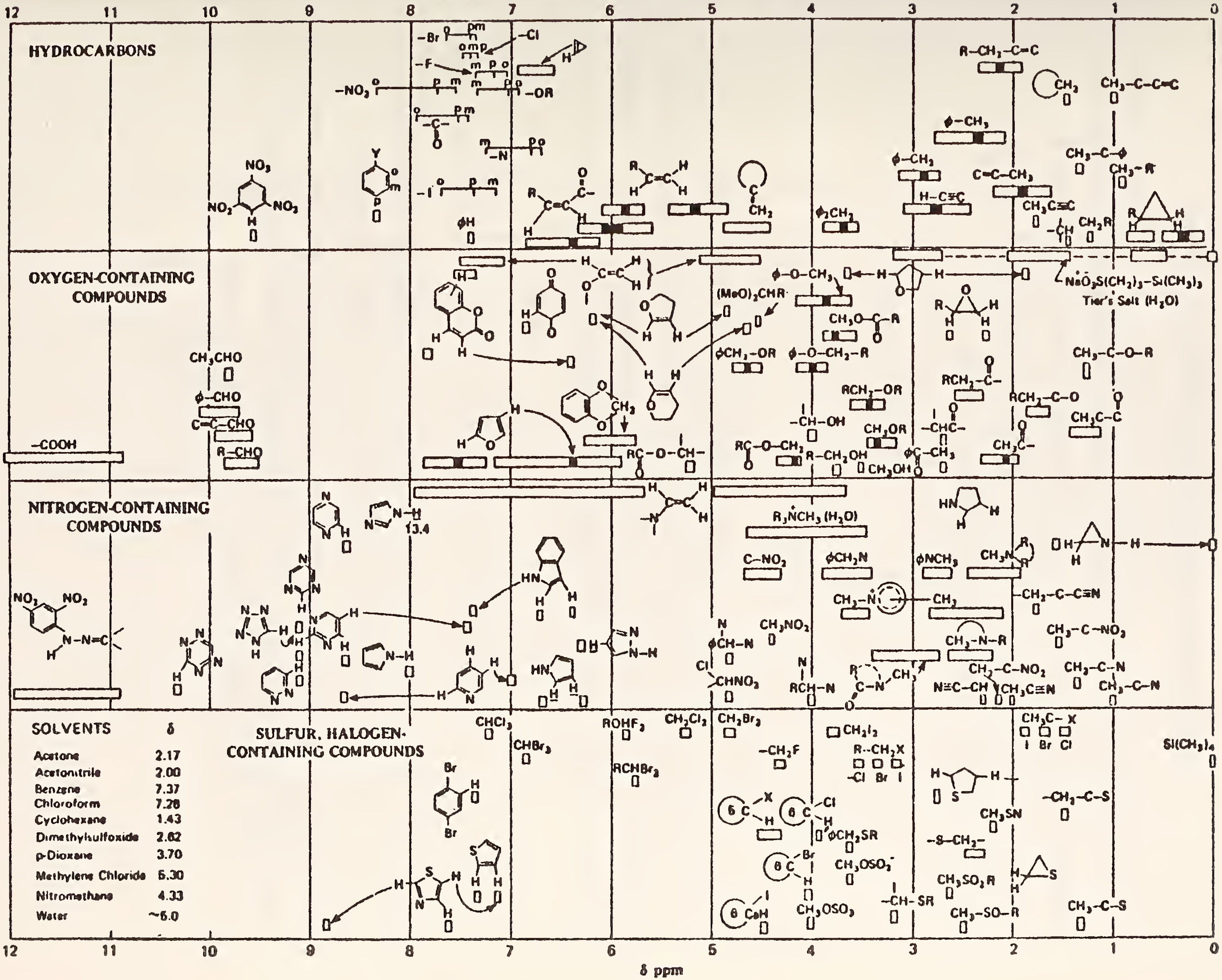
Element	Isotope	Abundance (%)	Spin Number (magnetic moment)	Resonance Frequency at 4.2276 Wb/m^2 (Hz)
Hydrogen	^{1}H	99.984	1/2	180.0
	^{2}H	0.016	1	27.6
				192.0
	^{3}H	$<10^{-3}$	1/2	19.34
Boron	^{10}B	18.83	3	57.75
	^{11}B	81.17	3/2	
Carbon	^{12}C	98.9	0	----
	^{13}C	1.1	1/2	45.3
Nitrogen	^{14}N	99.64	1	13.0
	^{15}N	0.36	1/2	18.24
Oxygen	^{16}O	99.76	0	----
	^{17}O	0.04	5/2	24.40
Fluorine	^{19}F	100	1/2	169.34
Silicon	^{28}Si	92.28	0	----
	^{29}Si	4.70	1/2	35.76
	^{30}Si	3.02	0	----
Phosphorus	^{31}P	100	1/2	72.87
Sulfur	^{32}S	95.06	0	----
	^{33}S	0.74	3/2	13.81
	^{34}S	4.2	0	----
Chlorine	^{35}Cl	75.4	3/2	17.64
	^{37}Cl	24.6	3/2	14.68
Bromine	^{79}Br	50.57	3/2	45.1
	^{81}Br	49.43	3/2	48.6
Iodine	^{127}I	100	5/2	36.0

REFERENCES:

[1.] Silverstein, R.M., Bassler, G.C., Morrill, T.C., Spectrometric Identification of Organic Compounds, 4th edition John Wiley, New York, 1981.

[1.] Streitwiesser, A, Heathcock, C.H., Introduction to Organic Chemistry, MacMillan, New York, 1985.

NMR Correlation Chart



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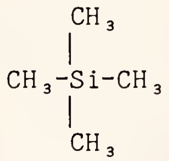
Proton NMR Absorptions of Major Chemical Families

The following tables give the region of the expected nuclear magnetic resonance absorbtions of major chemical families. These absorptions are reported in the dimensionless units of parts per million (ppm) versus the standard compound tetramethylsilane (TMS):



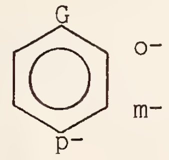
$$\begin{array}{c} CH_3 \\ | \\ CH_3\text{-}Si\text{-}CH_3 \\ | \\ CH_3 \end{array}$$

The use of this unit of measure makes the chemical shifts independent of the applied magnetic field strength or the radio frequency. For most proton NMR spectra, the protons in TMS are more shielded than almost all other protons. The chemical shift in this dimensionless unit system is then defined by:

$$\delta \equiv \frac{\nu_s - \nu_r}{\nu_r} \times 10^6 \qquad (V\ -1)$$

where ν_s and ν_r are the absorption frequencies of the sample proton and the reference (TMS) protons (twelve, magnetically equivalent), respectively. In these tables, the proton(s) in question are indicated by underscore. For more detail concerning these conventions, the reader is refered to the general references listed in the introduction of the tables for NMR.

Hydrocarbons

Family	δ of protons underlined	
Alkanes	$\underline{CH_3}$-R ~0.8 ppm -$\underline{CH_2}$-R ~1.1 ppm -$\underline{CH}$-R ~1.4 ppm (cyclopropane ~0.2 ppm)	
Alkenes	$\underline{CH_3}$ >C=C< ~1.6 ppm	$\underline{CH_3}$-C >C=C< ~1.0 ppm
	-$\underline{CH_2}$ >C=C< ~2.1 ppm	-$\underline{CH_2}$-C >C=C< ~1.4 ppm
	| -$\underline{CH}$ >C=C< ~2.5 ppm	| -$\underline{CH}$-C >C=C< ~1.8 ppm
	>C=C< $\underline{H}$ 4.2-6.2 ppm	
Alkynes	$\underline{CH_3}$-C≡C- ~1.7 ppm	$\underline{CH_3}$-C-C≡C- ~1.2 ppm
	-$\underline{CH_2}$-C≡C- ~2.2 ppm	-$\underline{CH_2}$-C-C≡C- ~1.5 ppm
	-$\underline{CH}$-C≡C- ~2.7 ppm	-$\underline{CH}$-C-C≡C- ~1.8 ppm
	R-C≡C-$\underline{H}$ ~2.4 ppm	
Aromatics	 Range: 8.5 -6.9 ppm	
	$\underline{G}$=Electron withdrawing (e.g., $-\underset{\underset{O}{\|}}{C}-$, -$NO_2$, -C≡N) o,p-closer to 8.5 ppm (more downfield)	$\underline{G}$=Electron donating (g., -NH_2, -OH, -OR, -R) o-p-closer to 7.3 ppm (more upfield)

Organic Oxygen Compounds

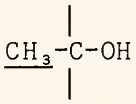
δ of protons underlined

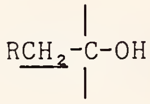
Alcohols

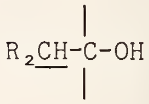
$\underline{CH_3}$-OH 3.2 ppm

$R\underline{CH_2}$-OH 3.4 ppm

$R_2\underline{CH}$-OH 3.6 ppm

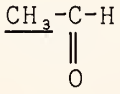

$\underline{CH_3}-\overset{|}{\underset{|}{C}}-OH$ 1.2 ppm

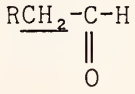

$R\underline{CH_2}-\overset{|}{\underset{|}{C}}-OH$ 1.5 ppm

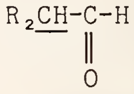

$R_2\underline{CH}-\overset{|}{\underset{|}{C}}-OH$ 1.8 ppm

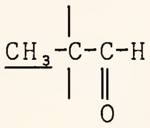
$R-\underline{O-H}$ (1-5 - depending on concentration)

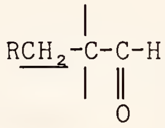
Aldehydes


$\underline{CH_3}-\underset{\underset{O}{\|}}{C}-H$ 2.2 ppm


$R\underline{CH_2}-\underset{\underset{O}{\|}}{C}-H$ 2.4 ppm


$R_2\underline{CH}-\underset{\underset{O}{\|}}{C}-H$ 2.5 ppm


$\underline{CH_3}-\overset{|}{\underset{|}{C}}-\underset{\underset{O}{\|}}{C}-H$ 1.1 ppm


$R\underline{CH_2}-\overset{|}{\underset{|}{C}}-\underset{\underset{O}{\|}}{C}-H$ 1.6 ppm

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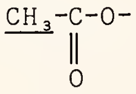
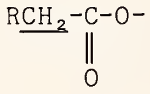
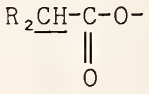
Amides

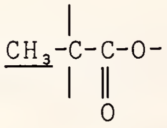
See Organic Nitrogen Compounds

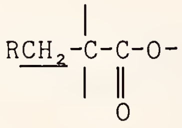
Anhydrides

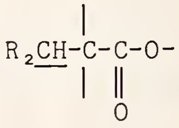

$\underline{CH_3}-\underset{\underset{O}{\|}}{C}-O-$ 1.8 ppm


$R\underline{CH_2}-\underset{\underset{O}{\|}}{C}-O-$ 2.1 ppm


$R_2\underline{CH}-\underset{\underset{O}{\|}}{C}-O-$ 2.3 ppm

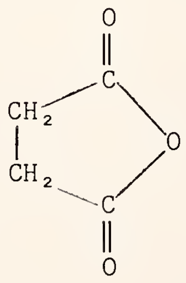

$\underline{CH_3}-\overset{|}{\underset{|}{C}}-\underset{\underset{O}{\|}}{C}-O-$ 1.2 ppm


$R\underline{CH_2}-\overset{|}{\underset{|}{C}}-\underset{\underset{O}{\|}}{C}-O-$ 1.8 ppm

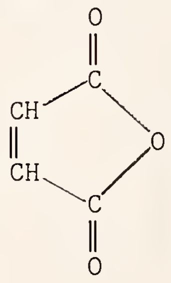

$R_2\underline{CH}-\overset{|}{\underset{|}{C}}-\underset{\underset{O}{\|}}{C}-O-$ 2.0 ppm

Cyclic

3.0 ppm



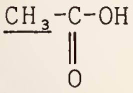
7.1 ppm

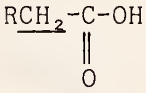


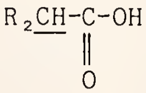
Organic Oxygen Compounds (cont.)

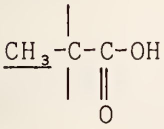
δ of protons underlined

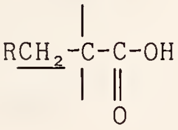
Carboxylic acids

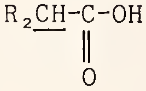

$\underline{\mathrm{CH_3}}-\underset{\underset{\mathrm{O}}{\|}}{\mathrm{C}}-\mathrm{OH}$ 2.1 ppm

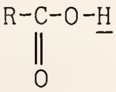

$\mathrm{R}\underline{\mathrm{CH_2}}-\underset{\underset{\mathrm{O}}{\|}}{\mathrm{C}}-\mathrm{OH}$ 2.3 ppm


$\mathrm{R_2}\underline{\mathrm{CH}}-\underset{\underset{\mathrm{O}}{\|}}{\mathrm{C}}-\mathrm{OH}$ 2.5 ppm


$\underline{\mathrm{CH_3}}-\overset{|}{\underset{|}{\mathrm{C}}}-\underset{\underset{\mathrm{O}}{\|}}{\mathrm{C}}-\mathrm{OH}$ 1.1 ppm


$\mathrm{R}\underline{\mathrm{CH_2}}-\overset{|}{\underset{|}{\mathrm{C}}}-\underset{\underset{\mathrm{O}}{\|}}{\mathrm{C}}-\mathrm{OH}$ 1.6 ppm


$\mathrm{R_2}\underline{\mathrm{CH}}-\underset{\underset{\mathrm{O}}{\|}}{\mathrm{C}}-\mathrm{OH}$ 2.0 ppm


$\mathrm{R}-\underset{\underset{\mathrm{O}}{\|}}{\mathrm{C}}-\mathrm{O}-\underline{\mathrm{H}}$ 11-12 ppm

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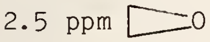
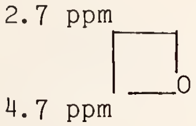
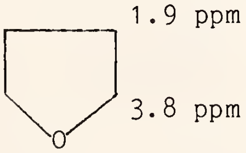
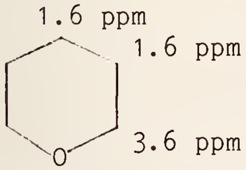
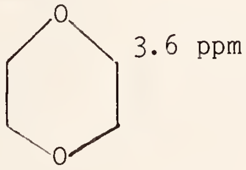
Cyclic Ethers

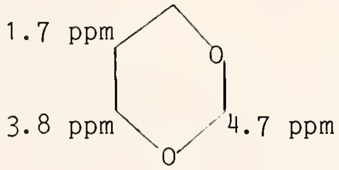


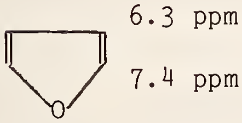


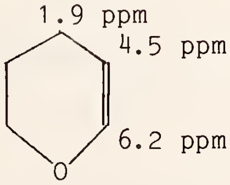










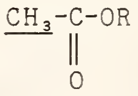


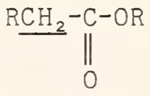
Epoxides
See Cyclic Ethers

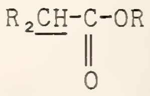
Organic Oxygen Compounds (cont.)

δ of protons underlined

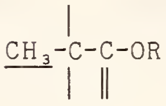
Esters

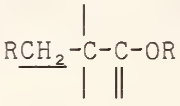

$\underline{CH_3}-\underset{\substack{\| \\ O}}{C}-OR$

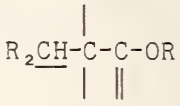

$R\underline{CH_2}-\underset{\substack{\| \\ O}}{C}-OR$

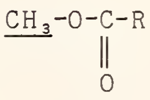

$R_2\underline{CH}-\underset{\substack{\| \\ O}}{C}-OR$

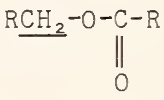
R = alkyl	1.9 ppm	2.1 ppm	2.3 ppm
R = aryl	2.0 ppm	2.2 ppm	2.4 ppm

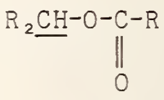

$\underline{CH_3}-\overset{|}{\underset{|}{C}}-\underset{\|}{C}-OR$ 1.1 ppm

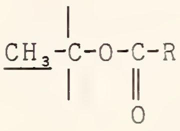

$R\underline{CH_2}-\overset{|}{\underset{|}{C}}-\underset{\|}{C}-OR$ 1.7 ppm

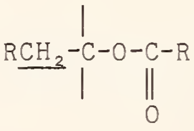

$R_2\underline{CH}-\overset{|}{\underset{|}{C}}-\underset{\|}{C}-OR$ 1.9 ppm

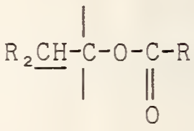

$\underline{CH_3}-O-\underset{\substack{\| \\ O}}{C}-R$ 3.6 ppm


$R\underline{CH_2}-O-\underset{\substack{\| \\ O}}{C}-R$ 4.1 ppm

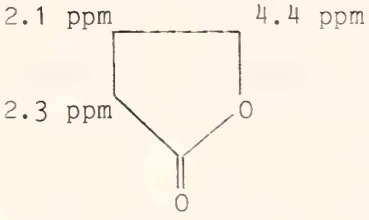

$R_2\underline{CH}-O-\underset{\substack{\| \\ O}}{C}-R$ 4.8 ppm

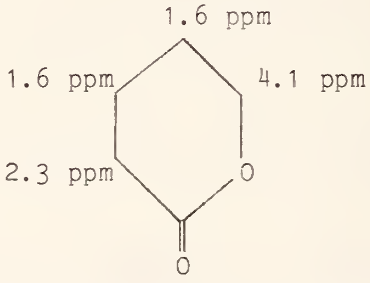

$\underline{CH_3}-\overset{|}{\underset{|}{C}}-O-\underset{\substack{\| \\ O}}{C}-R$ 1.3 ppm


$R\underline{CH_2}-\overset{|}{\underset{|}{C}}-O-\underset{\substack{\| \\ O}}{C}-R$ 1.6 ppm


$R_2\underline{CH}-\overset{|}{\underset{|}{C}}-O-\underset{\substack{\| \\ O}}{C}-R$ 1.8 ppm

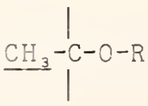
Cyclic

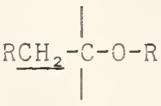


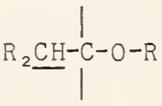


Ethers

$\underline{CH_3}-O-R$		$R\underline{CH_2}-O-R$	$R_2\underline{CH}-O-R$
R = alkyl	3.2 ppm	3.4 ppm	3.6 ppm
R = aryl	3.9 ppm	4.1 ppm	4.5 ppm


$\underline{CH_3}-\overset{|}{\underset{|}{C}}-O-R$


$R\underline{CH_2}-\overset{|}{\underset{|}{C}}-O-R$


$R_2\underline{CH}-\overset{|}{\underset{|}{C}}-O-R$

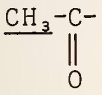
R = alkyl	1.2 ppm	1.5 ppm	1.8 ppm
R = aryl	1.3 ppm	1.6 ppm	2.0 ppm

Organic Oxygen Compounds (cont.)

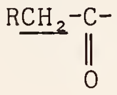
δ of protons underlined

Isocyanates
See Nitrogen Compounds

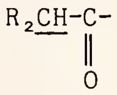
Ketones



$\underline{\mathrm{CH_3}}-\underset{\underset{\mathrm{O}}{\|}}{\mathrm{C}}-$

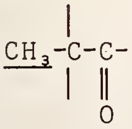


$\mathrm{R}\underline{\mathrm{CH_2}}-\underset{\underset{\mathrm{O}}{\|}}{\mathrm{C}}-$

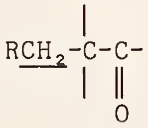


$\mathrm{R_2}\underline{\mathrm{CH}}-\underset{\underset{\mathrm{O}}{\|}}{\mathrm{C}}-$

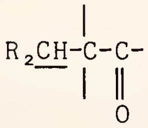
R = alkyl	1.9 ppm	2.1 ppm	2.3 ppm
R = aryl	2.4 ppm	2.7 ppm	3.4 ppm



$\underline{\mathrm{CH_3}}-\overset{|}{\underset{|}{\mathrm{C}}}-\underset{\underset{\mathrm{O}}{\|}}{\mathrm{C}}-$

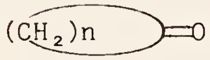


$\mathrm{R}\underline{\mathrm{CH_2}}-\overset{|}{\underset{|}{\mathrm{C}}}-\underset{\underset{\mathrm{O}}{\|}}{\mathrm{C}}-$



$\mathrm{R_2}\underline{\mathrm{CH}}-\overset{|}{\underset{|}{\mathrm{C}}}-\underset{\underset{\mathrm{O}}{\|}}{\mathrm{C}}-$

R = alkyl	1.1 ppm	1.6 ppm	2.0 ppm
R = aryl	1.2 ppm	1.6 ppm	1.9 ppm



α - hydrogens	2.0-2.3 ppm	(n>2)
	3.0 ppm	(n=2)
	1.7 ppm	(n=1)
β - hydrogens	1.9-1.5 ppm	

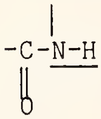
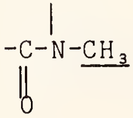
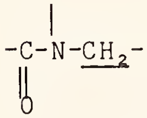
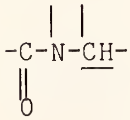
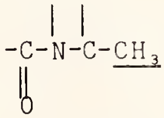
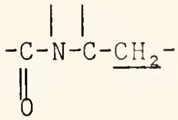
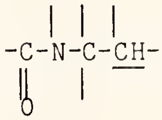
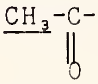
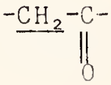
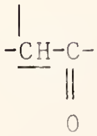
Lactones
See Esters, cyclic

Nitrocompounds
See Organic Nitrogen Compounds

Phenols
Ar-O-$\underline{\mathrm{H}}$ 9-10 ppm Ar = aryl

Organic Nitrogen Compounds

Amides

δ of proton(s) (underlined)	Primary R-C(=O)NH_2 δ,ppm	Secondary R-C(=O)NHR_1 δ,ppm	Tertiary R-C(=O)NR_1R_2 δ,ppm
(i) N-substitution			
 $-\underset{\underset{O}{\|}}{C}-\underline{\overset{|}{N}-H}$	5-12	5-12	---
a) alpha			
 $-\underset{\underset{O}{\|}}{C}-\overset{|}{N}-\underline{CH_3}$	---	~2.9	~2.9
 $-\underset{\underset{O}{\|}}{C}-\overset{|}{N}-\underline{CH_2}-$	---	~3.4	~3.4
 $-\underset{\underset{O}{\|}}{C}-\overset{|}{N}-\underline{\overset{|}{C}H}-$	---	~3.8	~3.8
b) beta			
 $-\underset{\underset{O}{\|}}{C}-\overset{|}{N}-\overset{|}{C}-\underline{CH_3}$	~1.1	~1.1	~1.1
 $-\underset{\underset{O}{\|}}{C}-\overset{|}{N}-\overset{|}{C}-\underline{CH_2}-$	~1.5	~1.5	~1.5
 $-\underset{\underset{O}{\|}}{C}-\overset{|}{N}-\underset{|}{\overset{|}{C}}-\underline{\overset{|}{C}H}-$	~1.9	~1.9	~1.9
(ii) C-substitution a) alpha			
 $\underline{CH_3}-\underset{\underset{O}{\|}}{C}-$	~1.9	~2.0	~2.1
 $-\underline{CH_2}-\underset{\underset{O}{\|}}{C}-$	~2.1	~2.1	~2.1
 $-\underline{\overset{|}{C}H}-\underset{\underset{O}{\|}}{C}-$	~2.2	~2.2	~2.2

Amides (cont.)

δ of proton(s) (underlined)	Primary $R-C(=O)NH_2$ δ, ppm	Secondary $R-C(=O)NHR_1$ δ, ppm	Tertiary $R-C(=O)NR_1R_2$ δ, ppm
b) beta			
$\underline{CH_3}-C-C(=O)-$	~1.1	~1.1	~1.1
$-\underline{CH_2}-C-C(=O)-$	~1.5	~1.5	~1.5
$-\underline{CH}-C-C(=O)-$	~1.8	~1.8	~1.8

Amines

δ of proton(s) (underlined)	Primary $R-NH_2$ δ, ppm	Secondary RN-HR δ, ppm	Tertiary RRRN δ, ppm
(i) alpha protons			
$>N-\underline{CH_3}$	~2.5	2.3-3.0	~2.2
$>N-\underline{CH_2}-$	~2.7	2.6-3.4	~2.4
$>N-\underline{CH}<$	~3.1	2.9-3.6	~2.8
(ii) beta protons			
$>N-C-\underline{CH_3}$			~1.1
$>N-C-\underline{CH_2}-$			~1.4
$>N-C-\underline{CH}<$			~1.7

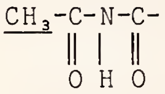
Cyanocompounds (Nitriles):

(i) Alpha hydrogens	δ, ppm
$\underline{CH_3}-C\equiv N$	~2.1
$-\underline{CH_2}-C\equiv N$	~2.5
$-CH-C\equiv N$	~2.9

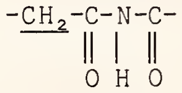
(ii) Beta hydrogens	δ, ppm
$\underline{CH_3}-C-C\equiv N$	~1.2
$-\underline{CH_2}-C-C\equiv N$	~1.6
$\underline{CH}-C-C\equiv N$	~2.0

Imides:

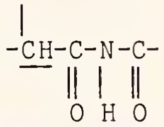
i) Alpha hydrogens δ, ppm



$\underline{CH_3}-\underset{\underset{O}{\|}}{C}-\underset{\underset{H}{|}}{N}-\underset{\underset{O}{\|}}{C}-$ ~2.0

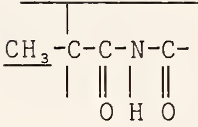


$-\underline{CH_2}-\underset{\underset{O}{\|}}{C}-\underset{\underset{H}{|}}{N}-\underset{\underset{O}{\|}}{C}-$ ~2.1

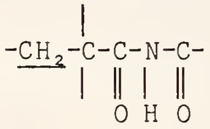


$-\overset{|}{\underline{CH}}-\underset{\underset{O}{\|}}{C}-\underset{\underset{H}{|}}{N}-\underset{\underset{O}{\|}}{C}-$ ~2.2

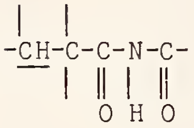
(ii) Beta hydrogens δ, ppm



$\underline{CH_3}-\overset{|}{\underset{|}{C}}-\underset{\underset{O}{\|}}{C}-\underset{\underset{H}{|}}{N}-\underset{\underset{O}{\|}}{C}-$ ~1.2



$-\underline{CH_2}-\overset{|}{\underset{|}{C}}-\underset{\underset{O}{\|}}{C}-\underset{\underset{H}{|}}{N}-\underset{\underset{O}{\|}}{C}-$ ~1.3



$-\overset{|}{\underline{CH}}-\overset{|}{\underset{|}{C}}-\underset{\underset{O}{\|}}{C}-\underset{\underset{H}{|}}{N}-\underset{\underset{O}{\|}}{C}-$ ~1.4

Isocyanates:

(i) Alpha hydrogens δ, ppm

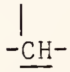
$\underline{CH_3}-N=C=O$	~3.0
$-\underline{CH_2}-N=C=O$	~3.3
$-CH-N=C=O$	~3.6

Isocyanides (Isonitriles):

(i) Alpha hydrogens δ, ppm

$\underline{CH_3}-N=C:$ ~2.9

$-\underline{CH_2}-N=C:$ ~3.3



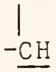
$-\overset{|}{\underline{CH}}-$ $N=C:$ ~4.9

Isonitriles: (See Isocyanides)

Isoniocyanates δ, ppm

$\underline{CH_3}-N=C=S$ ~3.4

$-\underline{CH_2}-N=C=S$ ~3.7



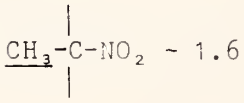
$-\overset{|}{\underline{CH}}$ $-N=C=S$ ~4.0

Nitriles δ, ppm

$-\underline{CH_2}-O-N=O$ ~4.8

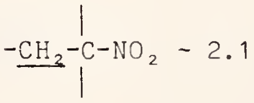
Nitrocompounds δ, ppm

$\underline{CH_3}-NO_2$ ~ 4.1

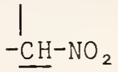


$\underline{CH_3}-\overset{|}{\underset{|}{C}}-NO_2$ ~ 1.6

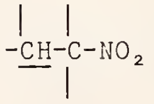
$-\underline{CH_2}-NO_2$ ~ 4.2



$-\underline{CH_2}-\overset{|}{\underset{|}{C}}-NO_2$ ~ 2.1



$-\overset{|}{\underline{CH}}-NO_2$ ~ 4.4

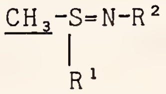


$-\overset{|}{\underline{CH}}-\overset{|}{\underset{|}{C}}-NO_2$ ~ 2.5

Organic Sulfur Compounds

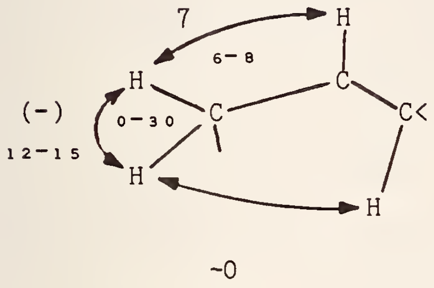
Family	δ of proton(s) underlined			
Disulfides	$\underline{CH_3}-S-S-R$	~2.4 ppm	$\underline{CH_3}-\overset{\vert}{\underset{\vert}{C}}-S-S-R$	~1.2 ppm
	$-\underline{CH_2}-S-S-R$	~2.7 ppm	$-\underline{CH_2}-\overset{\vert}{\underset{\vert}{C}}-S-S-R$	~1.6 ppm
	$-\underline{\overset{\vert}{C}H}-S-S-R$	~3.0 ppm	$-\underline{CH}-\overset{\vert}{\underset{\vert}{C}}-S-S-R$	~2.0 ppm
Isothiocyanates	$\underline{CH_3}-N=C=S$	~2.4 ppm		
	$-\underline{CH_2}-N=C=S$	~2.7 ppm		
	$-\underline{\overset{\vert}{C}H}-N=C=S$	~3.0 ppm		
Mercaptans (Thiols)	$\underline{CH_3}-S-H$	~2.1 ppm	$\underline{CH_3}-\overset{\vert}{\underset{\vert}{C}}-S-H$	~1.3 ppm
	$-\underline{CH_2}-S-H$	~2.6 ppm	$-\underline{CH_2}-\overset{\vert}{\underset{\vert}{C}}-S-H$	~1.6 ppm
	$-\underline{\overset{\vert}{C}H}-S-H$	~3.1 ppm	$-\underline{CH}-\overset{\vert}{\underset{\vert}{C}}-S-H$	~1.7 ppm
Sulfates	$(\underline{CH_3}-O)_2S(=O)_2$	~3.4 ppm		
Sulfides	$\underline{CH_3}-S-R$	~2.1 ppm	$\underline{CH_3}-\overset{\vert}{\underset{\vert}{C}}-S-R$	~1.2 ppm
	$-\underline{CH_2}-S-R$	~2.6 ppm	$-\underline{CH_2}-\overset{\vert}{\underset{\vert}{C}}-S-R$	~1.6 ppm
	$-\underline{\overset{\vert}{C}H}-S-R$	~3.1 ppm	$-\underline{CH}-\overset{\vert}{\underset{\vert}{C}}-S-H$	~1.9 ppm

Organic Sulfur Compounds (cont)

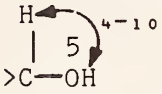
Family	δ of proton(s) underlined		
Sulfilimines	 $\underline{CH_3}-\underset{\underset{R^1}{\mid}}{S}=N-R^2$	~2.5 ppm	
Sulfonamides	$\underline{CH_3}-SO_2NH_2$	~3.0 ppm	
Sulfonates	$\underline{CH_3}-SO_2-OR$	~3.0 ppm	
Sulfones	$\underline{CH_3}-SO_2-R^2$	~2.6 ppm	
Sulfonic acids	$\underline{CH_3}-SO_3H$	~3.0 ppm	
Sulfoxides	$\underline{CH_3}-S(=O)R$	~2.5 ppm	
	$-\underline{CH_2}-S(=O)R$	~3.1 ppm	
Thiocyanates	$\underline{CH_3}-S-C\equiv N$	~2.7 ppm	
	$-\underline{CH_2}-S-C\equiv N$	~3.0 ppm	
	$-\underline{CH}-S-C\equiv N$	~3.3 ppm	
Thiols	See Mercaptans		

SOME USEFUL ^1H COUPLING CONSTANTS (IN H_z)

1) Freely Rotating Chains



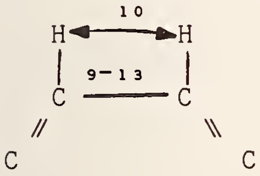
2) Alcohols with No-Exchange as in DMSO

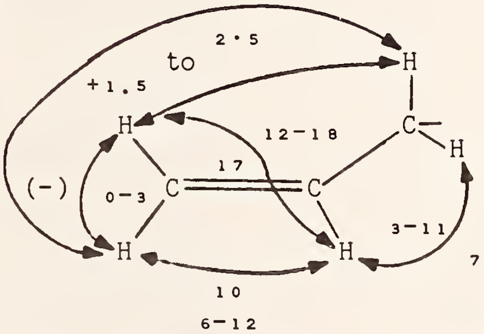


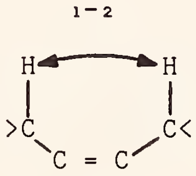
1° = triplet
2° = doublet } broad
3° = singlet

Then add TFA, all = sharp single

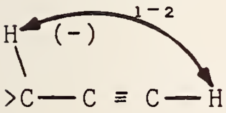
3) Alkenes

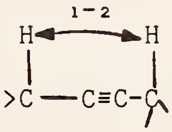




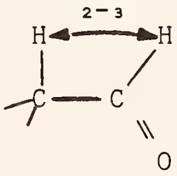


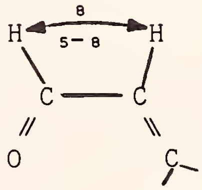
4) Alkynes



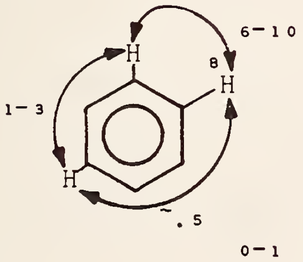


5) Aldehydes



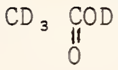
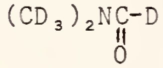
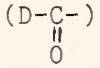
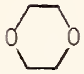


6) Aromatic

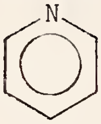
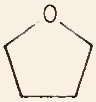


Adapted from the work of Professor C.F. Hammer, Georgetown University, Washington D.C.

Solvent Positions of Residual (Impurity) Protons in Incompletely Deuterated Solvents

Solvent	Formula	Group	δ (ppm)
d_4-acetic acid	 $CD_3\underset{\underset{O}{\|}}{C}OD$	Methyl (CD_3-)	2.05
		Hydroxyl (-OD)	10-12[1]
d_6-acetone	$(CD_3)_2C=O$	Methyl (CD_3-)	2.05
d_3-acetonitrile	CD_3CN	Methyl (CD_3-)	1.95-2.05
d_6-benzene	C_6D_6	Methine (CD-)	7.2-7.3
d_1-chloroform	$CDCl_3$	Methine (CD-)	7.25
d_{12}-cyclohexane	C_6D_{12}	Methylene (CD_2-)	1.40
d_4-dichloroethane	CD_2ClCD_2Cl	Methylene (CD_2-)	3.69
d_7-dimethylformamide (DMF)	 $(CD_3)_2N\underset{\underset{O}{\|}}{C}-D$	Methyl (CD_3-)	2.75
		Methyl (CD_3-)	2.95
		Formyl  $(D-\underset{\underset{O}{\|}}{C}-)$	8.05
d_6-dimethylsulfoxide (DMSO)	$(CD_3)_2SO$	Methyl (CD_3-)	2.5
		Absorbed water	3-4[1]
d_8-dioxane		Methylene	3.55
d_{18}-hexamethylphosphoramide	$[(CD_3)_2N]_3\ P=O$	Methyl (CD_3-)	2.60
d_4-methanol	CD_3OD	Methyl (CD_3-)	3.35
		Hydroxyl (-OD)	3-6[1]
d_2-methylene chloride	CD_2Cl_2	Methylene (CD_2-)	5.35
d_3-nitromethane	CD_3NO_2	Methyl (CH_3)	4.33

Solvent Positions of Residual (Impurity) Protons in Incompletely Common Deuterated Solvents (cont.)

Solvent	Formula	Group	δ (ppm)
d_5-pyridine		C-2 Methine	8.70
		C-3 Methine	7.20
		C-4 Methine	7.58
d_8-tetrahydrofuran		α-Methylene	3.60
		β-Methylene	0.75
d_8-toluene	$C_6D_5CD_3$	Methyl (CD_3-)	2.3
		Methine (CD-)	7.2
d_1-trifluoroacetic acid	CF_3COOD	Hydroxyl (-OD)	10-12[1]
d_2-water	D_2O	Hydroxyl (-OD)	3.5-6[1]

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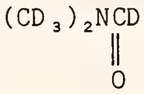
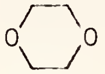
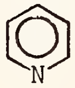
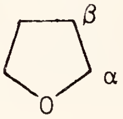
[1] Exact value depends on the solute nature and concentration.

^{13}C Chemical Shifts of Useful NMR Solvents

Solvent	Formula	Chemical Shift (ppm)
acetone-d_6	$(CD_3)_2C=O$	29.2 (CD_3) 204.1 (>C=O)
acetonitrile-d_3	$CD_3C\equiv N$	1.3 (CD_3) 117.7 ($C\equiv N$)
benzene-d_6	C_6D_6	128.4
carbon disulfide	CS_2	192.3
carbon tetrachloride	CCl_4	96.0
chloroform-d_3	$CDCl_3$	76.9
cyclohexane-d_{12}	C_6D_{12}	27.5
dichloromethane-d_2	CD_2Cl_2	53.6
dimethylformanide-d_7	 $(CD_3)_2NCD{=}O$	31 (CD_3) 36 (CD_3) 162.4 (DC=O)
dimethylsulfoxide-d_6	$(CD_3)_2$ S=O	39.6
dioxane-d_8		67.4
methanol-d_4	CD_3OD	49.3
nitromethane-d_3	CD_3-NO_2	57.3
pyridine-d_5		124.0 136.0 150.0
1,1,2,2-tetrachloro-ethane-d_2	$CDCl_2$-$CDCl_2$	75.5
tetrahydrofuran-d_8		25.8 (β-) 67.9 (α-)
trichlorofluoromethane	$CFCl_3$	117.6
Water (heavy)	D_2O	-

VI. Tables for Mass Spectrometry

Natural Abundance of Important Isotopes

The following table lists the atomic masses and relative percent concentrations of naturally occurring isotopes of importance in mass spectroscopy [1-3].

REFERENCES:

[1] Rose, M.E., Johnstone, R.A.W., Mass Spectrometry for Chemists and Biochemists, Cambridge University Press, Cambridge, 1982.

[2] Weast, R.C., ed., Handbook of Chemistry and Physics, 63rd Ed., The Chemical Rubber Co., Boca Raton, 1984.

[3] McLafferty, F.W., Interpretation of Mass Spectra, University Science Books, Mill Valley, 1980.

Element	Total # of isotopes	More important isotopes (mass [amu], percent abundance)		
Hydrogen	3	^{1}H (1.00783, 99.99)	^{2}H (2.01410, 0.015)	
Boron	6	^{10}B (10.01294, 19.8)	^{11}B (11.00931, 80.2)	
Carbon	7	^{12}C (12.00000, 98.9)	^{13}C (13.00335, 1.1)	
Nitrogen	7	^{14}N (14.00307, 99.6)	^{15}N (15.00011, 0.4)	
Oxygen	8	^{16}O (15.99491, 99.8)		^{18}O (17.9992, 0.2)
Fluorine	6	^{19}F (18.99840, 100.0)		
Silicon	8	^{28}Si (27.97693, 92.2)	^{29}Si (28.97649, 4.7)	^{30}Si (29.97376, 3.1)
Phosphorus	7	^{31}P (30.97376, 100.0)		
Sulfur	10	^{32}S (31.972017, 95.0)	^{33}S (32.97146, 0.7)	^{34}S (33.96786, 4.2)
Chlorine	11	^{35}Cl (34.96885, 75.5)		^{37}Cl (36.96590, 24.5)
Bromine	17	^{79}Br (78.9183, 50.5)		^{81}Br (80.91642, 49.5)
Iodine	23	^{127}I (126.90466, 100.0)		

Rules for Determination of Molecular Formula

The following rules are used in the mass spectroscopic determination of the molecular formula of an organic compound [1]. These rules should be applied to the molecular ion peak and its isotopic cluster. The molecular ion, in turn, should be the highest mass in the spectrum, must be an odd-electron ion and must be capable of yielding all other important ions of the spectrum via a logical neutral species loss. The elements that are assumed to (possibly) exist are carbon, hydrogen, nitrogen, the halogens, sulfur and/or oxygen. The molecular formula that can be derived is not the only possible one and consequently help from nuclear magnetic resonance spectrometry and infrared spectrophotometric data is necessary for the final determination.

Rule 1: An odd molecular ion value suggests the presence of an odd number of nitrogens. An even molecular ion is due to the presence of zero or an even number of nitrogens. Thus, $m/e = 141$ suggests 1, 3, 5, 7, etc., nitrogen atoms while $m/e = 142$ suggests 0, 2, 4, 6, etc., nitrogen atoms.

Rule 2: The maximum number of carbons can be calculated from the formula

$$\frac{\text{Relative Intensity of M + 1}}{\text{Relative Intensity of } M^+} \times \frac{100}{1.1}$$

where $M + 1$ is the peak next to that of the molecular ion (M^+). This rule gives the maximum number of carbons, but not necessarily the right number. Thus, if for example the relative intensities of M^+

and M + 1 are 100% and 9% respectively, then the maximum number of carbons is

$$\frac{9}{100} \times \frac{100}{1.1} = 8$$

There is a possibility for seven, six, etc., carbons but not for nine or more.

Rule 3: The maximum numbers of sulfurs can be calculated from the formula

$$\frac{\text{Relative Intensity of M + 2}}{\text{Relative Intensity of } M^{+}} \times \frac{100}{4.4}$$

where M + 2 is the peak next to that of the molecular ion M^{+}.

Rule 4: The number of chlorines and/or bromines can be derived from the table showing the relative ratio of the isotope cluster of the molecular ion.

Rule 5: The difference should be only oxygen and hydrogen. These rules assume absence of phosphorus silicon or any other elements.

REFERENCE:

[1] McLafferty, F.W., Interpretation of Mass Spectra, University Science Books, Mill Valley, 1980.

Chlorine - Bromine Combination Isotope Intensities

Due to the distinctive mass spectral patterns caused by the presence of chlorine and bromine in a molecule, interpretation can be much easier if the results of the relative isotope concentrations are known. The following table provides peak intensities (relative to the P^+ at an intensity normalized to 100 percent) for various combinations of chlorine and bromine molecules, assuming the absence of all other elements except carbon and hydrogen [1-3]. The mass abundance calculations were based upon the atomic mass data of Weast [4].

REFERENCES:

[1] McLafferty, F.W., Interpretation of Mass Spectra, University Science Books, Mill Valley, 1980.

[2] Silverstein, R.H., G.C. Bassler and T.C. Morrill, Spectrometric Identification of Organic Compounds, John Wiley and Sons, New York, 1981.

[3] Williams, D.H. and I. Fleming, Spectroscopic Methods in Organic Chemistry, McGraw-Hill, London, 1973.

[4] Weast, R.C., ed., Handbook of Chemistry and Physics, 63rd. Ed., The Chemical Rubber Company, Boca Raton, 1984.

Relative Intensities of Isotope Peaks for Combinations of Bromine and Chlorine ($P^+ = 100\%$)

		Br_0	Br_1	Br_2	Br_3	Br_4
Cl_0	P + 2		98.0	196.0	294.0	390.8
	P + 4			96.1	288.2	574.7
	P + 6				94.1	375.3
	P + 8					92.0
Cl_1	P + 2	32.5	130.6	228.0	326.1	424.6
	P + 4		31.9	159.0	383.1	704.2
	P + 6			31.2	187.4	564.1
	P + 8				30.7	214.8
	P + 10					30.3
Cl_2	P + 2	65.0	163.0	261.1	359.3	456.3
	P + 4	10.6	74.4	234.2	490.2	840.3
	P + 6		10.4	83.3	312.8	791.6
	P + 8			10.2	91.7	397.5
	P + 10				9.8	99.2
	P + 12					10.1
Cl_3	P + 2	97.5	195.3	294.0	393.3	
	P + 4	31.7	127.0	99.7	609.8	
	P + 6	3.4	34.4	159.4	473.8	
	P + 8		3.3	37.1	193.9	
	P + 10			3.2	39.6	
	P + 12				3.0	
	P + 14					
Cl_4	P + 2	130.0	228.3	326.6	4.2	
	P + 4	63.3	190.9	414.9	735.3	
	P + 6	13.7	75.8	263.1	670.0	
	P + 8	1.2	14.4	88.8	347.1	
	P + 10		1.1	15.4	102.2	
	P + 12			1.3	16.2	
	P + 14				0.7	

Relative Intensities of Isotope Peaks for Combinations of Bromine and Chlorine (P^+ = 100%)

		Br_0	Br_1	Br_2	Br_3	Br_4
Cl_5	P + 2	162.6	260.7	358.9		
	P + 4	105.7	265.3	520.8		
	P + 6	34.3	137.9	397.9		
	P + 8	5.5	39.3	174.5		
	P + 10	0.3	5.8	44.3		
	P + 12		0.3	5.7		
	P + 14			0.5		
Cl_6	P + 2	195.3				
	P + 4	158.6				
	P + 6	68.8				
	P + 8	16.6				
	P + 10	2.1				
	P + 12	0.1				
Cl_7	P + 2	227.8				
	P + 4	222.1				
	P + 6	120.3				
	P + 8	39.0				
	P + 10	7.5				
	P + 12	0.8				
	P + 14	0.05				

Common Fragmentation Patterns of Families of Organic Compounds

The following table provides a guide to the identification and interpretation of commonly observed mass spectral fragmentation patterns for common organic functional groups [1-4]. It is of course highly desirable to augment mass spectroscopic data with as much other structural information as is possible. Especially useful in this regard will be the confirmatory information of infrared and ultraviolet spectrophotometry and nuclear magnetic resonance spectrometry.

REFERENCES

[1] Pasto, D.J. and C.R. Johnson, Organic Structure Determination. Prentice-Hall, 1969.

[2] McLafferty, F.W., Interpretation of Mass Spectra, University Science Books, 1980.

[3] Rose, M.E. and R.A.W. Johnstone, Mass Spectrometry for Chemical and Biochemists, Cambridge University Press, 1982.

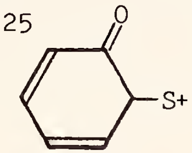
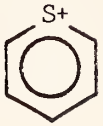
[4] Silverstein, R.M., G.C. Bassler and T.C. Morrill, Spectrometric Identification of Organic Compounds, John Wiley and Sons, 1981.

Family	Molecular Ion Peak	Common Fragments; Characteristic Peaks
Acetals		cleavage of all C-O, C-H & C-C bonds around the original aldehydic carbon.
Alcohols	weak for 1° & 2°; not detectable for 3°; strong for benzyl alcohols	loss of 18 (H_2O - usually by cyclic mechanism); loss of H_2O and olefin simultaneously with four (or more) carbon-chain alcohols; prominent peak at $^{m}/e = 31$ $(CH_2\ddot{O}H)^+$ for 1° alcohols; prominent peak at $^{m}/e = RCH\ddot{O}H^+$ for $^{+}$2° and $^{m}/e = R_2C\ddot{O}H^+$ for 3° alcohols.
Aldehydes	low intensity	loss of aldehydic hydrogen (strong M-1 peak, especially with aromatic aldehydes); strong peak at $^{m}/e = 29$ $(HC \equiv O^+)$; loss of chain attached to αlpha carbon (beta cleavage); McLafferty rearrangement via beta cleavage if gamma hydrogen is present.
Alkanes		
a) Chain	low intensity	loss of 14 units (CH_2).
b) Branched	low intensity	cleavage at the point of branch; low intensity ions from random rearrangements.
c) Alicyclic	rather intense	loss of 28 units ($CH_2{=}CH_2$) and side chains.
Alkenes (olefins)	rather high intensity (loss of π-electron) especially in case of cyclic olefins	loss of units of general formula C_nH_{2n-1}; formation of fragments of the composition C_nH_{2n} (via McLafferty rearrangement); retro Diels-Alder fragmentation.

Family	Molecular Ion Peak	Common Fragments; Characteristic Peaks
Alkyl halides	abundance of molecular ion $F < Cl < Br < I$ intensity decreases with increase in size and branching	loss of fragments equal to the mass of the halogen until all halogens are cleared off.
a) fluorides	very low intensity	loss of 20 (HF); loss of C_2H_2 in case of fluorobenzenes.
b) chlorides	low intensity; characteristic isotope cluster	loss of 35 (Cl) or 36 (HCl); loss of chain attached to gamma carbon to the carbon carrying the Cl.
c) bromides	low intensity; characteristic isotope cluster	loss of 79 (Br); loss of chain attached to gamma carbon to the carbon carrying the Br.
d) iodides	higher than other corresponding halides	loss of 127 (I).
Alkynes	rather high intensity (loss of π-electron)	fragmentation similar to that of alkenes.
Amides	rather high intensity	strong peak at $^m/e$ indicative of a 1° amide $(O = C = \overset{+}{N}H_2)$; base peak at $^m/e = 59$ $(CH_2 = \underset{OH}{C} - \underset{\bullet}{\overset{+}{N}}H_2)$; possibility of McLafferty rearrangement; loss of C_2H_2O for amides of the form $RNHCOCH_3$ when R is aromatic ring.
Amines	hardly detectable in case of acyclic aliphatic amines; high intensity for aromatic and cyclic amines	beta cleavage yielding $>C = \underset{+}{N}<$; base peak for all 1° amines at $^m/e = 30$ $(CH_2 = \underset{+}{N}H_2)$; moderate M-1 peak for aromatic amines; loss of 27 (HCN) in aromatic amines; fragmentation at alpha carbons in cyclic amines

Family	Molecular Ion Peak	Common Fragments; Characteristic Peaks
Aromatic hydrocarbons (arenes)	rather intense	loss of side chain; formation of RCH = CHR' (via McLafferty rearrangement); cleavage at the bonds beta to the aromatic ring; peaks at $^{m}/e = 77$ (benzene ring; especially mono-substituted), 91 (tropyllium); the ring position of alkyl substitution has very little effect on the spectrum.
Carboxylic acids	weak for straight-chain monocarboxylic acids; large if aromatic acids	base peak at $^{m}/e = 60$ $(CH_2 = C(OH)_2)$ if δ-hydrogen is present; peak at $^{m}/e = 45$ $(CO\dot{O}H)$; loss of 17 (-OH) in case of aromatic acids or short-chain acids.
Disulfides	rather low intensity	loss of olefins ($^{m}/e$ equal to $R\text{-}S\text{-}S\text{-}H^{+\cdot}$); strong peak at $^{m}/e = 66$ $(HSSH^{+\cdot})$.
Phenols	high intensity (base peak (generally)	loss of 28 (C = O) and 29 (-CHO); strong peak at $^{m}/e = 65$ $(C_5H_5^{+})$.
Sulfides (thioethers)	rather low intensity but higher than that of corresponding ether	similar to those of ethers (-O- substituted by -S-); aromatic sulfides show strong peaks at $^{m}/e = 109$ $(C_6H_5S^{+\cdot})$; 65 $(C_5H_5^{+\cdot})$; 91 (tropyllium ion).
Sulfonamides	rather intense	loss of $^{m}/e = 64$ (SO_2NH_2) and $^{m}/e = 27$ (HCN) in case of benzenesulfonamide.

Family	Molecular Ion Peak	Common Fragments; Characteristic Peaks
Esters $R\text{-}\underset{\underset{O}{\Vert}}{C}\text{-}OR'$	rather weak intensity	base peak at $^{m}/e$ equal to the mass of $R\text{-}C \equiv O^{+}$; peaks at $^{m}/e$ equal to the mass of $^{+}O \equiv C\text{-}OR'$, the mass of OR' and R'; McLafferty rearrangement possible in case of, a) presence of a beta hydrogen in R' (peak at $^{m}/e$ equal to the mass of R-C-OH), and b) presence of a gamma +OH hydrogen in R (peak at $^{m}/e$ equal to the mass of $(CH_2 = \underset{+O\text{-}H}{C}\text{-}OR)$; loss of 42 $(CH_2 = C = O)$ in case of benzyl esters; loss of ROH via the ortho effect in case of O-substituted benzoates.
Ethers	rather low intensity	cleavage of a bond beta to the oxygen and formation of $CH_2 = \underset{+}{O}\text{-}R$ species; cleavage of C-O bond and loss of R-groups; loss of $^{m}/e = 30$ (CH_2O), $^{m}/e = 29$ (CHO) and $^{m}/e = 15$ (CH_3) in case of anisoles; loss of $^{m}/e = 1$ (H), 28 (CO) and 29 (CHO) in diphenyl ethers.
Ketones	rather high intensity	loss of R-groups attached to the $>C = O$ (alpha cleavage); peak at $^{m}/e = 43$ for all methyl ketones (CH_3CO^{+}); McLafferty rearrangement via beta cleavage if gamma hydrogen is present; loss of $^{m}/e = 28$ $(>C = O)$ for cyclic ketones after initial alpha cleavage and McLafferty rearrangement.
Mercaptans (thiols)	rather low intensity but higher than that of corresponding alcohol	similar to those of alcohols (-OH substituted by -SH); loss of $^{m}/e = 45$ (CHS) and $^{m}/e = 44$ (CS) for aromatic thiols.

Family	Molecular Ion Peak	Common Fragments; Characteristic Peaks
Nitriles	unlikely to be detected except in case of acetonitrile (CH_3CN) and propionitrile (C_2H_5CN)	M + 1 ion may appear (especially at higher pressures); M − 1 peak is weak but detectable ($R{-}CH{=}C{=}N^+$); base peak at $^m/e = 41$ ($CH_2{=}C{=}\overset{+}{\underset{\bullet}{N}}{-}H$); McLafferty rearrangement possible; loss of HCN in case of cyanobenzenes.
Nitrites	absent (or very weak at best)	base peak at $^m/e = 30$ (NO^+); large peak at $^m/e = 60$ ($CH_2{=}\underset{+}{O}NO$) in all unbranched at the alpha carbon nitrites; absence of $^m/e = 46$ permits differentiation from nitrocompounds.
Nitro compounds	seldom observed	loss of 30 (NO); subsequent loss of CO (in case of aromatic nitrocompounds; loss of NO_2 from molecular ion peak.
Sulfones	high intensity	similar to sulfoxides; loss of mass equal to RSO_2.
Sulfoxides	high intensity	loss of 17 (OH); loss of alkene ($^m/e$ equal to $RSOH^{+\bullet}$); peak at $^m/e = 63$ ($CH_2 = \underset{+}{S}OH$); aromatic sulfoxides show peak at $^m/e = 125$  ;97  93 ($C_6H_5\overset{+}{\underset{\bullet}{O}}H$).

VII. Tables for Qualitative Analysis

Organic Group Qualitative Tests

The following flow charts and notes provide a step by step process for the identification of functional groups which may be present in an unknown sample [1-7]. These are meant to augment and confirm information obtainable using instrumental methods of analysis. It will usually be necessary to use gas or liquid chromatography before these "wet" chemical tests in order to determine the number of components present in a given sample. Since many of these tests require the use of dangerous compounds, the strictest rules of laboratory safety must be observed at all times. The use of a fume hood is required.

Note: ppt = precipitate

conc = concentrated

dil = dilute

REFERENCES:

[1] Pasto, D.J., Johnson, C.R., Laboratory Text for Organic Chemistry, Prentice Hall, Englewood Cliffs, 1979.

[2] Sarlo, E., Svoronos, P.D.N., Experiments for Organic Chemistry, Burgess Publishing, Minneapolis, 1983.

[3] Roberts, R.M., Gilbert, J.C., Rodewald, L.B., Wingrove, A.S., An Introduction to Modern Experimental Organic Chemistry, Holt, Rinehart, and Winston, New York, 1969.

[4] Hopkins and Williams Research Laboratory, Organic Reagents for Organic Analysis, Chemical Publishing Co., Brooklyn, 1946.

[5] Hodgman, C.D., Weast, R.C., Selby, S.M., Tables for Identification of Organic Compounds, Chemical Rubber Publishing Co., Cleveland, 1950.

[6] Kamm, O., Qualitative Organic Analysis, John Wiley and Sons, Inc., New York, 1932.

[7] Vogel, A.I., *A Textbook of Practical Organic Chemistry*, Longmans, Green, and Co., London, 1951.

Protocol For Chemical Tests

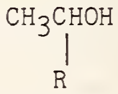
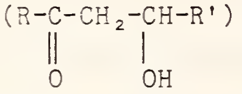
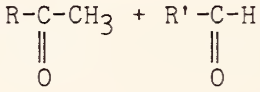
Ceric ammonium nitrate: To 1-2 ml 5% ceric ammonium nitrate add 10 drops of the compound to be tested. A change to an orange/red color is indicative of an alcohol (detection limit 100 mg - compounds tested C_1-C_{10}).

Dichromate test: Add ten drops of the alcohol to be tested to a mixture of 1 ml 1% $Na_2Cr_2O_7$ and 5 drops conc. H_2SO_4. A blue-green solution is positive test for a 1° or 2° alcohol. 3° alcohols do not react and, therefore, the solution stays orange. (Detection limit 20 μg - compounds tested C_1-C_8).

2,4-Dinitrophenylhydrazine test (2,4-DNP): Add 10 drops of the compound to be tested to 1 ml of the 2,4-DNP reagent. A yellow to orange-red ppt is considered a positive test. The 2,4-DNP reagent can be prepared by dissolving 1 g 2,4-dinitrophenylhydrazine in 5 ml conc. H_2SO_4 and then mixing it with 8 ml of water and 20 ml 95% ethanol. The solution should be filtered before reacting it with the unknown compound. (Detection limit 20 μg - compounds tested C_1-C_8).

Ferric chloride test: Add 10 drops of 3% aqueous $FeCl_3$ solution to 1 ml of a 5% aqueous (ethanol) solution of the compound in question. Phenols give red, blue, purple or green colorations. The same test can be done by using chloroform as a solvent (detection limit 50 μg).

Hinsberg test: To 0.5 ml of the amine (0.5 g, if solid) in a test tube add 1 g of p-toluenesulfonyl chloride and 8 ml 10% NaOH. Stopper the tube and shake for 3-5 minutes. Remove the stopper and warm the tube with shaking in a hot water bath (70°C) for about one minute. No reaction is indicative of a 3° amine, which is usually soluble upon acidification (pH = 2-4) with 10% HCl. If a precipitate is present in the alkaline solution, dilute with 5-8 ml H_2O and shake. If the precipitate does not dissolve the original amine is, probably, a 2° one. If the solution is clear acidify (pH = 4) with 10% HCl. The formation of a precipitate is an indication of a 1° amine. (Detection limit 100 mg - compounds tested C_1-C_{10}.)

Iodoform test: The reagent calls for the mixture of 10 g I_2 and 20 g KI in 100 ml water. The reagent is then added dropwise to a mixture of 10 drops of the compound in question in 2 ml of water (or dioxane, to facilitate the solubility) and 1 ml 10% aqueous NaOH solution until a persistent brown color remains (even when heating in a hot water bath at 60°C.) A yellow precipitate is indicative of iodoform (CHI_3) formation and is characteristic of a methyl ketone, acetaldehyde or an alcohol of the general formula  $CH_3\underset{\displaystyle R}{\underset{|}{C}}HOH$ (R = alkyl, hydrogen). Aldols  $(R\text{-}\underset{O}{\underset{\|}{C}}\text{-}CH_2\text{-}\underset{OH}{\underset{|}{C}}H\text{-}R')$ also give a positive iodoform test by a retro aldol condensation first yielding  $R\text{-}\underset{O}{\underset{\|}{C}}\text{-}CH_3 + R'\text{-}\underset{O}{\underset{\|}{C}}\text{-}H$ (detection limit 100 mg).

Lucas test: The reagent is made by dissolving 16 g anhydrous $ZnCl_2$ in 10 ml conc. HCl with cooling to avoid HCl loss. Add 10-15 drops of the alcohol to 2 ml of the reagent. 3° alcohols form an emulsion (the alkyl halide) almost immediately, 2° alcohols form it after 2-5 minutes while 1° alcohols react after a very long time.

Sodium fusion test: 10 mg of the compound to be analyzed are mixed with a fresh piece of sodium metal of the size of a small pea in a 4-inch test tube.

The test tube is warmed gently until melting of the sodium metal and decomposition (indicated by charring) of the compound occurs. When it appears that all the volatile material has been decomposed, the test tube is strongly heated until the residue becomes red. After 3 minutes of constant heating, the mixture is left to cool to room temperature, then a few drops of methanol are added. If no smoke appears, an excess of sodium metal was not present and incomplete conversion of the elements (N, S, halogens} to their anions (CN^-, S^{-2}, halides) is very likely. Addition of another tiny piece of sodium metal and repetition of the heating process is necessary. If smoke appears then the test tube is plunged in a small beaker containing 10-15 ml <u>distilled water</u> and covered with a watch glass or a wire gauze. The test tube might shatter and, therefore, having the small beaker inside a larger one is recommended. The contents of the test tube together with the broken glass are ground in a mortar using a pestle, then transferred in the small beaker and heated for a few minutes. The solution is then filtered and the solution divided into <u>two</u> larger parts and <u>one</u> 1-ml part.

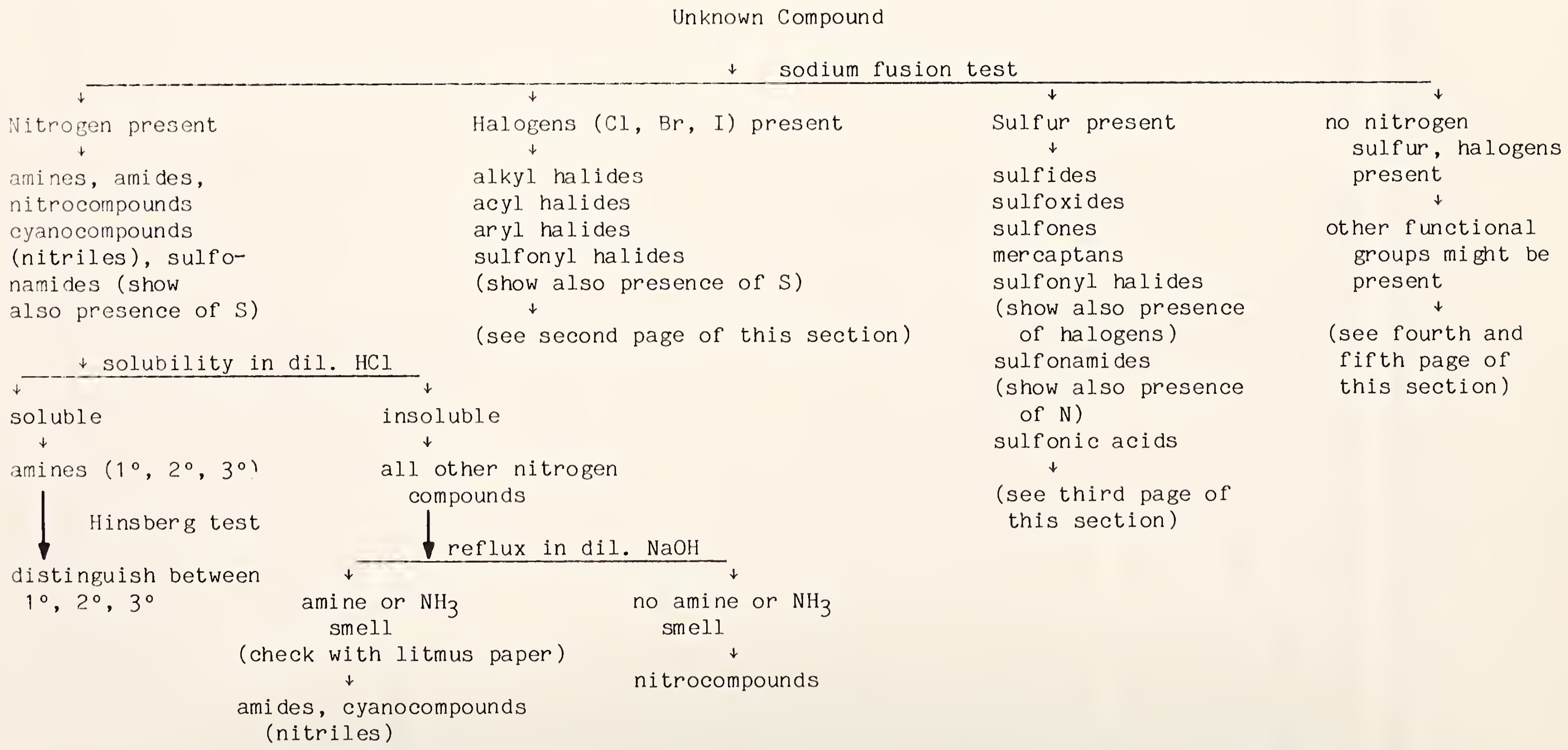
<u>Detection of nitrogen</u>: To one of the larger parts add 0.5 ml of 6M NaOH (pH adjusted to 13), five drops of saturated $Fe(NH_4)_2(SO_4)_2$ and five drops 30% KF solution. The mixture is boiled for 30 seconds and immediately acidified with 6M H_2SO_4 with stirring until the colloidal iron hydroxides are dissolved. The formation of a blue color is indicative of the presence of nitrogen. presence.

<u>Detection of sulfur</u>: To the 1-ml part add 10 drops of 6M acetic acid and 2-3 drops of 5% lead acetate solution. A black precipitate is indicative of sulfur presence.

Detection of halogens: To the other larger part add 10% H_2SO_4 until the solution is acidic. Boil off the solution to 1/3 its volume to secure evaporation of H_2S and HCN gases. Formation of a precipitate upon addition of 10% $AgNO_3$ solution is indicative of the presence of a halogen - white for a chloride (which is soluble in 6M NH_4OH), pale yellow for a bromide (which is only slightly soluble in 6M NH_4OH) and canary yellow for iodide (which is insoluble in 6M NH_4OH). Should the color of the precipitate be difficult to provide satisfactory identification of the halogen, proceed as follows: the working solution which has been acidified with 10% H_2SO_4 and boiled down is treated with 4-5 drops 0.1 N $KMnO_4$ solution, with enough oxalic acid added to discharge the color of excess permanganate and 0.5 ml carbon disulfide. The presence of a color in the carbon disulfide layer indicates the presence of bromine or iodine - purple if iodine is present, red-brown if bromine is present, colorless if chlorine is present. Should the compound to be tested carry both bromine and iodine the identification will be difficult (red-brown to purple carbon disulfide layer). Addition of a few drops of allyl alcohol decolorizes bromine but does not decolorize iodine.

Tollen's test: The reagent is actually made by mixing two solutions (A and B). Solution A is a 10% aqueous $AgNO_3$ solution and Solution B is a 10% aqueous NaOH solution. When the test is required, one ml of solution A and one ml of solution B are mixed, and the silver oxide thus formed is dissolved by dropwise addition of 10% aqueous NH_4OH. To the clear solution, 10 drops of the compound to be tested are added. A silver mirror is indicative of the presence of an aldehyde. The reagent mixture (A + B) is to be prepared immediately prior to use, otherwise explosive silver fulminate might be formed.

The silver mirror is usually deposited on the walls of the test tube immediately or after a short warming period in a hot water bath. It is to be disposed of immediately with water and/or dil. HNO_3. (Detection limit 50 mg - compounds tested C_1-C_6.)



Unknown Compound

↓ sodium fusion test

↓
Nitrogen present
↓
amines, amides,
nitrocompounds
cyanocompounds
(nitriles), sulfonamides (show
also presence of S)

↓ solubility in dil. HCl

↓
soluble
↓
amines (1°, 2°, 3°)

Hinsberg test

distinguish between
1°, 2°, 3°

↓
insoluble
↓
all other nitrogen
compounds

reflux in dil. NaOH

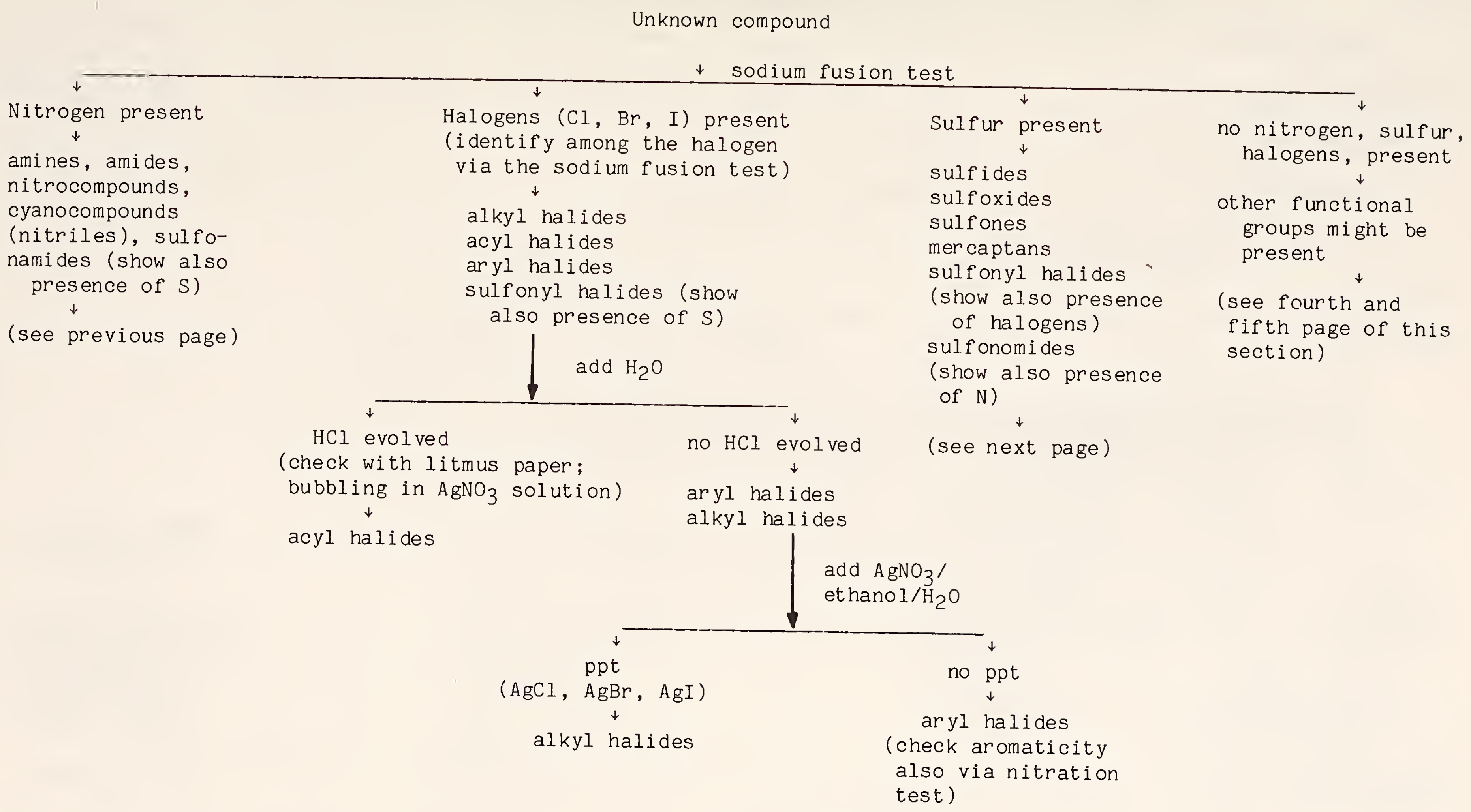
↓
amine or NH_3
smell
(check with litmus paper)
↓
amides, cyanocompounds
(nitriles)

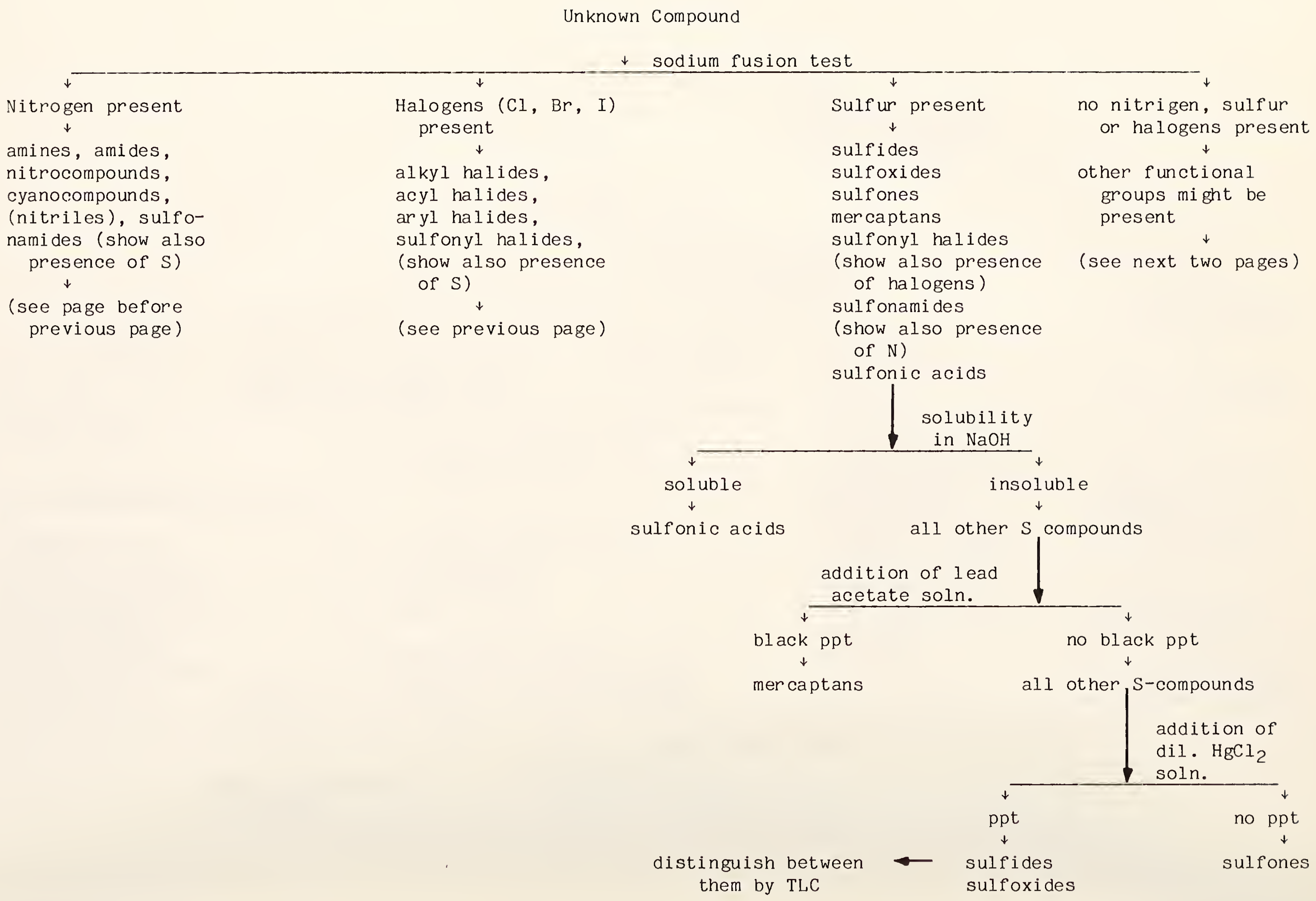
↓
no amine or NH_3
smell
↓
nitrocompounds

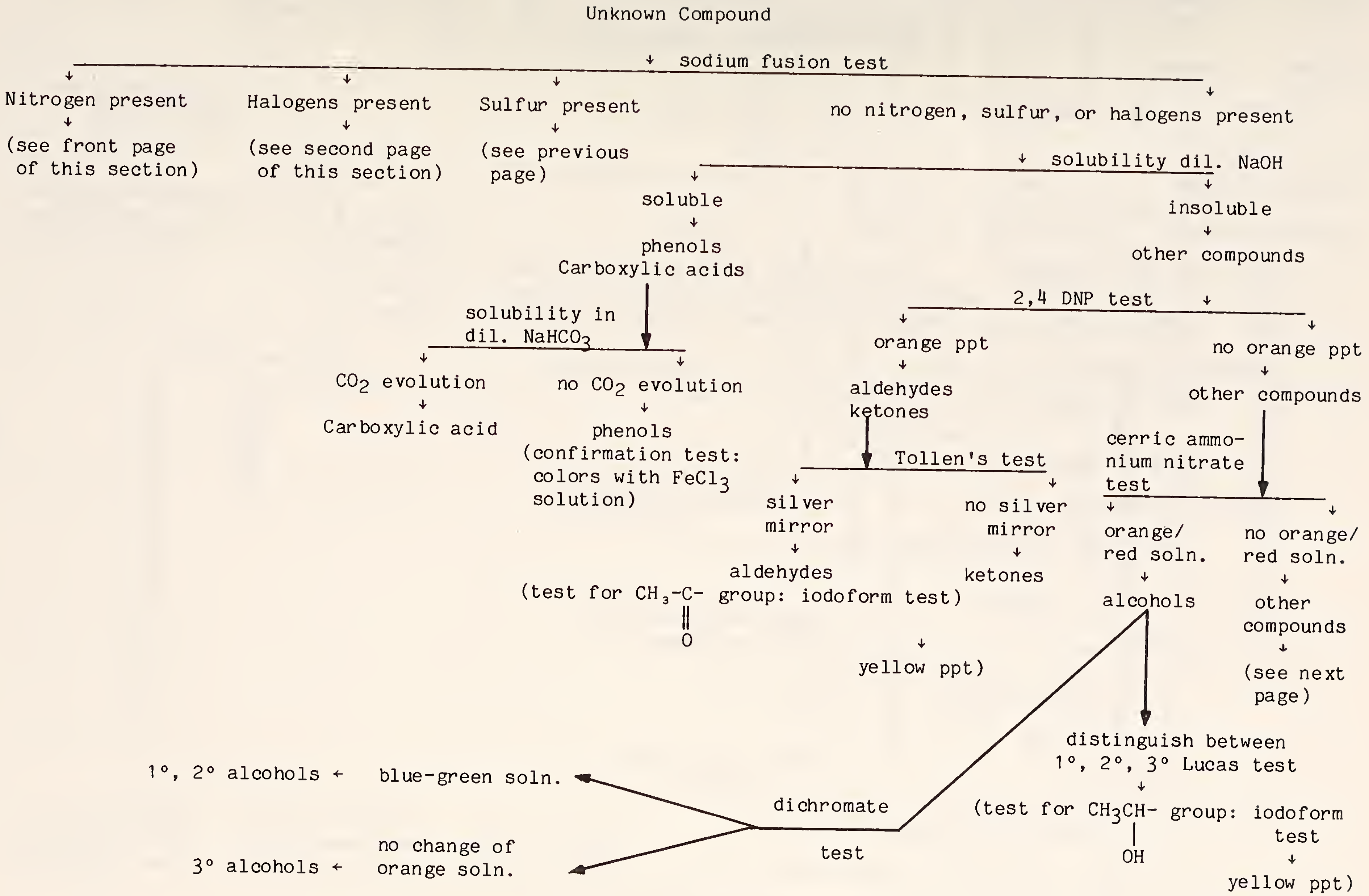
↓
Halogens (Cl, Br, I) present
↓
alkyl halides
acyl halides
aryl halides
sulfonyl halides
(show also presence of S)
↓
(see second page of this section)

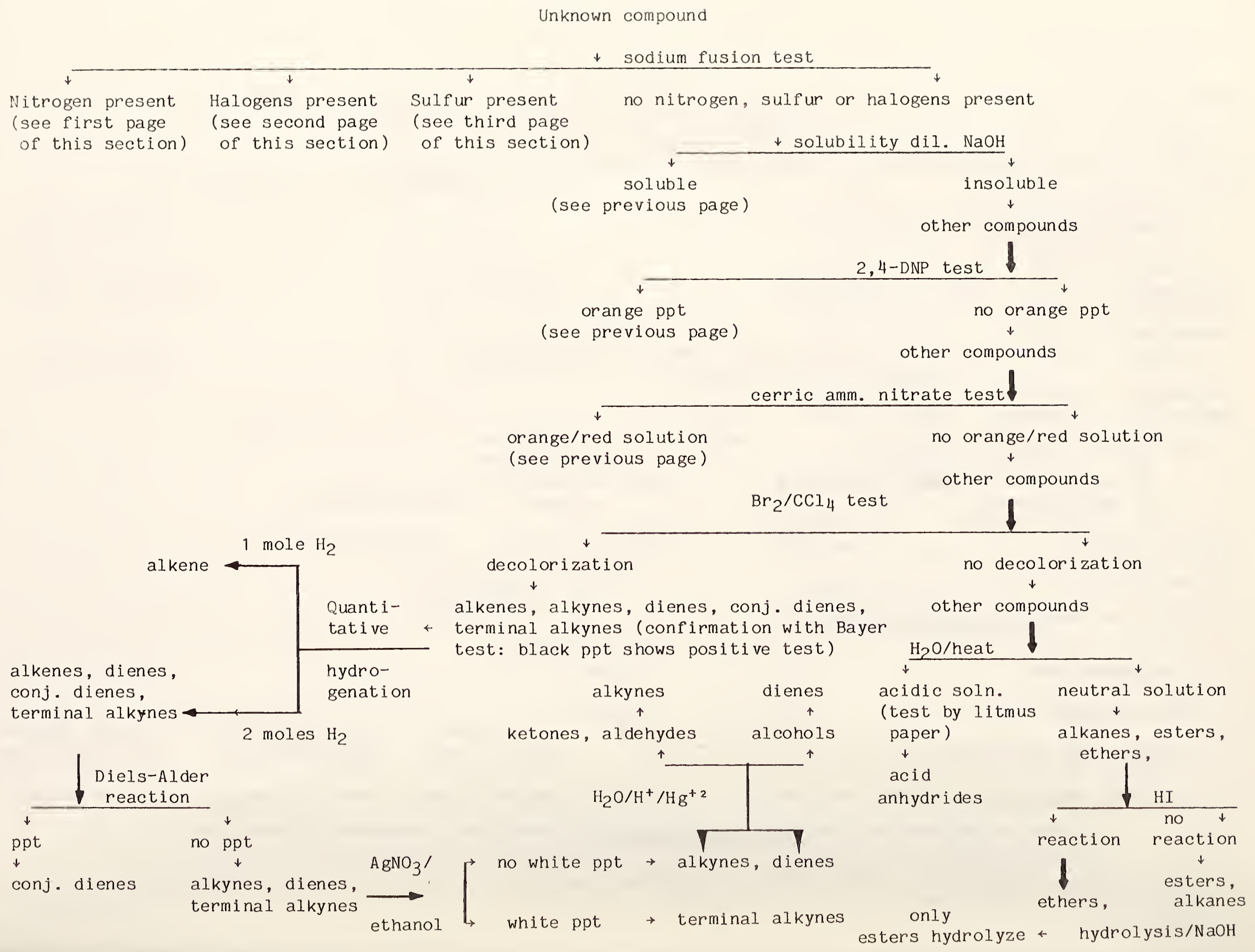
↓
Sulfur present
↓
sulfides
sulfoxides
sulfones
mercaptans
sulfonyl halides
(show also presence
of halogens)
sulfonamides
(show also presence
of N)
sulfonic acids
↓
(see third page of
this section)

↓
no nitrogen
sulfur, halogens
present
↓
other functional
groups might be
present
↓
(see fourth and
fifth page of
this section)


Unknown compound
sodium fusion test
Nitrogen present
amines, amides, nitrocompounds, cyanocompounds (nitriles), sulfonamides (show also presence of S)
(see previous page)
Halogens (Cl, Br, I) present (identify among the halogen via the sodium fusion test)
alkyl halides
acyl halides
aryl halides
sulfonyl halides (show also presence of S)
add H_2O
HCl evolved (check with litmus paper; bubbling in $AgNO_3$ solution)
acyl halides
no HCl evolved
aryl halides
alkyl halides
add $AgNO_3$/ ethanol/H_2O
ppt ($AgCl$, $AgBr$, AgI)
alkyl halides
no ppt
aryl halides (check aromaticity also via nitration test)
Sulfur present
sulfides
sulfoxides
sulfones
mercaptans
sulfonyl halides (show also presence of halogens)
sulfonomides (show also presence of N)
(see next page)
no nitrogen, sulfur, halogens, present
other functional groups might be present
(see fourth and fifth page of this section)


Unknown Compound
sodium fusion test
Nitrogen present
amines, amides, nitrocompounds, cyanocompounds, (nitriles), sulfonamides (show also presence of S)
(see page before previous page)
Halogens (Cl, Br, I) present
alkyl halides, acyl halides, aryl halides, sulfonyl halides, (show also presence of S)
(see previous page)
Sulfur present
sulfides
sulfoxides
sulfones
mercaptans
sulfonyl halides (show also presence of halogens)
sulfonamides (show also presence of N)
sulfonic acids
no nitrigen, sulfur or halogens present
other functional groups might be present
(see next two pages)
solubility in NaOH
soluble
sulfonic acids
insoluble
all other S compounds
addition of lead acetate soln.
black ppt
mercaptans
no black ppt
all other S-compounds
addition of dil. HgCl2 soln.
ppt
sulfides
sulfoxides
distinguish between them by TLC
no ppt
sulfones


Unknown Compound
sodium fusion test
Nitrogen present
(see front page of this section)
Halogens present
(see second page of this section)
Sulfur present
(see previous page)
no nitrogen, sulfur, or halogens present
solubility dil. NaOH
soluble
phenols
Carboxylic acids
insoluble
other compounds
solubility in dil. $NaHCO_3$
CO_2 evolution
Carboxylic acid
no CO_2 evolution
phenols
(confirmation test: colors with $FeCl_3$ solution)
2,4 DNP test
orange ppt
aldehydes
ketones
no orange ppt
other compounds
Tollen's test
silver mirror
aldehydes
(test for $CH_3-C(=O)-$ group: iodoform test)
yellow ppt)
no silver mirror
ketones
cerric ammonium nitrate test
orange/red soln.
alcohols
no orange/red soln.
other compounds
(see next page)
distinguish between 1°, 2°, 3° Lucas test
(test for $CH_3CH(OH)-$ group: iodoform test
yellow ppt)
dichromate test
blue-green soln.
1°, 2° alcohols
no change of orange soln.
3° alcohols


Unknown compound
sodium fusion test
Nitrogen present (see first page of this section)
Halogens present (see second page of this section)
Sulfur present (see third page of this section)
no nitrogen, sulfur or halogens present
solubility dil. NaOH
soluble (see previous page)
insoluble
other compounds
2,4-DNP test
orange ppt (see previous page)
no orange ppt
other compounds
cerric amm. nitrate test
orange/red solution (see previous page)
no orange/red solution
other compounds
Br$_2$/CCl$_4$ test
decolorization
no decolorization
alkenes, alkynes, dienes, conj. dienes, terminal alkynes (confirmation with Bayer test: black ppt shows positive test)
other compounds
Quantitative hydrogenation
1 mole H$_2$
alkene
2 moles H$_2$
alkenes, dienes, conj. dienes, terminal alkynes
Diels-Alder reaction
ppt
conj. dienes
no ppt
alkynes, dienes, terminal alkynes
AgNO$_3$/ethanol
no white ppt
alkynes, dienes
white ppt
terminal alkynes
H$_2$O/H$^+$/Hg^{+2}
ketones, aldehydes
alkynes
alcohols
dienes
H$_2$O/heat
acidic soln. (test by litmus paper)
acid anhydrides
neutral solution
alkanes, esters, ethers,
HI
reaction
ethers,
no reaction
esters, alkanes
hydrolysis/NaOH
only esters hydrolyze

Inorganic Group Qualitative Tests

The following tables list some simple chemical tests which will indicate the presence or absence of a given inorganic cation or anion [1]. For most of these tests, the anion or cation must be present at a relatively high concentration (approximate lower bound is 0.05 percent). It may therefore be necessary to concentrate more dilute samples before successful results can be obtained. These tests should be used in conjunction with other methods such as the chromatographic methods or spectrometry and spectrophotometry. Since many of these tests require the use of dangerous compounds, the strictest rules of laboratory safety must be observed at all times. The use of fume hood is required.

REFERENCES:

[1] Barber, H.H., Taylor, T.I., Semimicro Qualitative Analysis, Harper Brothers, New York, 1953.

ACID (ANION) TESTS

	$BaCl_2$	$AgNO_3$	Concentrated H_2SO_4	SPECIAL TESTS
Carbonates, CO_3^{-2}	White, soluble in dilute HCl	Grey	Effervescence, liberating CO_2 (odorless)	Effervescence with all acids, giving CO_2 which renders limewater cloudy
Nitrites NO_2^{-}	....	Dirty yellow precipitate, soluble in hot water	Liberate NO_2 (brown)	Acidified solutions liberate l_2 from KI (brown)
Sulfites SO_3^{-2}	If pure, no precipitate	White precipitate, darkens upon heating (slow)	Liberate SO_2 (pungent)	Acidified solutions decolorize $KMnO_4$ solution
Sulfides S^{-2}	....	Black	Liberate H_2S	Cu or Pb salt solution gives black precipitate
Borates BO_3^{-3}	White, soluble in dilute HCl or $HC_2H_3O_2$	White, soluble in HNO_3 or NH_4OH	....	Free acid gives green color to flame
Chromates CrO_4^{-2}	Yellow	Red brown	....	1. Pb or Ba salt solution give a yellow precipitate 2. H_2S gives a dirty yellow deposit of S

ACID (ANION) TESTS (continued)

	$BaCl_2$	$AgNO_3$	Concentrated H_2SO_4	SPECIAL TESTS
Fluorides F^-	White, insolubel in $HC_2H_3O_2$	....	If concentrated, evolve HF	HF etches glass (only visible after drying)
Silicates SiO_3^{-2}	White	Dirty Yellow	Gelatinous precipitate	Gelatinous precipitate with NH_4Cl
Oxalates $C_2O_4^{-2}$	White, insoluble in $HC_2H_3O_2$	White, slightly soluble in HNO_3	$CO + CO_2$ gas (on ignition, blue flame)	Acidified soluble decolorizes $KMnO_4$ solution
Phosphates PO_4^{-3}	White, soluble in dilute HCl or $HC_2H_3O_2$	Yellow, soluble in HNO_3 or NH_4OH	....	1. White precipitate with Mg^{+2} in presence of an NH_4^+ salt 2. Yellow precipitate with ammonium molybdate in presence of HNO_3
Sulfates SO_4^{-2}	White precipitate	....	....	$BaCl_2$ insoluble--white precipitate, soluble in HCl
Tartarates $C_4H_4O_6^{-2}$	White	Reduce to Ag in alkaline solution	Odor of burned sugar	If very concentrated, precipitate when shaken with a K salt
Bromides Br^-	....	Yellowish, slightly soluble in NH_4OH; insoluble in HNO_3	If concentrated, evolve HBr, Br_2	1. $MnO_2 + H_2SO_4 \rightarrow Br_2$ 2. Cl water in $CS_2 \rightarrow Br_2$ in CS_2 (orange)

ACID (ANION) TESTS (continued)

	$BaCl_2$	$AgNO_3$	Concentrated H_2SO_4	SPECIAL TESTS
Chlorides Cl^-	....	White, soluble in NH_4OH, reprecipitate with HNO_3	If concentrated, evolve HCl (pungent)	1. $MnO_2 + H_2SO_4 \rightarrow Cl_2$ 2. Cl_2 water + CS_2, no coloration
Iodides I^-	....	Yellowish, slightly soluble in NH_4OH; insoluble in HNO_3	If concentrated, evolve HI, I_2	1. $MnO_2 + H_2SO_4 \rightarrow I_2$ 2. Cl_2 water + $CS_2 \rightarrow I_2$ in CS_2 (violet) 3. Starch paste + Cl_2 water-deep blue
Acetates $C_2H_3O_2^-$	....	....	Odor of vinegar	1. $H_2SO_4 + C_2H_6OH \rightarrow C_2H_6C_2H_3O_2$ (pleasing odor) 2. Strong neutral solution gives red coloration with $FeCl_3$ (coagulates on boiling)
Chlorates ClO_3^-	....	....	Liberate ClO_2 (green); Solids decrepitate when warmed with H_2SO_4	1. Solids give off O_2 when heated 2. Acidified solutions bleach litmus paper
Nitrates NO_3^-	....	....	....	1. Add $FeSO_4$, shake; then add concentrated H_2SO_4 (brown ring) 2. Warmed with H_2SO_4 + Cu, produces $NO \rightarrow NO_2$ (brown fumes)

METAL (CATION) TESTS

Group I (precipitate by dilute HCl)--Pb, Ag, Hg (ous)

	LEAD (Pb^{+2})	SILVER (Ag^{+})	MERCURY I (Hg_2^{+2})
	White, soluble in hot water	White, insoluble in hot H_2O, soluble in NH_4OH	White, darkens with NH_4OH
Confirmatory Tests	1. K_2CrO_4--yellow precipitate 2. KI--yellow precipitate 3. H_2SO_4--white precipitate 4. H_2S--black precipitate	1. K_2CrO_4--red, brown precipitate 2. KI--light yellow precipitate 3. Na_2HPO_4--yellow precipitate 4. H_2S--black precipitate	1. K_2CrO_4--orange precipitate 2. KI--grey-green precipitate 3. H_2SO_4--white precipitate 4. Amalgamates Cu or Zn

Group II (Precipitate by H_2S in presence of dilute HCl)--Cu, Hg, Bi, As, Sb, Sn

	COPPER II (Cu^{+2})	MERCURY II (Hg^{+2})	BISMUTH (Bi^{+3})
	Black	Yellow-Black	Brown-Black
Confirmatory Tests	1. Green flame 2. Deposits on Zn or Fe 3. NH_4OH--blue, soluble in excess	1. KI--red precipitate, soluble in excess 2. Amalgamates Cu or Zn 3. NH_4OH--heavy white precipitate	1. KI--brown 2. K_2CrO_4--yellow 3. NH_4OH--white

METAL (CATION) TESTS (continued)

Group II (Precipitate by H_2S in presence of dilute HCl)--Cu, Hg, Bi, As, Sb, Sn (continued)

	ARSENIC (As^{+3})	ANTIMONY (Sb^{+3})	STANNOUS (Sn^{+2})	STANNIC (Sn^{+4})
	Yellow	Orange	Brown	Yellow
Confirmatory Tests	1. H_2S precipitate soluble in yellow $(NH_4)_2S$ 2. Black deposit on Cu 3. (Gives Marsh test)	1. H_2S precipitate soluble in yellow $(NH_4)_2S$ 2. Black deposit on Cu 3. (Gives Marsh test)	1. H_2S precipitate soluble in yellow $(NH_4)_2S$ 2. Spongy deposit on Zn 3. NH_4OH--white 4. Stannous salts reduce $HgCl_2$ and $KMnO_4$	

Group III (Precipitate by NH_4OH in presence of NH_4Cl)--Al, Cr, Fe (ic)

	ALUMINUM (Al^{+3})	CHROMIUM (Cr^{+3})	IRON III (Fe^{+3})
	White gelatinous, soluble in NaOII	Grey-green, soluble in NaOH	Red-brown, insoluble in NaOH
Confirmatory Tests	1. $(NH_4)_2CO_3$--white gelatinous precipitate 2. Na_2HPO_4--white precipitate 3. $Co(NO_3)_2$ test--blue	1. $(NH_4)_2CO_3$--greenish precipitate 2. Na_2HPO_4--green precipitate 3. Borax bead--green	1. KSCN--dark red coloration 2. $K_4Fe(CN)_6$--deep blue 3. Zn and HCl--reduced to Fe^{++} by the nascent H_2

METAL (CATION) TESTS (continued)

Group IV (Precipitate by $NH_4)_2S$ in presence of NH_4Cl)--Zn, Mn, Co, Ni, Fe (ous)

	ZINC (Zn^{+2})	MANGANESE II (Mn^{+2})	COBALT II (Co^{+2})	NICKEL (Ni^{+2})	IRON II (Fe^{+2})
	White, soluble in dilute HCl	Pinkish, soluble in dilute HCl	Black, insoluble in dilute HCl	Black, insoluble in HCl	Black, soluble in HCl
Confirmatory Tests	1. NH_4OH--white soluble in NH_4Cl or $HC_8H_2O_2$ 2. H_2S in presence of $NH_4C_2H_3O_2$--white precipitate	1. NH_4OH--white precipitate, rapidly oxidizing to brown 2. Borax bead--amethyst	1. NH_4OH--green precipitate, quickly dissolving in excess 2. Borax bead--blue	1. NH_4OH--blue precipitate, quickly dissolving in excess 2. Borax bead--brown	1. $K_2Fe(CN)_4$--deep blue 2. KSCN--no color (see 3) 3. Readily oxidized to Fe^{+3} by HNO_3, slowly in air

Group V (Precipitate by $(NH_4)_2CO_3$ in presence of NH_4Cl)--Ba, Sr, Ca

	BARIUM (Ba^{+2})	STRONTIUM (Sr^{+2})	CALCIUM (Ca^{+2})
	White, soluble in dilute HCl	White, soluble in dilute HCl	White, soluble in dilute HCl
Confirmatory Tests	1. $(NH_4)_2C_2O_4$--white, soluble in $HC_2H_3O_2$ 2. $HC_2H_3O_2$ and $K_2Cr_2O_7$--yellow precipitate 3. Green flame (uncertain)	1. $(NH_4)_2C_2O_4$--white, soluble in $HC_2H_3O_2$ 2. $HC_2H_3O_2$ and $K_2Cr_2O_7$--no precipitate 3. Bright red flame	1. $(NH_4)_2C_2O_4$--white, insoluble in $HC_2H_3O_2$ 2. $HC_2H_3O_2$ and $K_2Cr_2O_7$--no precipitate 3. Orange flame

METAL (CATION) TESTS (continued)

Group VI (Precipitate by Na_2HPO_4 in presence of NH_4Cl)--Mg		Group VII (not readily precipitated)--The Alkalies, K, Na, NH_4		
	MAGNESIUM (Mg^{+2})	POTASSIUM (K^+)	SODIUM (Na^+)	AMMONIUM (NH_4^+)
	White, soluble in dilute HCl	Lilac flame	Persistent yellow flame	Gives NH_3 gas on warming with NaOH solution
	Na_2CO_3--white precipitate, soluble in NH_4Cl solution			

VIII. Miscellaneous Tables

Common Drying Agents for Organic Liquids [1,2]

Family	Na_2CO_3 a	K_2CO_3 a	$MgSO_4$ b	$CaSO_4$ c	Na_2SO_4 c	$CaCl_2$	Na	P_2O_5	NaOH (solid)	KOH (solid)	Quick-lime	CaH_2
Alcohols		••••••••	••••••••	••••••••		d	never	never			••••••••	
Aldehydes			••••••••	••••••••	••••••••	d		never				
Alkylhalides						••••••••	••••••••	••••••••				
Amines						d	never	never	••••••••	••••••••	••••••••	f
Arylhalides						••••••••	••••••••	••••••••				
Carboxylic-acids			••••••••	••••••••	••••••••	e	never	never				
Esters			••••••••		••••••••	d						

KEY

a Excellent in salting out
b Best all purpose solvent
c High Capacity, but slow reacting
d Forms complexes
e Lime (common impurity) reacts with acidic hydrogen
f Only for 3° amines ($R_3\ddot{N}$)

REFERENCES:

[1] Vogel, A.I., A Textbook of Practical Organic Chemistry. Longmans, Green & Co., London, 1951.

[2] Brewster, R.Q., Vanderwerf, C.A.; McEwen, W.E., Unitized Experiments in Organic Chemistry, D. Van Nostrand Co., New York, 1977.

Common Drying Agents for Organic Liquids (cont.)

Ethers				•••••		•••••	•••••	•••••				•••••
Hydrocarbons, aromatic				•••••	poor	•••••	•••••	•••••				
Hydrocarbons, saturated				•••••	poor	•••••	•••••	•••••				
Hydrocarbons, unsaturated	•••••	•••••			poor	•••••		•••••				
Ketones		•••••	•••••	•••••	•••••	d		never				
Nitriles								•••••				

KEY

a Excellent in salting out
b Best all purpose solvent
c High Capacity, but slow reacting
d Forms complexes
e Lime (common impurity) reacts with acidic hydrogen
f Only for 3° amines ($R_3\ddot{N}$)

Flammability Hazards of Common Liquids

The following table lists relevant data regarding the flammability of common organic liquids [1,2].

REFERENCES:

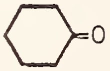
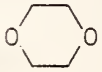
[1] Turner, C. F., McCreery, J. W., The Chemistry of Fire and Hazardous Materials, Allyn and Bacon, Boston, 1981.

[2] E.I. du Pont de Nemours & Co., Inc., Data Safety Sheet, Wilmington, Delaware, 1985.

Solvent	Formula	Specific gravity	Boiling point (°C)	Flash point (°C)	Auto-ignition point (°C)	How to extinguish flames
acetaldehyde	CH_3CHO	0.8	21	-38	185	a,b,c
acetone	$(CH_3)_2CO$	0.8	57	-18	538	a,b
acetonitrile	$CH_3C\equiv N$	0.79	82	6	---	a,c,d
acetylacetone	$CH_3COCH_2COCH_3$	1.0	139	41	---	a,b,c
acrolein	$CH_2{=}CHCHO$	0.8	53	-26	277	a,b,c
acrylonitrile	$CH_2{=}CH{-}CHC\equiv N$	0.81	77	0	481	a,c,d
allylamine	$CH_2{=}CHCH_2NH_2$	0.8	53	-29	374	a,b
amylmercaptan	$CH_3(CH_2)_4SH$	0.8	127	18	---	a,b
aniline	$C_6H_5NH_2$	1.0	184	70	768	a,b,c use masks
anisole	$C_6H_5OCH_3$	1.0	154	52	---	a,b,c
benzaldehyde	C_6H_5CHO	1.1	179	65	192	a,b,c
benzene	C_6H_6	0.88	79	-11	563	a,b,c
bromine	Br_2	3.0	59	---	---	CO_2 (never H_2O)
butyl alcohol	C_4H_9OH	0.8	117	29	366	a,b,c

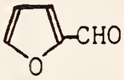
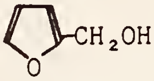
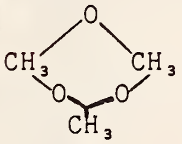
a - alcohol foam, b - carbon dioxide,
c - dry chemical, d - water

Flammability Hazards of Common Liquids (cont.)

Solvent	Formula	Specific gravity	Boiling point (°C)	Flash point (°C)	Auto-ignition point (°C)	How to extinguish flames
t-butylperacetate	$CH_3CO(O_2)C(CH_3)_3$	---	---	<27	---	b,c
t-butylperbenzoate	$C_6H_5CO(O_2)C(CH_3)_3$	>1.0	112	88	8	a,b,c
butyraldehyde	$CH_3(CH_2)_2CHO$	0.8	76	7	230	a,b,c
carbon disulfide	CS_2	1.3	47	-30	100	b,d, use masks
crotonaldehyde	$CH_3CH=CHCHO$	0.9	104	13	232	a,b,c
cumene hydroperoxide	---	1.0	153	175	---	a,b,c
cyclohexanone		0.9	156	43	420	a,b,c
diacetyl	$(CH_3CO)_2$	1.0	88	27	---	a,b,c
diethanolamine	$(HOCH_2CH_2)_2NH$	1.1	269	152	662	b,c
diethylene glycol diethylether	$CH_3(CH_2OCH_2)_3CH_3$	0.9	189	83	---	a, halons
diethylether	$(C_2H_5)_2O$	0.7	34	-45	180	a,b, halons
diethylketone	$(C_2H_5)_2CO$	0.8	101	13	452	a,b,c
dimethyl sulfate	$(CH_3)_2SO_4$	1.3	188	83	188	a,b,c,d
dimethyl sulfide	$(CH_3)_2S$	0.8	37	-18	206	b,c
1,4-dioxane		1.0	101	2	180	a,b,c
ethanol	C_2H_5OH	0.8	78	13	423	a,b,c
ethylacetone (2-pentanone)	$CH_3COCH_2CH_2CH_3$	0.8	102	7	504	a,b,c
ethylamine	$C_2H_5NH_2$	0.7	31	-18	384	a,b,c

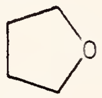
a - alcohol foam, b - carbon dioxide,
c - dry chemical, d - water

Flammability Hazards of Common Liquids (cont.)

Solvent	Formula	Specific gravity	Boiling point (°C)	Flash point (°C)	Auto-ignition point (°C)	How to extinguish flames
ethylenediamine	$H_2NCH_2CH_2NH_2$	0.9	117	34	385	a,b,c
ethyleneglycol	$HOCH_2CH_2OH$	1.1	198	111	413	a,b,c,d
formaldehyde	HCHO	1.0	99	88	427	a,b,c
furfural		1.2	162	60	316	a,b,c,d
furfuryl alcohol		1.1	171	75	491	a,b,c
gasoline	C_7H_{16} (isomers)	<1.0	38-218	-43	257	a,b,c
hexylamine	$C_6H_{13}NH_2$	0.8	132	29	---	a,b
isopropanol	$(CH_3)_2CHOH$	0.8	82	12	399	b,c
isopropyl ether	$((CH_3)_2CH)_2O$	0.7	68	-28	443	a,b
kerosene	CH_4 series mixture	<1.0	149-316	38-71	229	a,b,c
methanol	CH_3OH	0.8	65	11	464	a,b
methylamine (aq)	CH_3NH_2	0.7	31	-18	384	a,b,c
methylaniline	$CH_3NHC_6H_5$	0.8	151	49	533	a,b
methylethyl ketone	$CH_3COCH_2CH_3$	0.8	79	-6	516	a,b,c
methylethyl ketone peroxide	$C_4H_8O_2$	---	---	63	---	a,b
naphtha (mixture)	---	0.8-0.9	149-216	38-46	277-496	a,b,c
paraldehyde		1.0	124	36	238	a,b,c

a - alcohol foam, b - carbon dioxide,
c - dry chemical, d - water

Flammability Hazards of Common Liquids (cont.)

Solvent	Formula	Specific gravity	Boiling point (°C)	Flash point (°C)	Auto-ignition point (°C)	How to extinguish flames
2-pentanone	See Ethylacetone	---	---	---	---	---
3-pentene nitrile	$CH_3CH=CHCH_2C\equiv N$	0.83	14.5	40	---	b,c,d
peracetic acid	CH_3COOOH	1.2	105	40	---	a,b,c
petroleum ether	---	<0.7	38-79	<0	288	a,b,c
propionaldehyde	CH_3CH_2CHO	0.8	49	8	207	a,b,c
propylamine	$CH_3CH_2CH_2NH_2$	0.7	49	-37	318	a,b,c
propylene glycol	$CH_3CHOHCH_2OH$	1.0	188	99	421	a,b
sulfur chloride	S_2Cl_2	1.7	138	118	234	b,c
sulfuryl chloride	$SOCl_2$	1.7	69	---	---	a,b,c
tetrahydrofuran		0.9	60	-17	321	a,b,c
thionylchloride	$SOCl_2$	1.6	79	---	---	---
toluene	$C_6H_5CH_3$	0.87	111	4	510	a,b,c
triethanolamine	$(HOCH_2CH_2)_3N$	1.1	360	179	---	b,c,d
triethylamine	$(C_2H_5)_3N$	0.7	89	7	---	a,b,c
xylene (o-)	$C_6H_4(CH_3)_2$	0.88	144	32	463	a,b,c
xylene (m-)	$C_6H_4(CH_3)_2$	0.86	139	29	527	a,b,c
xylene (p-)	$C_6H_4(CH_3)_2$	0.86	138	39	529	a,b,c

a - alcohol foam, b - carbon dioxide,
c - dry chemical, d - water

Properties of Hazardous Solids

The following table lists some of the more important properties of hazardous room temperature solids commonly used in the analytical laboratory [1,2]

Name	Formula	Specific Gravity at(20°C)	Melting Point, °C	Boiling Point, °C	Flash Point, °C	Autoignition Point, °C	Ignition/Explosion Mechanism	Emergency Procedures
acetyl peroxide	$(CH_3CO)_2O_2$	1.2	30	63	--	--	heat, shock	a,c
adipic acid	$(CH_2)_4(COOH_2$	1.3	152	330	196	420	heat	a,b,c
aluminum	Al	2.7	660	2270	--	--	mixing with iron oxides	a
aluminum chlorate	$Al(ClO_3)_3$	--	--	--	--	--	heat, impact, red agents	a
aluminum chloride	$AlCl_3$	2.4	192	180	--	--	heat, moisture	a
ammonium nitrate	NH_4NO_3	1.7	169	210	--	--	heat	b
ammonium nitrite	NH_4NO_2	1.7	dec	--	70	--	heat, shock, impact	a
ammonium perchlorate	NH_4ClO_4	--	dec	--	--	--	shock, impact	--

a	dry chemicals
b	H_2O
c	CO_2
d	H_2O as a for
e	wet sand
f	chlorinated hydrocarbons

REFERENCES:

[1] Turner, C.F., McCreery, J.W., The Chemistry of Fire and Hazardous Materials, Allyn and Bacon, Boston, 1981.

[2] E.I. du Pont de Nemours & Co., Inc., Safety Sheet, Wilmington, Delaware, 1985.

Name	Formula	Specific Gravity at(20°C)	Melting Point, °C	Boiling Point, °C	Flash Point, °C	Autoignition Point, °C	Ignition/Explosion Mechanism	Emergency Procedures
antimony	Sb	6.7	630	1375	--	--	heat, water	a
antimony trisulfide	SbS_3	4.6	--	--	--	--	heat, strong organic acids, oxidizers	b
antimony pentasulfide	SbS_5	4.1	--	--	--	--	heat, strong oxidizers, acids	a
barium	Ba	3.6	850	1530	--	--	heat	a
beryllium	Be	1.87	1280	1500	--	--	heat, friction	a
cadmium	Cd	8.6	321	765	--	--	heat	a
calcium hypochlorite	$CaCl(C\ell O)\cdot 4H_2O$	--	dec	--	--	--	heat, contact with combustible material, acid	--
camphor	$C_{10}H_{16}O$	1.0	177	sub	66	466	high conc. in air	a,c
cesium	Cs	1.9	29	670	--	--	water	f
iodine	I_2	4.9	113	183	--	--	heat	c(never
lithium	Li	0.53	179	1335	--	--	water, inorg. acids	a
magnesium	Mg	1.75	651	1107	--	--	water	a
phosphorus, red	P_4	2.2	600	sub	--	260	heat, oxidizers	b,e

a	dry chemicals
b	H_2O
c	CO_2
d	H_2O as a for
e	wet sand
f	chlorinated hydrocarbons

Name	Formula	Specific Gravity at(20°C)	Melting Point, °C	Boiling Point, °C	Flash Point, °C	Autoignition Point, °C	Ignition/Explosion Mechanism	Emergency Proecedures
phosphorus, white	P_4	1.82	44	279	ambient	30	heat, oxidizers, dry atmosphere	b
phosphorus, pentachloride	PCl_5	4.7	167	sub	--	--	moist air, heat	a,c
phosphorus, pentasulfide	P_2S_5	2.03	276	514	142	287	water, acids	--
potassium chlorate	$KClO_3$	2.3	368	dec	--	--	charcoal, sulfur and phosphorous	b
potassium nitrate	KNO_3	2.1	334	400	--	999	friction, contact with organics	b
potassium nitrite	KNO_2	1.9	388	dec	--	999	friction, impact	
sodium	Na	0.97	98	890	--	--	moisture	a
sodium hydride	NaH	0.9	800	--	--	--	water, oxidizers	a
sodium nitrate	$NaNO_3$	2.3	307	379	--	--	contact with organics	b
sodium nitrite	$NaNO_2$	2.17	271	318	--	--	contact with organics	b
sodium styrene sulfonate	$C_8H_7SO_3Na$	--	225(dec)	--	--	462	hot surfaces, flames, sparks	a,b,c

a	dry chemicals
b	H_2O
c	CO_2
d	H_2O as a for
e	wet sand
f	chlorinated hydrocarbons

Name	Formula	Specific Gravity at(20°C)	Melting Point, °C	Boiling Point, °C	Flash Point, °C	Autoignition Point, °C	Ignition/Explosion Mechanism	Emergency Proecedures
sulfur	S/S_8	2.07	115	445	207	232	heat	a,d
triphenylboron	$(C_6H_5)_3B$	--	136	347	--	220	water (produces benzene) heat	a,b,c,d

a dry chemicals
b H_2O
c CO_2
d H_2O as a for
wet sand
f chlorinated hydrocarbons

Hazardous Material Log Sheet

The many chemical hazards present in the analytical laboratory must be subject to strict control. To assist in this vital function, a log sheet for each hazardous compound is helpful. The following example, adapted from that suggested by Pfaff [1], is currently used in the analytical laboratory of the Thermophysics Division (774.03) of the National Bureau of Standards, Boulder Laboratories.

[1] Pfaff, R.C., J. Chem. Educ., 62, A282, 1985.

Analytical Laboratory

Hazardous Materials Log Sheet

Name of Material: ____________________

Date of Receipt: __________ Name of Receiver: ____________________

Quantity: __________ Container Size: ____________________

Form of Shipment (i.e., Federal Express, UPS, etc.): ____________________

Condition of Shipment or Sample: ____________________

Distribution of Material: Amount: __________ Building: __________

Room Number: ________ Name of Principal Investigator: ____________________

Date: __________ Signature of Recipient: ____________________

Exact Storage Location: ____________________

Material Safety Data Sheet Available: Yes ______ No ______

Approved Safety Plan Available: Yes ______ No ______

Disposal: Amount: __________ Date: ________ Program: ____________________

Disposal Data: ____________________

Health and Safety Impact: ____________________

Unit Conversions

The international system of units is described in detail in NBS Special Publication 330 [1] and lists of physical constants and conversions factors are tabulated by Mechtly [2]. The American Society for Testing and Materials (ASTM), American National Standards Institute (ANSI), and 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 are given in the following tables.

References:

[1] The International System of Units, National Bureau of Standards (U.S.) Special Publication SP-330 (Aug. 1977).

[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).

Density

kg/m^3	g/cm^3	Amagat	lb/ft^3
16.018	0.016018	178.216	1
1	0.001	11.126	0.062428
1,000	1	1.1126×10^{4}	62.428
2,015.9	2.0159	2.2428×10^{4}	125.85
0.089881	8.9881×10^{-5}	1	5.6111×10^{-3}

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
4.9605×10^{-4}	0.49605	7.9458×10^{-3}

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

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
0.49605	0.11856	0.21341
4.1840	1	1.8

Specific Heat, Entropy

kJ/kg-K (J/g-K)	Btu/°R
4.184	1
1	0.23901
0.49605	0.11856
2.0755	0.49605

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

Viscosity

kg/m-s ($N-s/m^2$)	Centipoise (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

Velocity of Sound

m/s	ft/s
0.3048	1
1	3.2808

Surface Tension

N/m	dyne/cm	lb_f/in.
175.13	175.13×10^3	1
1	1,000	5.7102×10^{-3}
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

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Tables of important data for use in the analytical chemistry laboratory are provided. These tables contain information for use in gas chromatography, liquid chromatography, infrared and ultraviolet spectrophotometry, mass spectrometry, and wet chemical techniques. Tables relating to safe practice in the analytical laboratory are also included.

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The National Bureau of Standards[1] was established by an act of Congress on March 3, 1901. The Bureau's overall goal is to strengthen and advance the nation's science and technology and facilitate their effective application for public benefit. To this end, the Bureau conducts research and provides: (1) a basis for the nation's physical measurement system, (2) scientific and technological services for industry and government, (3) a technical basis for equity in trade, and (4) technical services to promote public safety. The Bureau's technical work is performed by the National Measurement Laboratory, the National Engineering Laboratory, the Institute for Computer Sciences and Technology, and the Institute for Materials Science and Engineering.

The National Measurement Laboratory

Provides the national system of physical and chemical measurement; coordinates the system with measurement systems of other nations and furnishes essential services leading to accurate and uniform physical and chemical measurement throughout the Nation's scientific community, industry, and commerce; provides advisory and research services to other Government agencies; conducts physical and chemical research; develops, produces, and distributes Standard Reference Materials; and provides calibration services. The Laboratory consists of the following centers:

- Basic Standards[2]
- Radiation Research
- Chemical Physics
- Analytical Chemistry

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- Applied Mathematics
- Electronics and Electrical Engineering[2]
- Manufacturing Engineering
- Building Technology
- Fire Research
- Chemical Engineering[2]

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- Inorganic Materials
- Fracture and Deformation[3]
- Polymers
- Metallurgy
- Reactor Radiation

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[1] Headquarters and Laboratories at Gaithersburg, MD, unless otherwise noted; mailing address Gaithersburg, MD 20899.

[2] Some divisions within the center are located at Boulder, CO 80303.

[3] Located at Boulder, CO, with some elements at Gaithersburg, MD.

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