

**J. Gmehling
U. Onken
W. Arlt**

VAPOR-LIQUID EQUILIBRIUM DATA COLLECTION

Halogen, Nitrogen, Sulfur and other Compounds



Chemistry Data Series

Vol. I, Part 8

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Editors: Dieter Behrens, Reiner Eckermann**

Vapor-Liquid Equilibrium Data Collection

8

**Halogen, Nitrogen, Sulfur and other
Compounds**

Tables and diagrams of data for binary and multicomponent mixtures up to moderate pressures. Constants of correlation equations for computer use.

J. Gmehling, U. Onken, W. Arlt

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8

Halogen, Nitrogen, Sulfur and other Compounds

Systems with:

Halogenated Hydrocarbons

Silanes, Siloxanes

Nitro Compounds, Amines, Imines, Oximes, Nitriles,
Isocyanates, Amides, Pyrrolidines, Pyridines,
Quinolines

Mercaptans, Sulfides, Sulfoxides, Carbon Disulfide,
Thiophenes, Thiazoles

SUBJECTS OF VOLUME I

The table lists all parts of Volume I with year of publication.

Subtitle	Vol. I, Part
Aqueous-Organic Systems	1 (1980)
Supplement 1	1a (1981)
Organic Hydroxy Compounds	
Alcohols	2a (1977)
Alcohols and Phenols	2b (1978)
Supplement 1	2c (1982)
Supplement 2	2d (1982)
Aldehydes, Ketones, Ethers	3/4 (1979)
Carboxylic Acids, Anhydrides, Esters	5 (1982)
Aliphatic Hydrocarbons C ₄ -C ₆	6a (1980)
Aliphatic Hydrocarbons C ₇ -C ₁₈	6b (1980)
Supplement 1	6c (1984)
Aromatic Hydrocarbons	7 (1980)
Halogen, Nitrogen, Sulfur and other Compounds	8 (1984)

AUTHORS' PREFACE

The appearance of this volume marks the completion of our VLE data collection. When we began publishing this series in 1977, we were not aware of the amount of work ahead. Perhaps if we really had known then what we were embarking upon, we might not have started. And we were able to continue during these years because we have been lucky enough to obtain collaboration and to find encouragement from all the members of our team and from many colleagues.

In preparing this part we were helped by Dipl.-Chem. J. Berg, Dipl.-Ing. P. Grenzheuser, Mrs. Dr. B. Kolbe, Mrs. L. Kunzner, Dipl.-Chem. J. Menke, Mrs. Dipl.-Chem. U. Schwaitzer, Dipl.-Chem. D. Tiegs, Dipl.-Chem. U. Weidlich and by the students R. Rarey and J. Schomschor. For translating some sources of VLE data we were able to draw on the help of two of our foreign guests during their research stay with us: Ing. Yang Zhendong from the People's Republic of China, who translated several publications from Chinese, and Ing. C. Osorio Bastiades, who assisted us in understanding some Spanish nomenclature. They and all co-workers mentioned in the other parts of our data collection deserve our wholehearted thanks. Likewise we should again like to express our gratitude to the computer center of the University of Dortmund, especially to Mr. T. Blaszyk for his co-operation, and to Dr. R. Eckermann and Dipl.-Ing. C. Hammer (both DECHEMA, Frankfurt/M.) for their efforts in the editing of our data collection.

Finally, we must not forget the numerous suggestions and the stimulation coming from colleagues from all over the world. We shall continue our work on the DDB (Dortmund VLE Data Bank), adding newly published results and publishing supplements to the data collection from time to time. On this occasion we should again like to ask all workers in the field of vapour-liquid equilibrium to send us reprints containing new results. This will help to ensure that this truly international partnership can grow and continue.

Dortmund, May 1984

Ulfert Onken

Jürgen Gmehling

Wolfgang Art

PREFACE OF EDITORS

Subjects of the Dechema Chemistry Data Series are the physical and thermodynamic property data of chemical compounds and mixtures essentially for the fluid state covering PVT data, heat capacity, enthalpy, and entropy data, phase equilibrium data, transport and interfacial tension data.

The main purpose is to provide chemists and engineers with data for process design and development. For computer based calculations in process design appropriate correlation methods and accurate data must be used. These are only in some cases available in the open literature. For that reason the most urgent requirement regarding the publication of data is to offer classified and critically evaluated data, thus giving an impression which of them are reliable or not. This will be the goal of the series.

DECHEMA gives the opportunity to authors especially from universities to publish not only their theoretical results, but also their measured or compiled data, most often a large amount, that would otherwise never have been published.

The research work of Dr. Gmehling, Prof. Onken and co-workers on vapor-liquid equilibria which was partly supported by the Federal Ministry of Research and Technology and DECHEMA has been very fruitful; in particular, it led to an extension of the UNIFAC method. The authors have produced what is probably the largest collection of vapor-liquid equilibrium data that is today available with evaluation programs and experimental data.

We present the evaluation of this material in several parts of the first volume of the series. We hope that this gives particularly the users an instrument that will allow them to solve their problems considerably more easily and quickly than before.

Frankfurt/Main, May 1984

Dieter Behrens
Reiner Eckermann

CONTENTS
Vol. I, Part 8

Subjects of Volume I	VI
Authors' Preface	VII
Preface of Editors	VIII
Contents Volume I, Part 8	IX
Contents Volume I, Part 1	XIII
Contents Volume I, Part 1a	XIV
Contents Volume I, Part 2a	XV
Contents Volume I, Part 2b	XVI
Contents Volume I, Part 2c	XVIII
Contents Volume I, Part 2d	XX
Contents Volume I, Parts 3 + 4	XXIII
Contents Volume I, Part 5	XXV
Contents Volume I, Part 6a	XXVIII
Contents Volume I, Part 6b	XXX
Contents Volume I, Part 6c	XXXII
Contents Volume I, Part 7	XXXV
Guide to Tables	XXXVII
List of Symbols	XLVII
References	IL
Data Tables	1
Binary Systems	1
Trifluorobromomethane	1
Cyanogen Chloride	17
Dichlorodifluoromethane	18
Tetrachloromethane	55
Tribromomethane	193
Difluorochloromethane	197
Dichlorofluoromethane	201
Chloroform	202
Hydrogen Cyanide	248
Bromochloromethane	250
Dibromomethane	252
Dichloromethane	255
Methyltrichlorosilane	269
N-Deuteromethylamine	273

Methyl Iodide	278
Nitromethane	279
Methyldichlorosilane	302
Methanethiol	305
Methylamine	312
Carbon Disulfide	316
1,1,2-Trichloro-1,2,2-Trifluoroethane	323
Tetrachloroethylene	324
Trichloroethylene	348
1,1-Dichloroethylene	353
cis-1,2-Dichloroethylene	355
trans-1,2-Dichloroethylene	357
1,1,1,2-Tetrachloroethane	358
1,1,2,2-Tetrachloroethane	359
Vinyl Chloride	362
1,1,1-Trichloroethane	363
Acetonitrile	364
Methyl Isocyanate	388
1,2-Dibromoethane	390
1,1-Dichloroethane	397
Ethyl Bromide	400
Ethyl Iodide	401
N-Methylformamide	402
Dimethyldichlorosilane	405
Dimethyl Sulfoxide	407
Dimethyl Sulfide	408
Ethanethiol	409
Ethylamine	410
Acrylonitrile	414
1,1,1,3-Tetrachloropropane	417
3-Bromo-1-Propene	418
3-Chloro-1-Propene	419
Acetone Oxime	421
N,N-Dimethylformamide	425
Propionaldehyde Oxime	430
1-Nitropropane	434
Trimethylchlorosilane	436
Isopropylamine	437
2,2,3-Trichloroheptafluorobutane	439

Thiophene	440
2-Chloro-1,3-Butadiene	441
2,3,4-Trichloro-1-Butene	444
Allyl Cyanide	445
Butyl Bromide	447
tert-Butyl Bromide	448
Butyl Chloride	452
sec-Butyl Chloride	456
Pyrrolidine	461
Methyl Ethyl Ketoxime	463
tert-Butylhydroperoxide	464
(Bromomethyl)Trimethylsilane	465
Butylamine	472
Diethylamine	474
Pyridine	497
Piperidine	504
Hexafluorobenzene	505
Perfluorohexane	514
o-Dichlorobenzene	515
Bromobenzene	516
Chlorobenzene	517
Trichlorophenylsilane	536
Nitrobenzene	540
m-Chloroaniline	545
p-Chloroaniline	546
Aniline	547
2-Methylpyridine	559
3-Methylpyridine	560
Adiponitrile	562
Chlorocyclohexane	566
Hexamethylene Imine	568
Benzoyl Chloride	573
Benzyl Chloride	574
o-Chlorotoluene	577
N-Methylaniline	578
Isoquinoline	582
Lepidine	584
Trichlorosilane	585

Ternary Systems	
Tetrachloromethane	586
Chloroform	590
Bromochloromethane	595
Appendix A: Pure Component Parameters	597
Formula Index of Systems	603
Alphabetical Index of Systems	623

Formula Index of Systems

R = RECOMMENDED VALUES

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE		
CBRF3	TRIFLUOROBROMOMETHANE				
	CHCLF2	DI FLUOROCHLOROMETHANE	1- 16		
CCLN	CYANOGEN CHLORIDE				
	CHN	HYDROGEN CYANIDE	17		
CCL2F2	DICHLORODIFLUOROMETHANE				
	CHCLF2	DI FLUOROCHLOROMETHANE	18- 37 37		
	CHF3	FLUOROFORM	38- 42		
	C2CL3F3	1,1,2-TRICHLORO-1,2,2-TRIFLUOROETHANE	43- 45		
	C2H4F2	1,1-DIFLUOROETHANE	46		
	C3F6	PERFLUOROPROPYLENE	47		
	C4F8	PERFLUOROCYCLOBUTANE	48- 54		
CCL4	TETRACHLOROMETHANE				
	CHCL3	CHLOROFORM	55- 61		
		CH2CL2	DICHLOROMETHANE	586-587	
	CH2CL2	DICHLOROMETHANE	62- 67		
		CHCL3	CHLOROFORM	586-587	
	CH3I	METHYL IODIDE	68		
	CH3NO2	NITROMETHANE	69		
	CH5N	METHYLAMINE	70- 72		
	CS2	CARBON DISULFIDE	73- 76		
	C2CL4	TETRACHLOROETHYLENE	77- 79 79		
	C2HCL3	TRICHLOROETHYLENE	80- 81		
		C2H4CL2	1,2-DICHLOROETHANE	588-589	
	C2H3CL3	1,1,1-TRICHLOROETHANE	82- 84		
	C2H3N	ACETONITRILE	85- 87		
	C2H3NO	METHYL ISOCYANATE	88- 89		
	C2H4BR2	1,2-DIBROMOETHANE	90- 92		
	C2H4CL2	1,1-DICHLOROETHANE	93- 98		
	C2H4CL2	1,2-DICHLOROETHANE	C2HCL3	TRICHLOROETHYLENE	588-589
	C2H5I	ETHYL IODIDE	99		
	C2H5NO	N-METHYLFORMAMIDE	100-104 104		
	C2H5NO2	NITROETHANE	105		

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
=====			
CCL4	TETRACHLOROMETHANE		
C2H6OS	DIMETHYL SULFOXIDE		106-107
C2H7N	DIMETHYLAMINE		108-110
C3H3N	ACRYLONITRILE		111-112
C3H3NS	THIAZOLE		113
C3H7NO	N,N-DIMETHYLFORMAMIDE		114-118 118 R
C3H7NO2	1-NITROPROPANE		119-120
C3H9N	TRIMETHYLAMINE		121-123
C4H4S	THIOPHENE		124
C4H9CL	TERT-BUTYL CHLORIDE		125-128
C4H9NO	METHYL ETHYL KETOXIME		129
C4H11N	DIETHYLAMINE		130-133 133 R
C5H5N	PYRIDINE		134-143 143 R
C6F6	HEXAFLUOROBENZENE		144-151
C6H5BR	BROMOBENZENE		152-157 157 R
C6H5CL	CHLOROBENZENE		158-167 167 R
C6H5NO2	NITROBENZENE		168
C6H7N	ANILINE		169-174
C6H15N	TRIETHYLAMINE		175-176
C7H9N	N-METHYLANILINE		177-180 180 R
C8H24O4Si4	OCTAMETHYLCYCLOTETRASILOXANE		181-185
CL4Si	SILICON TETRACHLORIDE		186-192 192 R
=====			
CHBR3	TRIBROMOMETHANE		
C2H6OS	DIMETHYL SULFOXIDE		193
C5H5N	PYRIDINE		194-196
=====			
CHCLF2	DIFLUOROCHLOROMETHANE		
CBRF3	TRIFLUOROBROMOMETHANE		1- 16
CCL2F2	DICHLORODIFLUOROMETHANE		18- 37 37 R
C2CL2F4	1,2-DICHLOROTETRAFLUOROETHANE		197-198
C3F6	PERFLUOROPROPYLENE		199
C4F8	PERFLUOROCYCLOBUTANE		200
=====			
CHCL2F	DICHLOROFLUOROMETHANE		
C4F8	PERFLUOROCYCLOBUTANE		201

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE	
CHCL3	CHLOROFORM			
CCL4	TETRACHLOROMETHANE		55- 61	
		CH2CL2	DICHLOROMETHANE	586-587
CH2CL2	DICHLOROMETHANE		202-203	
		CCL4	TETRACHLOROMETHANE	586-587
CH3I	METHYL IODIDE		204-205	
CS2	CARBON DISULFIDE		206-214	
		C6H18OSI2	HEXAMETHYLDISILOXANE	590-591
C2CL4	TETRACHLOROETHYLENE		215	
C2H3N	ACETONITRILE		216-218	
C2H4CL2	1,1-DICHLOROETHANE		219-224	
		C2H4CL2	1,2-DICHLOROETHANE	592-594
C2H4CL2	1,2-DICHLOROETHANE	C2H4CL2	1,1-DICHLOROETHANE	592-594
C2H6OS	DIMETHYL SULFOXIDE		225-235 235	
C3H8S	METHYL ETHYL SULFIDE		236	
C5H5N	PYRIDINE		237-243	
C6H5CL	CHLOROBENZENE		244	
C6H7N	2-METHYLPYRIDINE		245-246	
C6H15N	TRIETHYLAMINE		247	
C6H18OSI2	HEXAMETHYLDISILOXANE	CS2	CARBON DISULFIDE	590-591
CHF3	FLUOROFORM			
CCL2F2	DICHLORODIFLUOROMETHANE		38- 42	
CHN	HYDROGEN CYANIDE			
CCLN	CYANOGEN CHLORIDE		17	
C3H5CL	3-CHLORO-1-PROPENE		248	
C4H5N	ALLYL CYANIDE		249	
CH2BRCL	BROMOCHLOROMETHANE			
CH2BR2	DIBROMOMETHANE		250	
		CH2CL2	DICHLOROMETHANE	595-596
CH2CL2	DICHLOROMETHANE		251	
		CH2BR2	DIBROMOMETHANE	595-596
CH2BR2	DIBROMOMETHANE			
CH2BRCL	BROMOCHLOROMETHANE		250	
		CH2CL2	DICHLOROMETHANE	595-596
CH2CL2	DICHLOROMETHANE		252	
		CH2BRCL	BROMOCHLOROMETHANE	595-596
C2H6OS	DIMETHYL SULFOXIDE		253-254	

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
CH2CL2	DICHLOROMETHANE		
CCL4	TETRACHLOROMETHANE		62-67
		CHCL3 CHLOROFORM	586-587
CHCL3	CHLOROFORM		202-203
		CCL4 TETRACHLOROMETHANE	586-587
CH2BRCL	BROMOCHLOROMETHANE		251
		CH2BR2 DIBROMOMETHANE	595-596
CH2BR2	DIBROMOMETHANE		252
		CH2BRCL BROMOCHLOROMETHANE	595-596
CH3I	METHYL IODIDE		255
C2CL4	TETRACHLOROETHYLENE		256
C2H3N	ACETONITRILE		257-259
C2H4CL2	1,2-DICHLOROETHANE		260-263
C2H6OS	DIMETHYL SULFOXIDE		264
C3H7NO	N,N-DIMETHYLFORMAMIDE		265
C4H8O2S	SULFOLANE		266
C5H5N	PYRIDINE		267
C6H15N	TRIETHYLAMINE		268
CH3CL3SI	METHYLTRICHLOROSILANE		
C3H9CL3SI	TRIMETHYLCHLOROSILANE		269-270
CL4SI	SILICON TETRACHLORIDE		271-272
CH3D2N	N-DEUTEROMETHYLAMINE		
C3H9N	TRIMETHYLAMINE		273-277
CH3I	METHYL IODIDE		
CCL4	TETRACHLOROMETHANE		68
CHCL3	CHLOROFORM		204-205
CH2CL2	DICHLOROMETHANE		255
CS2	CARBON DISULFIDE		278
CH3NO2	NITROMETHANE		
CCL4	TETRACHLOROMETHANE		69
CS2	CARBON DISULFIDE		279
C2HCL3	TRICHLOROETHYLENE		280
C2H3N	ACETONITRILE		281-284
C2H5I	ETHYL IODIDE		285-286
C2H5NO2	NITROETHANE		287-290
C3H7NO	N,N-DIMETHYLFORMAMIDE		291

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE	
CH3NO2	NITROMETHANE			
C4H4S	THIOPHENE		292-293	
C4H9CL	BUTYL CHLORIDE		294-296	
C5H6N2	GLUTARONITRILE		297	
C6H5CL	CHLOROBENZENE		298-300	
C6H5NO2	NITROBENZENE		301	
CH4CL2SI	METHYLDICHLOROSILANE			
CL3HSI	TRICHLOROSILANE		302	
CL4SI	SILICON TETRACHLORIDE		303-304	
CH4S	METHANETHIOL			
CH5N	METHYLAMINE		305	
C2H3N	ACETONITRILE		306	
C2H6OS	DIMETHYL SULFOXIDE		307	
C2H6S	DIMETHYL SULFIDE		308-310	
C3H7NO	N,N-DIMETHYLFORMAMIDE		311	
CH5N	METHYLAMINE			
CCL4	TETRACHLOROMETHANE		70-72	
CH4S	METHANETHIOL		305	
C3H9N	TRIMETHYLAMINE		312-315	
CS2	CARBON DISULFIDE			
CCL4	TETRACHLOROMETHANE		73-76	
CHCL3	CHLOROFORM		206-214	
		C6H18OSI2	HEXAMETHYLDISILOXANE	590-591
CH3I	METHYL IODIDE		278	
CH3NO2	NITROMETHANE		279	
C2CL4	TETRACHLOROETHYLENE		316-319 319	
C2H3N	ACETONITRILE		320	
C4H9CL	ISOBUTYL CHLORIDE		321-322	
C6H18OSI2	HEXAMETHYLDISILOXANE	CHCL3	CHLOROFORM	590-591
C2CL2F4	1,2-DICHLOROTETRAFLUOROETHANE			
CHCLF2	DIFLUOROCHLOROMETHANE		197-198	
C2CL3F3	1,1,2-TRICHLORO-1,2,2-TRIFLUOROETHANE			
CCL2F2	DICHLORODIFLUOROMETHANE		43-45	
C12F27N	PERFLUOROTRIBUTYLAMINE		323	

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
C2CL4	TETRACHLOROETHYLENE		
CCL4	TETRACHLOROMETHANE		77-79 79 R
CHCL3	CHLOROFORM		215
CH2CL2	DICHLOROMETHANE		256
CS2	CARBON DISULFIDE		316-319 319 R
C2HCL3	TRICHLOROETHYLENE		324-332 332 R
C2H2CL4	1,1,2,2-TETRACHLOROETHANE		333-337
C2H3CL3	1,1,2-TRICHLOROETHANE		338-339
C2H4CL2	1,2-DICHLOROETHANE		340
C3H3N	ACRYLONITRILE		341-342
C5H5N	PYRIDINE		343-347 347 R
C2HCL3	TRICHLOROETHYLENE		
CCL4	TETRACHLOROMETHANE		80-81
		C2H4CL2 1,2-DICHLOROETHANE	588-589
CH3NO2	NITROMETHANE		280
C2CL4	TETRACHLOROETHYLENE		324-332 332 R
C2H2CL2	TRANS-1,2-DICHLOROETHYLENE		348
C2H3N	ACETONITRILE		349-350
C2H4CL2	1,2-DICHLOROETHANE		351
		CCL4 TETRACHLOROMETHANE	588-589
C4H10S	DIETHYL SULFIDE		352
C2H2CL2	1,1-DICHLOROETHYLENE		
C2H3CL	VINYL CHLORIDE		353
C3H3N	ACRYLONITRILE		354
C2H2CL2	CIS-1,2-DICHLOROETHYLENE		
C2H2CL2	TRANS-1,2-DICHLOROETHYLENE		355
C2H3CL3	1,1,1-TRICHLOROETHANE		356
C2H2CL2	TRANS-1,2-DICHLOROETHYLENE		
C2HCL3	TRICHLOROETHYLENE		348
C2H2CL2	CIS-1,2-DICHLOROETHYLENE		355
C2H3CL3	1,1,1-TRICHLOROETHANE		357
C2H2CL4	1,1,1,2-TETRACHLOROETHANE		
C2H2CL4	1,1,2,2-TETRACHLOROETHANE		358

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
C2H2CL4	1,1,2,2-TETRACHLOROETHANE		
C2CL4	TETRACHLOROETHYLENE		333-337
C2H2CL4	1,1,1,2-TETRACHLOROETHANE		358
CL2O2S	SULFURYL CHLORIDE		359-361
C2H3CL	VINYL CHLORIDE		
C2H2CL2	1,1-DICHLOROETHYLENE		353
C2H4CL2	1,2-DICHLOROETHANE		362
C2H3CL3	1,1,1-TRICHLOROETHANE		
CCL4	TETRACHLOROMETHANE		82- 84
C2H2CL2	CIS-1,2-DICHLOROETHYLENE		356
C2H2CL2	TRANS-1,2-DICHLOROETHYLENE		357
C2H4CL2	1,2-DICHLOROETHANE		363
C2H3CL3	1,1,2-TRICHLOROETHANE		
C2CL4	TETRACHLOROETHYLENE		338-339
C2H3N	ACETONITRILE		
CCL4	TETRACHLOROMETHANE		85- 87
CHCL3	CHLOROFORM		216-218
CH2CL2	DICHLOROMETHANE		257-259
CH3NO2	NITROMETHANE		281-284
CH4S	METHANETHIOL		306
CS2	CARBON DISULFIDE		320
C2HCL3	TRICHLOROETHYLENE		349-350
C2H4CL2	1,2-DICHLOROETHANE		364
C3H3N	ACRYLONITRILE		365-374 374 R
C4H9CL	BUTYL CHLORIDE		375-377
C6H5CL	CHLOROBENZENE		378-382
C6H7N	ANILINE		383-385
C6H7N	2-METHYLPYRIDINE		386
CL4SI	SILICON TETRACHLORIDE		387
C2H3NO	METHYL ISOCYANATE		
CCL4	TETRACHLOROMETHANE		88- 89
C2H4CL2	1,2-DICHLOROETHANE		388
C6H5CL	CHLOROBENZENE		389

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
C2H4BR2	1,2-DIBROMOETHANE		
CCL4	TETRACHLOROMETHANE		90-92
C3H6BR2	1,2-DIBROMOPROPANE		390-391
C3H7NO2	1-NITROPROPANE		392-394 394
C6H5CL	CHLOROBENZENE		395-396
C2H4CL2	1,1-DICHLOROETHANE		
CCL4	TETRACHLOROMETHANE		93-98
CHCL3	CHLOROFORM		219-224
		C2H4CL2 1,2-DICHLOROETHANE	592-594
C2H4CL2	1,2-DICHLOROETHANE		397-399
		CHCL3 CHLOROFORM	592-594
C2H4CL2	1,2-DICHLOROETHANE		
CCL4	TETRACHLOROMETHANE	C2HCL3 TRICHLOROETHYLENE	588-589
CHCL3	CHLOROFORM	C2H4CL2 1,1-DICHLOROETHANE	592-594
CH2CL2	DICHLOROMETHANE		260-263
C2CL4	TETRACHLOROETHYLENE		340
C2HCL3	TRICHLOROETHYLENE		351
		CCL4 TETRACHLOROMETHANE	588-589
C2H3CL	VINYL CHLORIDE		362
C2H3CL3	1,1,1-TRICHLOROETHANE		363
C2H3N	ACETONITRILE		364
C2H3NO	METHYL ISOCYANATE		388
C2H4CL2	1,1-DICHLOROETHANE		397-399
		CHCL3 CHLOROFORM	592-594
C2H4F2	1,1-DIFLUOROETHANE		
CCL2F2	DICHLORODIFLUOROMETHANE		46
C2H5BR	ETHYL BROMIDE		
C2H5I	ETHYL IODIDE		400
C2H5I	ETHYL IODIDE		
CCL4	TETRACHLOROMETHANE		99
CH3NO2	NITROMETHANE		285-286
C2H5BR	ETHYL BROMIDE		400
C6H5NO2	NITROBENZENE		401

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
C2H5NO	N-METHYLFORMAMIDE		
	CCL4	TETRACHLOROMETHANE	100-104 104 R
	C2H6OS	DIMETHYL SULFOXIDE	402
	C3H7NO	N-METHYLACETAMIDE	403-404
C2H5NO2	NITROETHANE		
	CCL4	TETRACHLOROMETHANE	105
	CH3NO2	NITROMETHANE	287-290
C2H6CL2SI	DIMETHYLDICHLOROSILANE		
	C3H9CLSI	TRIMETHYLCHLOROSILANE	405
	CL4SI	SILICON TETRACHLORIDE	406
C2H6OS	DIMETHYL SULFOXIDE		
	CCL4	TETRACHLOROMETHANE	106-107
	CHBR3	TRIBROMOMETHANE	193
	CHCL3	CHLOROFORM	225-235 235 R
	CH2BR2	DIBROMOMETHANE	253-254
	CH2CL2	DICHLOROMETHANE	264
	CH4S	METHANETHIOL	307
	C2H5NO	N-METHYLFORMAMIDE	402
	C3H7NO	N,N-DIMETHYLFORMAMIDE	407
C2H6S	DIMETHYL SULFIDE		
	CH4S	METHANETHIOL	308-310
	C2H6S	ETHANETHIOL	408
C2H6S	ETHANETHIOL		
	C2H6S	DIMETHYL SULFIDE	408
	C3H7NO	N,N-DIMETHYLFORMAMIDE	409
C2H7N	DIMETHYLAMINE		
	CCL4	TETRACHLOROMETHANE	108-110
C2H7N	ETHYLAMINE		
	C4H11N	DIETHYLAMINE	410-411
	C6H15N	TRIETHYLAMINE	412-413

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
C3F6	PERFLUOROPROPYLENE		
	CCL2F2	DICHLORODIFLUOROMETHANE	47
	CHCLF2	DIFLUOROCHLOROMETHANE	199
C3H3N	ACRYLONITRILE		
	CCL4	TETRACHLOROMETHANE	111-112
	C2CL4	TETRACHLOROETHYLENE	341-342
	C2H2CL2	1,1-DICHLOROETHYLENE	354
	C2H3N	ACETONITRILE	365-374 374
	C3H5N	PROPIONITRILE	414-415
	C4H5CL	2-CHLORO-1,3-BUTADIENE	416
C3H3NS	THIAZOLE		
	CCL4	TETRACHLOROMETHANE	113
C3H4CL4	1,1,1,3-TETRACHLOROPROPANE		
	C5H8CL4	1,1,1,5-TETRACHLOROPENTANE	417
C3H5BR	3-BROMO-1-PROPENE		
	C3H5CL	3-CHLORO-1-PROPENE	418
C3H5CL	3-CHLORO-1-PROPENE		
	CHN	HYDROGEN CYANIDE	248
	C3H5BR	3-BROMO-1-PROPENE	418
	C3H7CL	ISOPROPYL CHLORIDE	419
	C4H5N	ALLYL CYANIDE	420
C3H5N	PROPIONITRILE		
	C3H3N	ACRYLONITRILE	414-415
C3H6BR2	1,2-DIBROMOPROPANE		
	C2H4BR2	1,2-DIBROMOETHANE	390-391
C3H7CL	ISOPROPYL CHLORIDE		
	C3H5CL	3-CHLORO-1-PROPENE	419
C3H7NO	ACETONE OXIME		
	C3H7NO	PROPIONALDEHYDE OXIME	421-422
	C4H9NO	BUTYRALDEHYDE OXIME	423-424

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
C3H7NO	N,N-DIMETHYLFORMAMIDE		
CCL4	TETRACHLOROMETHANE		114-118 118 R
CH2CL2	DICHLOROMETHANE		265
CH3NO2	NITROMETHANE		291
CH4S	METHANETHIOL		311
C2H6OS	DIMETHYL SULFOXIDE		407
C2H6S	ETHANETHIOL		409
C4H4S	THIOPHENE		425
C5H6N2	GLUTARONITRILE		426
C6H7N	ANILINE		427-428
C7H9N	N-METHYLANILINE		429
C3H7NO	N-METHYLACETAMIDE		
C2H5NO	N-METHYLFORMAMIDE		403-404
C3H7NO	PROPIONALDEHYDE OXIME		
C3H7NO	ACETONE OXIME		421-422
C4H9NO	BUTYRALDEHYDE OXIME		430-431
C4H9NO	METHYL ETHYL KETOXIME		432-433
C3H7NO2	1-NITROPROPANE		
CCL4	TETRACHLOROMETHANE		119-120
C2H4BR2	1,2-DIBROMOETHANE		392-394 394 R
C6H5CL	CHLOROBENZENE		434-435
C3H8S	METHYL ETHYL SULFIDE		
CHCL3	CHLOROFORM		236
C3H9CLSI	TRIMETHYLCHLOROSILANE		
CH3CL3SI	METHYLTRICHLOROSILANE		269-270
C2H6CL2SI	DIMETHYLDICHLOROSILANE		405
CL4SI	SILICON TETRACHLORIDE		436
C3H9N	ISOPROPYLAMINE		
C6H15N	DIISOPROPYLAMINE		437-438
C3H9N	TRIMETHYLAMINE		
CCL4	TETRACHLOROMETHANE		121-123
CH3D2N	N-DEUTEROMETHYLAMINE		273-277
CH5N	METHYLAMINE		312-315

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
C4CL3F7	2,2,3-TRICHLOROHEPTAFLUOROBUTANE		
	C5CL2F6	1,2-DICHLOROHEXAFLUOROCYCLOPENTENE	439
C4F8	PERFLUOROCYCLOBUTANE		
	CCL2F2	DICHLORODIFLUOROMETHANE	48-54
	CHCLF2	DIFLUOROCHLOROMETHANE	200
	CHCL2F	DICHLOROFLUOROMETHANE	201
C4H4S	THIOPHENE		
	CCL4	TETRACHLOROMETHANE	124
	CH3NO2	NITROMETHANE	292-293
	C3H7NO	N,N-DIMETHYLFORMAMIDE	425
	C5H5N	PYRIDINE	440
C4H5CL	2-CHLORO-1,3-BUTADIENE		
	C3H3N	ACRYLONITRILE	416
	C4H6CL2	1,3-DICHLORO-2-BUTENE	441-443
C4H5CL3	2,3,4-TRICHLORO-1-BUTENE		
	C4H6CL2	1,3-DICHLORO-2-BUTENE	444
C4H5N	ALLYL CYANIDE		
	CHN	HYDROGEN CYANIDE	249
	C3H5CL	3-CHLORO-1-PROPENE	420
	C4H5N	CIS-CROTONONITRILE	445
	C4H5N	TRANS-CROTONONITRILE	446
C4H5N	CIS-CROTONONITRILE		
	C4H5N	ALLYL CYANIDE	445
C4H5N	TRANS-CROTONONITRILE		
	C4H5N	ALLYL CYANIDE	446
C4H6CL2	1,3-DICHLORO-2-BUTENE		
	C4H5CL	2-CHLORO-1,3-BUTADIENE	441-443
	C4H5CL3	2,3,4-TRICHLORO-1-BUTENE	444
C4H8O2S	SULFOLANE		
	CH2CL2	DICHLOROMETHANE	266

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
C4H9BR	BUTYL BROMIDE		
	C4H9CL	BUTYL CHLORIDE	447
C4H9BR	TERT-BUTYL BROMIDE		
	C4H9CL	TERT-BUTYL CHLORIDE	448-451
C4H9CL	BUTYL CHLORIDE		
	CH3NO2	NITROMETHANE	294-296
	C2H3N	ACETONITRILE	375-377
	C4H9BR	BUTYL BROMIDE	447
	C6H5CL	CHLOROBENZENE	452-454
	C6H7N	ANILINE	455
C4H9CL	SEC-BUTYL CHLORIDE		
	C6H5NO2	NITROBENZENE	456-460
C4H9CL	TERT-BUTYL CHLORIDE		
	CCL4	TETRACHLOROMETHANE	125-128
	C4H9BR	TERT-BUTYL BROMIDE	448-451
C4H9CL	ISOBUTYL CHLORIDE		
	CS2	CARBON DISULFIDE	321-322
C4H9N	PYRROLIDINE		
	C6H18OSi2	HEXAMETHYLDISILOXANE	461-462
C4H9NO	BUTYRALDEHYDE OXIME		
	C3H7NO	ACETONE OXIME	423-424
	C3H7NO	PROPIONALDEHYDE OXIME	430-431
C4H9NO	METHYL ETHYL KETOXIME		
	CCL4	TETRACHLOROMETHANE	129
	C3H7NO	PROPIONALDEHYDE OXIME	432-433
	C5H5N	PYRIDINE	463
C4H10O2	TERT-BUTYLHYDROPEROXIDE		
	C8H18O2	DI-TERT-BUTYLPEROXIDE	464
C4H10S	DIETHYL SULFIDE		
	C2HCL3	TRICHLOROETHYLENE	352

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
C4H11BRSI	(BROMOMETHYL-)TRIMETHYLSILANE		
	C4H12SI	TETRAMETHYLSILANE	465-471
C4H11N	BUTYLAMINE		
	C6H5CL	CHLOROBENZENE	472-473
C4H11N	DIETHYLAMINE		
	CCL4	TETRACHLOROMETHANE	130-133 133 R
	C2H7N	ETHYLAMINE	410-411
	C6H5CL	CHLOROBENZENE	474-476
	C6H5F	FLUOROBENZENE	477
	C6H15N	TRIETHYLAMINE	478-496 496 R
C4H12SI	TETRAMETHYLSILANE		
	C4H11BRSI	(BROMOMETHYL-)TRIMETHYLSILANE	465-471
C5CL2F6	1,2-DICHLOROHEXAFLUOROCYCLOPENTENE		
	C4CL3F7	2,2,3-TRICHLOROHEPTAFLUOROBUTANE	439
C5H5N	PYRIDINE		
	CCL4	TETRACHLOROMETHANE	134-143 143 R
	CHBR3	TRIBROMOMETHANE	194-195
	CHCL3	CHLOROFORM	237-243
	CH2CL2	DICHLOROMETHANE	267
	C2CL4	TETRACHLOROETHYLENE	343-347 347 R
	C4H4S	THIOPHENE	440
	C4H9NO	METHYL ETHYL KETOXIME	463
	C5H11N	PIPERIDINE	497-499
	C6H7N	ANILINE	500
	C6H7N	2-METHYLPYRIDINE	501
	C6H7N	3-METHYLPYRIDINE	502-503
C5H6N2	GLUTARONITRILE		
	CH3NO2	NITROMETHANE	297
	C3H7NO	N,N-DIMETHYLFORMAMIDE	426
C5H8CL4	1,1,1,5-TETRACHLOROPENTANE		
	C3H4CL4	1,1,1,3-TETRACHLOROPROPANE	417

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
C5H11N	PIPERIDINE		
C5H5N	PYRIDINE		497-499
C6H18OSi2	HEXAMETHYLDISILOXANE		504
C6F6	HEXAFLUOROBENZENE		
CCL4	TETRACHLOROMETHANE		144-151
C6H15N	TRIETHYLAMINE		505
C7F14	PERFLUOROMETHYLCYCLOHEXANE		506-512
C8H11N	N,N-DIMETHYLANILINE		513
C6F14	PERFLUOROHEXANE		
C12F27N	PERFLUOROTRIBUTYLAMINE		514
C6H4CL2	O-DICHLOROBENZENE		
C6H4CL2	P-DICHLOROBENZENE		515
C6H4CL2	P-DICHLOROBENZENE		
C6H4CL2	O-DICHLOROBENZENE		515
C6H5BR	BROMOBENZENE		
CCL4	TETRACHLOROMETHANE		152-157 157 R
C6H5CL	CHLOROBENZENE		516
C6H5CL	CHLOROBENZENE		
CCL4	TETRACHLOROMETHANE		158-167 167 R
CHCL3	CHLOROFORM		244
CH3NO2	NITROMETHANE		298-300
C2H3N	ACETONITRILE		378-382
C2H3NO	METHYL ISOCYANATE		389
C2H4BR2	1,2-DIBROMOETHANE		395-396
C3H7NO2	1-NITROPROPANE		434-435
C4H9CL	BUTYL CHLORIDE		452-454
C4H11N	BUTYLAMINE		472-473
C4H11N	DIETHYLAMINE		474-476
C6H5BR	BROMOBENZENE		516
C6H7N	ANILINE		517-528 528 R
C6H11CL	CHLOROCYCLOHEXANE		529-530
C6H13N	CYCLOHEXYLAMINE		531-533 533 R
C6H15N	TRIETHYLAMINE		534-535

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
C6H5CL3SI	TRICHLOROPHENYLSILANE		
	C6H6CL2SI	DICHLOROPHENYLSILANE	536-539 539 R
C6H5F	FLUOROBENZENE		
	C4H11N	DIETHYLAMINE	477
C6H5NO2	NITROBENZENE		
	CCL4	TETRACHLOROMETHANE	168
	CH3NO2	NITROMETHANE	301
	C2H5I	ETHYL IODIDE	401
	C4H9CL	SEC-BUTYL CHLORIDE	456-460
	C6H7N	ANILINE	540-544
C6H6CLN	M-CHLOROANILINE		
	C6H7N	ANILINE	545
C6H6CLN	P-CHLOROANILINE		
	C6H7N	ANILINE	546
C6H6CL2SI	DICHLOROPHENYLSILANE		
	C6H5CL3SI	TRICHLOROPHENYLSILANE	536-539 539 R
C6H7N	ANILINE		
	CCL4	TETRACHLOROMETHANE	169-174
	C2H3N	ACETONITRILE	383-385
	C3H7NO	N,N-DIMETHYLFORMAMIDE	427-428
	C4H9CL	BUTYL CHLORIDE	455
	C5H5N	PYRIDINE	500
	C6H5CL	CHLOROBENZENE	517-528 528 R
	C6H5NO2	NITROBENZENE	540-544
	C6H6CLN	M-CHLOROANILINE	545
	C6H6CLN	P-CHLOROANILINE	546
	C6H13N	CYCLOHEXYLAMINE	547-548
	C7H9N	N-METHYLANILINE	549-552 552 R
	C8H11N	N,N-DIMETHYLANILINE	553-556 556 R
	C9H7N	QUINOLINE	557
	C10H15N	N,N-DIETHYLANILINE	558

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
C6H7N	2-METHYLPYRIDINE		
	CHCL3	CHLOROFORM	245-246
	C2H3N	ACETONITRILE	386
	C5H5N	PYRIDINE	501
	C7H9N	2,6-DIMETHYLPYRIDINE	559
C6H7N	3-METHYLPYRIDINE		
	C5H5N	PYRIDINE	502-503
	C7H9N	2,6-DIMETHYLPYRIDINE	560
	C8H11N	2-METHYL-5-ETHYLPYRIDINE	561
C6H8N2	ADIPONITRILE		
	C6H16N2	HEXAMETHYLENEDIAMINE	562-565 565 R
C6H11CL	CHLOROCYCLOHEXANE		
	C6H5CL	CHLOROBENZENE	529-530
	C6H13N	CYCLOHEXYLAMINE	566-567
C6H13N	CYCLOHEXYLAMINE		
	C6H5CL	CHLOROBENZENE	531-533 533 R
	C6H7N	ANILINE	547-548
	C6H11CL	CHLOROCYCLOHEXANE	566-567
C6H13N	HEXAMETHYLENE IMINE		
	C6H16N2	HEXAMETHYLENEDIAMINE	568-572 572 R
C6H15N	DIISOPROPYLAMINE		
	C3H9N	ISOPROPYLAMINE	437-438
C6H15N	TRIETHYLAMINE		
	CCL4	TETRACHLOROMETHANE	175-176
	CHCL3	CHLOROFORM	247
	CH2CL2	DICHLOROMETHANE	268
	C2H7N	ETHYLAMINE	412-413
	C4H11N	DIETHYLAMINE	478-496 496 R
	C6F6	HEXAFLUOROBENZENE	505
	C6H5CL	CHLOROBENZENE	534-535

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE	
C6H16N2	HEXAMETHYLENEDIAMINE			
C6H8N2	ADIPONITRILE		562-565 565 R	
C6H13N	HEXAMETHYLENE IMINE		568-572 572 R	
C6H18OSi2	HEXAMETHYLDISILOXANE			
CHCL3	CHLOROFORM	CS2	CARBON DISULFIDE	590-591
CS2	CARBON DISULFIDE	CHCL3	CHLOROFORM	590-591
C4H9N	PYRROLIDINE			461-462
C5H11N	PIPERIDINE			504
C7F14	PERFLUOROMETHYLCYCLOHEXANE			
C6F6	HEXAFLUOROBENZENE			506-512
C7H5ClO	BENZOYL CHLORIDE			
CL2OS	THIONYL CHLORIDE			573
C7H7Cl	BENZYL CHLORIDE			
C8H7N	BENZYL CYANIDE			574-576
C7H7Cl	O-CHLOROTOLUENE			
C7H7Cl	P-CHLOROTOLUENE			577
C7H7Cl	P-CHLOROTOLUENE			
C7H7Cl	O-CHLOROTOLUENE			577
C7H9N	2,6-DIMETHYLPYRIDINE			
C6H7N	2-METHYLPYRIDINE			559
C6H7N	3-METHYLPYRIDINE			560
C7H9N	N-METHYLANILINE			
CCL4	TETRACHLOROMETHANE			177-180 180 R
C3H7NO	N,N-DIMETHYLFORMAMIDE			429
C6H7N	ANILINE			549-552 552 R
C8H11N	N,N-DIMETHYLANILINE			578-581 581 R
C8H7N	BENZYL CYANIDE			
C7H7Cl	BENZYL CHLORIDE			574-576

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
C8H11N	N,N-DIMETHYLANILINE		
	C6F6	HEXAFLUOROBENZENE	513
	C6H7N	ANILINE	553-556 556 R
	C7H9N	N-METHYLANILINE	578-581 581 R
C8H11N	2-METHYL-5-ETHYLPYRIDINE		
	C6H7N	3-METHYLPYRIDINE	561
C8H18O2	DI-TERT-BUTYLPEROXIDE		
	C4H10O2	TERT-BUTYLHYDROPEROXIDE	464
C8H24O4Si4	OCTAMETHYLCYCLOTETRASILOXANE		
	CCL4	TETRACHLOROMETHANE	181-185
C9H7N	ISOQUINOLINE		
	C9H7N	QUINOLINE	582
	C10H9N	QUINALDINE	583
C9H7N	QUINOLINE		
	C6H7N	ANILINE	557
	C9H7N	ISOQUINOLINE	582
C10H9N	LEPIDINE		
	C10H9N	7-METHYLQUINOLINE	584
C10H9N	7-METHYLQUINOLINE		
	C10H9N	LEPIDINE	584
C10H9N	QUINALDINE		
	C9H7N	ISOQUINOLINE	583
C10H15N	N,N-DIETHYLANILINE		
	C6H7N	ANILINE	558
C12F27N	PERFLUOROTRIBUTYLAMINE		
	C2CL3F3	1,1,2-TRICHLORO-1,2,2-TRIFLUOROETHANE	323
	C6F14	PERFLUOROHEXANE	514

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
CL2OS		THIONYL CHLORIDE	
	C7H5ClO	BENZOYL CHLORIDE	573
CL2O2S		SULFURYL CHLORIDE	
	C2H2Cl4	1,1,2,2-TETRACHLOROETHANE	359-361
CL3HSI		TRICHLOROSILANE	
	CH4CL2SI	METHYLDICHLOROSILANE	302
	CL4SI	SILICON TETRACHLORIDE	585
CL4SI		SILICON TETRACHLORIDE	
	CCL4	TETRACHLOROMETHANE	186-192 192
	CH3CL3SI	METHYLTRICHLOROSILANE	271-272
	CH4CL2SI	METHYLDICHLOROSILANE	303-304
	C2H3N	ACETONITRILE	387
	C2H6CL2SI	DIMETHYLDICHLOROSILANE	406
	C3H9CLSI	TRIMETHYLCHLOROSILANE	436
	CL3HSI	TRICHLOROSILANE	585

Alphabetical Index of Systems

R = RECOMMENDED VALUES

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
ACETONE OXIME		C3H7NO	
	BUTYRALDEHYDE OXIME	C4H9NO	423-424
	PROPIONALDEHYDE OXIME	C3H7NO	421-422
ACETONITRILE		C2H3N	
	ACRYLONITRILE	C3H3N	365-374 374 R
	ANILINE	C6H7N	383-385
	BUTYL CHLORIDE	C4H9CL	375-377
	CARBON DISULFIDE	CS2	320
	CHLOROBENZENE	C6H5CL	378-382
	CHLOROFORM	CHCL3	216-218
	1,2-DICHLOROETHANE	C2H4CL2	364
	DICHLOROMETHANE	CH2CL2	257-259
	METHANETHIOL	CH4S	306
	2-METHYLPYRIDINE	C6H7N	386
	NITROMETHANE	CH3NO2	281-284
	SILICON TETRACHLORIDE	CL4SI	387
	TETRACHLOROMETHANE	CCL4	85- 87
	TRICHLOROETHYLENE	C2HCL3	349-350
ACRYLONITRILE		C3H3N	
	ACETONITRILE	C2H3N	365-374 374 R
	2-CHLORO-1,3-BUTADIENE	C4H5CL	416
	1,1-DICHLOROETHYLENE	C2H2CL2	354
	PROPIONITRILE	C3H5N	414-415
	TETRACHLOROETHYLENE	C2CL4	341-342
	TETRACHLOROMETHANE	CCL4	111-112
ADIPONITRILE		C6H8N2	
	HEXAMETHYLENEDIAMINE	C6H16N2	562-565 565 R
ALLYL CYANIDE		C4H5N	
	3-CHLORO-1-PROPENE	C3H5CL	420
	CIS-CROTONONITRILE	C4H5N	445
	TRANS-CROTONONITRILE	C4H5N	446
	HYDROGEN CYANIDE	CHN	249

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE	
ANILINE		C6H7N		
	ACETONITRILE	C2H3N	383-385	
	BUTYL CHLORIDE	C4H9CL	455	
	M-CHLOROANILINE	C6H6CLN	545	
	P-CHLOROANILINE	C6H6CLN	546	
	CHLOROBENZENE	C6H5CL	517-528 528 R	
	CYCLOHEXYLAMINE	C6H13N	547-548	
	N,N-DIETHYLANILINE	C10H15N	558	
	N,N-DIMETHYLANILINE	C8H11N	553-556 556 R	
	N,N-DIMETHYLFORMAMIDE	C3H7NO	427-428	
	N-METHYLANILINE	C7H9N	549-552 552 R	
	NITROBENZENE	C6H5NO2	540-544	
	PYRIDINE	C5H5N	500	
	QUINOLINE	C9H7N	557	
	TETRACHLOROMETHANE	CCL4	169-174	
BENZOYL CHLORIDE		C7H5CLO		
	THIONYL CHLORIDE	CL2OS	573	
BENZYL CHLORIDE		C7H7CL		
	BENZYL CYANIDE	C8H7N	574-576	
BENZYL CYANIDE		C8H7N		
	BENZYL CHLORIDE	C7H7CL	574-576	
BROMOBENZENE		C6H5BR		
	CHLOROBENZENE	C6H5CL	516	
	TETRACHLOROMETHANE	CCL4	152-157 157 R	
BROMOCHLOROMETHANE		CH2BRCL		
	DIBROMOMETHANE	CH2BR2	250	
		DICHLOROMETHANE	CH2CL2	595-596
	DICHLOROMETHANE	CH2CL2	251	
		DIBROMOMETHANE	CH2BR2	595-596
3-BROMO-1-PROPENE		C3H5BR		
	3-CHLORO-1-PROPENE	C3H5CL	418	

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
(BROMOMETHYL-)TRIMETHYLSILANE		C4H11BR SI	
	TETRAMETHYLSILANE	C4H12SI	465-471
BUTYLAMINE		C4H11N	
	CHLOROBENZENE	C6H5CL	472-473
BUTYL BROMIDE		C4H9BR	
	BUTYL CHLORIDE	C4H9CL	447
TERT-BUTYL BROMIDE		C4H9BR	
	TERT-BUTYL CHLORIDE	C4H9CL	448-451
BUTYL CHLORIDE		C4H9CL	
	ACETONITRILE	C2H3N	375-377
	ANILINE	C6H7N	455
	BUTYL BROMIDE	C4H9BR	447
	CHLOROBENZENE	C6H5CL	452-454
	NITROMETHANE	CH3NO2	294-296
SEC-BUTYL CHLORIDE		C4H9CL	
	NITROBENZENE	C6H5NO2	456-460
TERT-BUTYL CHLORIDE		C4H9CL	
	TERT-BUTYL BROMIDE	C4H9BR	448-451
	TETRACHLOROMETHANE	CCl4	125-128
TERT-BUTYLHYDROPEROXIDE		C4H10O2	
	DI-TERT-BUTYLPEROXIDE	C8H18O2	464
DI-TERT-BUTYLPEROXIDE		C8H18O2	
	TERT-BUTYLHYDROPEROXIDE	C4H10O2	464
BUTYRALDEHYDE OXIME		C4H9NO	
	ACETONE OXIME	C3H7NO	423-424
	PROPIONALDEHYDE OXIME	C3H7NO	430-431
CARBON DISULFIDE		CS2	
	ACETONITRILE	C2H3N	320
	CHLOROFORM	CHCl3	206-214
	HEXAMETHYLDISILOXANE	C6H18OSi2	590-591

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
=====			
CARBON DISULFIDE	CS2		
	HEXAMETHYLDISILOXANE	C6H18OSI2	CHLOROFORM
			CHCL3
			590-591
	ISOBUTYL CHLORIDE	C4H9CL	
			321-322
	METHYL IODIDE	CH3I	
			278
	NITROMETHANE	CH3NO2	
			279
	TETRACHLOROETHYLENE	C2CL4	
			316-319
			319
	TETRACHLOROMETHANE	CCL4	
			73- 76
=====			
M-CHLOROANILINE	C6H6CLN		
	ANILINE	C6H7N	
			545
=====			
P-CHLOROANILINE	C6H6CLN		
	ANILINE	C6H7N	
			546
=====			
CHLOROBENZENE	C6H5CL		
	ACETONITRILE	C2H3N	
			378-382
	ANILINE	C6H7N	
			517-528
			528
	BROMOBENZENE	C6H5BR	
			516
	BUTYLAMINE	C4H11N	
			472-473
	BUTYL CHLORIDE	C4H9CL	
			452-454
	CHLOROCYCLOHEXANE	C6H11CL	
			529-530
	CHLOROFORM	CHCL3	
			244
	CYCLOHEXYLAMINE	C6H13N	
			531-533
			533
	1,2-DIBROMOETHANE	C2H4BR2	
			395-396
	DIETHYLAMINE	C4H11N	
			474-476
	METHYL ISOCYANATE	C2H3NO	
			389
	NITROMETHANE	CH3NO2	
			298-300
	1-NITROPROPANE	C3H7NO2	
			434-435
	TETRACHLOROMETHANE	CCL4	
			158-167
			167
	TRIETHYLAMINE	C6H15N	
			534-535
=====			
2-CHLORO-1,3-BUTADIENE	C4H5CL		
	ACRYLONITRILE	C3H3N	
			416
	1,3-DICHLORO-2-BUTENE	C4H6CL2	
			441-443
=====			
CHLOROCYCLOHEXANE	C6H11CL		
	CHLOROBENZENE	C6H5CL	
			529-530
	CYCLOHEXYLAMINE	C6H13N	
			566-567

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
CHLOROFORM	CHCL3		
	ACETONITRILE	C2H3N	216-218
	CARBON DISULFIDE	CS2	206-214
		HEXAMETHYLDISILOXANE	C6H18OSI2 590-591
	CHLOROBENZENE	C6H5CL	244
1,1-DICHLOROETHANE	C2H4CL2		219-224
		1,2-DICHLOROETHANE	C2H4CL2 592-594
1,2-DICHLOROETHANE	C2H4CL2	1,1-DICHLOROETHANE	C2H4CL2 592-594
	DICHLOROMETHANE	CH2CL2	202-203
		TETRACHLOROMETHANE	CCL4 586-587
	DIMETHYL SULFOXIDE	C2H6OS	225-235 235 R
	HEXAMETHYLDISILOXANE	C6H18OSI2	CARBON DISULFIDE CS2 590-591
	METHYL ETHYL SULFIDE	C3H8S	236
	METHYL IODIDE	CH3I	204-205
2-METHYLPYRIDINE	C6H7N		245-246
	PYRIDINE	C5H5N	237-243
	TETRACHLOROETHYLENE	C2CL4	215
	TETRACHLOROMETHANE	CCL4	55-61
		DICHLOROMETHANE	CH2CL2 586-587
	TRIETHYLAMINE	C6H15N	247
3-CHLORO-1-PROPENE	C3H5CL		
	ALLYL CYANIDE	C4H5N	420
3-BROMO-1-PROPENE	C3H5BR		418
	HYDROGEN CYANIDE	CHN	248
	ISOPROPYL CHLORIDE	C3H7CL	419
0-CHLOROTOLUENE	C7H7CL		
	P-CHLOROTOLUENE	C7H7CL	577
P-CHLOROTOLUENE	C7H7CL		
	0-CHLOROTOLUENE	C7H7CL	577
CIS-CROTONONITRILE	C4H5N		
	ALLYL CYANIDE	C4H5N	445
TRANS-CROTONONITRILE	C4H5N		
	ALLYL CYANIDE	C4H5N	446

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE	
CYANOGEN CHLORIDE		CCLN		
	HYDROGEN CYANIDE	CHN	17	
CYCLOHEXYLAMINE		C6H13N		
	ANILINE	C6H7N	547-548	
	CHLOROBENZENE	C6H5CL	531-533 533	
	CHLOROCYCLOHEXANE	C6H11CL	566-567	
N-DEUTEROMETHYLAMINE		CH3D2N		
	TRIMETHYLAMINE	C3H9N	273-277	
1,2-DIBROMOETHANE		C2H4BR2		
	CHLOROBENZENE	C6H5CL	395-396	
	1,2-DIBROMOPROPANE	C3H6BR2	390-391	
	1-NITROPROPANE	C3H7NO2	392-394 394	
	TETRACHLOROMETHANE	CCL4	90-92	
DIBROMOMETHANE		CH2BR2		
	BROMOCHLOROMETHANE	CH2BRCL	250	
		DICHLOROMETHANE	CH2CL2	595-596
	DICHLOROMETHANE	CH2CL2	252	
		BROMOCHLOROMETHANE	CH2BRCL	595-596
	DIMETHYL SULFOXIDE	C2H6OS	253-254	
1,2-DIBROMOPROPANE		C3H6BR2		
	1,2-DIBROMOETHANE	C2H4BR2	390-391	
O-DICHLOROBENZENE		C6H4CL2		
	P-DICHLOROBENZENE	C6H4CL2	515	
P-DICHLOROBENZENE		C6H4CL2		
	O-DICHLOROBENZENE	C6H4CL2	515	
1,3-DICHLORO-2-BUTENE		C4H6CL2		
	2-CHLORO-1,3-BUTADIENE	C4H5CL	441-443	
	2,3,4-TRICHLORO-1-BUTENE	C4H5CL3	444	

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE		
DICHLORODIFLUOROMETHANE	CCL2F2				
	DIFLUOROCHLOROMETHANE	CHCLF2	18- 37 37		
1,1-DIFLUOROETHANE	C2H4F2		46		
	FLUOROFORM	CHF3	38- 42		
	PERFLUOROCYCLOBUTANE	C4F8	48- 54		
	PERFLUOROPROPYLENE	C3F6	47		
1,1,2-TRICHLORO-1,2,2-TRI- FLUOROETHANE	C2CL3F3		43- 45		
1,1-DICHLOROETHANE	C2H4CL2				
	CHLOROFORM	CHCL3	219-224		
		1,2-DICHLOROETHANE	C2H4CL2	592-594	
1,2-DICHLOROETHANE	C2H4CL2		397-399		
		CHLOROFORM	CHCL3	592-594	
	TETRACHLOROMETHANE	CCL4	93- 98		
1,2-DICHLOROETHANE	C2H4CL2				
	ACETONITRILE	C2H3N	364		
	CHLOROFORM	CHCL3	1,1-DICHLOROETHANE	C2H4CL2	592-594
1,1-DICHLOROETHANE	C2H4CL2		397-399		
		CHLOROFORM	CHCL3	592-594	
	DICHLOROMETHANE	CH2CL2	260-263		
	METHYL ISOCYANATE	C2H3NO	388		
	TETRACHLOROETHYLENE	C2CL4	340		
	TETRACHLOROMETHANE	CCL4	TRICHLOROETHYLENE	C2HCL3	588-589
1,1,1-TRICHLOROETHANE	C2H3CL3		363		
	TRICHLOROETHYLENE	C2HCL3	351		
		TETRACHLOROMETHANE	CCL4	588-589	
	VINYL CHLORIDE	C2H3CL	362		
1,1-DICHLOROETHYLENE	C2H2CL2				
	ACRYLONITRILE	C3H3N	354		
	VINYL CHLORIDE	C2H3CL	353		
CIS-1,2-DICHLOROETHYLENE	C2H2CL2				
	TRANS-1,2-DICHLOROETHYLENE	C2H2CL2	355		
	1,1,1-TRICHLOROETHANE	C2H3CL3	356		

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE	
TRANS-1,2-DICHLOROETHYLENE		C2H2CL2		
	CIS-1,2-DICHLOROETHYLENE	C2H2CL2	355	
	1,1,1-TRICHLOROETHANE	C2H3CL3	357	
	TRICHLOROETHYLENE	C2HCL3	348	
DICHLOROFUOROMETHANE		CHCL2F		
	PERFLUOROCYCLOBUTANE	C4F8	201	
1,2-DICHLOROHEXAFLUOROCYCLOPENTENE		C5CL2F6		
	2,2,3-TRICHLOROHEPTAFLUORO- BUTANE	C4CL3F7	439	
DICHLOROMETHANE		CH2CL2		
	ACETONITRILE	C2H3N	257-259	
	BROMOCHLOROMETHANE	CH2BRCL	251	
		DIBROMOMETHANE	CH2BR2	595-596
	CHLOROFORM	CHCL3	202-203	
		TETRACHLOROMETHANE	CCL4	586-587
	DIBROMOMETHANE	CH2BR2	252	
		BROMOCHLOROMETHANE	CH2BRCL	595-596
	1,2-DICHLOROETHANE	C2H4CL2	260-263	
	N,N-DIMETHYLFORMAMIDE	C3H7NO	265	
	DIMETHYL SULFOXIDE	C2H6OS	264	
	METHYL IODIDE	CH3I	255	
	PYRIDINE	C5H5N	267	
	SULFOLANE	C4H8O2S	266	
	TETRACHLOROETHYLENE	C2CL4	256	
	TETRACHLOROMETHANE	CCL4	62-67	
		CHLOROFORM	CHCL3	586-587
	TRIETHYLAMINE	C6H15N	268	
DICHLOROPHENYLSILANE		C6H6CL2SI		
	TRICHLOROPHENYLSILANE	C6H5CL3SI	536-539 539 R	
1,2-DICHLOROTETRAFLUROETHANE		C2CL2F4		
	DIFLUOROCHLOROMETHANE	CHCLF2	197-198	
DIETHYLAMINE		C4H11N		
	CHLOROENZENE	C6H5CL	474-476	
	ETHYLAMINE	C2H7N	410-411	

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
DIETHYLAMINE		C4H11N	
	FLUOROBENZENE	C6H5F	477
	TETRACHLOROMETHANE	CCL4	130-133 133 R
	TRIETHYLAMINE	C6H15N	478-496 496 R
N,N-DIETHYLANILINE		C10H15N	
	ANILINE	C6H7N	558
DIETHYL SULFIDE		C4H10S	
	TRICHLOROETHYLENE	C2HCL3	352
DIFLUOROCHLOROMETHANE		CHCLF2	
	DICHLORODIFLUORO- METHANE	CCL2F2	18- 37 37 R
	1,2-DICHLOROTETRAFLURO- ETHANE	C2CL2F4	197-198
	PERFLUOROCYCLOBUTANE	C4F8	200
	PERFLUOROPROPYLENE	C3F6	199
	TRIFLUOROBROMOMETHANE	CBRF3	1- 16
1,1-DIFLUOROETHANE		C2H4F2	
	DICHLORODIFLUORO- METHANE	CCL2F2	46
DIISOPROPYLAMINE		C6H15N	
	ISOPROPYLAMINE	C3H9N	437-438
DIMETHYLAMINE		C2H7N	
	TETRACHLOROMETHANE	CCL4	108-110
N,N-DIMETHYLANILINE		C8H11N	
	ANILINE	C6H7N	553-556 556 R
	HEXAFLUOROBENZENE	C6F6	513
	N-METHYLANILINE	C7H9N	578-581 581 R
DIMETHYLDICHLOROSILANE		C2H6CL2SI	
	SILICON TETRACHLORIDE	CL4SI	406
	TRIMETHYLCHLOROSILANE	C3H9CLSI	405

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
N,N-DIMETHYLFORMAMIDE		C3H7NO	
	ANILINE	C6H7N	427-428
	DICHLOROMETHANE	CH2CL2	265
	DIMETHYL SULFOXIDE	C2H6OS	407
	ETHANETHIOL	C2H6S	409
	GLUTARONITRILE	C5H6N2	426
	METHANETHIOL	CH4S	311
	N-METHYLANILINE	C7H9N	429
	NITROMETHANE	CH3NO2	291
	TETRACHLOROMETHANE	CCL4	114-118 118 R
	THIOPHENE	C4H4S	425
2,6-DIMETHYLPYRIDINE		C7H9N	
	2-METHYLPYRIDINE	C6H7N	559
	3-METHYLPYRIDINE	C6H7N	560
DIMETHYL SULFIDE		C2H6S	
	ETHANETHIOL	C2H6S	408
	METHANETHIOL	CH4S	308-310
DIMETHYL SULFOXIDE		C2H6OS	
	CHLOROFORM	CHCL3	225-235 235 R
	DIBROMOMETHANE	CH2BR2	253-254
	DICHLOROMETHANE	CH2CL2	264
	N,N-DIMETHYLFORMAMIDE	C3H7NO	407
	METHANETHIOL	CH4S	307
	N-METHYLFORMAMIDE	C2H5NO	402
	TETRACHLOROMETHANE	CCL4	106-107
	TRIBROMOMETHANE	CHBR3	193
ETHANETHIOL		C2H6S	
	N,N-DIMETHYLFORMAMIDE	C3H7NO	409
	DIMETHYL SULFIDE	C2H6S	408
ETHYLAMINE		C2H7N	
	DIETHYLAMINE	C4H11N	410-411
	TRIETHYLAMINE	C6H15N	412-413

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE		
ETHYL BROMIDE		C2H5BR			
	ETHYL IODIDE	C2H5I	400		
ETHYL IODIDE		C2H5I			
	ETHYL BROMIDE	C2H5BR	400		
	NITROBENZENE	C6H5NO2	401		
	NITROMETHANE	CH3NO2	285-286		
	TETRACHLOROMETHANE	CCL4	99		
FLUOROBENZENE		C6H5F			
	DIETHYLAMINE	C4H11N	477		
FLUOROFORM		CHF3			
	DICHLORODIFLUORO- METHANE	CCL2F2	38- 42		
GLUTARONITRILE		C5H6N2			
	N,N-DIMETHYLFORMAMIDE	C3H7NO	426		
	NITROMETHANE	CH3NO2	297		
HEXAFLUOROBENZENE		C6F6			
	N,N-DIMETHYLANILINE	C8H11N	513		
	PERFLUOROMETHYLCYCLO- HEXANE	C7F14	506-512		
	TETRACHLOROMETHANE	CCL4	144-151		
	TRIETHYLAMINE	C6H15N	505		
HEXAMETHYLDISILOXANE		C6H18OSi2			
	CARBON DISULFIDE	CS2	CHLOROFORM	CHCL3	590-591
	CHLOROFORM	CHCL3	CARBON DISULFIDE	CS2	590-591
	PIPERIDINE	C5H11N			504
	PYRROLIDINE	C4H9N			461-462
HEXAMETHYLENEDIAMINE		C6H16N2			
	ADIPONITRILE	C6H8N2			562-565 565 R
	HEXAMETHYLENE IMINE	C6H13N			568-572 572 R
HEXAMETHYLENE IMINE		C6H13N			
	HEXAMETHYLENEDIAMINE	C6H16N2			568-572 572 R

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
HYDROGEN CYANIDE		CHN	
	ALLYL CYANIDE	C4H5N	249
	3-CHLORO-1-PROPENE	C3H5CL	248
	CYANOGEN CHLORIDE	CCLN	17
ISOBUTYL CHLORIDE		C4H9CL	
	CARBON DISULFIDE	CS2	321-322
ISOPROPYLAMINE		C3H9N	
	DIISOPROPYLAMINE	C6H15N	437-438
ISOPROPYL CHLORIDE		C3H7CL	
	3-CHLORO-1-PROPENE	C3H5CL	419
ISOQUINOLINE		C9H7N	
	QUINALDINE	C10H9N	583
	QUINOLINE	C9H7N	582
LEPIDINE		C10H9N	
	7-METHYLQUINOLINE	C10H9N	584
METHANETHIOL		CH4S	
	ACETONITRILE	C2H3N	306
	N,N-DIMETHYLFORMAMIDE	C3H7NO	311
	DIMETHYL SULFIDE	C2H6S	308-310
	DIMETHYL SULFOXIDE	C2H6OS	307
	METHYLAMINE	CH5N	305
N-METHYLACETAMIDE		C3H7NO	
	N-METHYLFORMAMIDE	C2H5NO	403-404
METHYLAMINE		CH5N	
	METHANETHIOL	CH4S	305
	TETRACHLOROMETHANE	CCL4	70-72
	TRIMETHYLAMINE	C3H9N	312-315
N-METHYLANILINE		C7H9N	
	ANILINE	C6H7N	549-552 552 R
	N,N-DIMETHYLANILINE	C8H11N	578-581 581 R

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
N-METHYLANILINE		C7H9N	
	N,N-DIMETHYLFORMAMIDE	C3H7NO	429
	TETRACHLOROMETHANE	CCL4	177-180 180 R
METHYLDICHLOROSILANE		CH4CL2SI	
	SILICON TETRACHLORIDE	CL4SI	303-304
	TRICHLOROSILANE	CL3HSI	302
METHYL ETHYL KETOXIME		C4H9NO	
	PROPIONALDEHYDE OXIME	C3H7NO	432-433
	PYRIDINE	C5H5N	463
	TETRACHLOROMETHANE	CCL4	129
2-METHYL-5-ETHYLPYRIDINE		C8H11N	
	3-METHYLPYRIDINE	C6H7N	561
METHYL ETHYL SULFIDE		C3H8S	
	CHLOROFORM	CHCL3	236
N-METHYLFORMAMIDE		C2H5NO	
	DIMETHYL SULFOXIDE	C2H6OS	402
	N-METHYLACETAMIDE	C3H7NO	403-404
	TETRACHLOROMETHANE	CCL4	100-104 104 R
METHYL IODIDE		CH3I	
	CARBON DISULFIDE	CS2	278
	CHLOROFORM	CHCL3	204-205
	DICHLOROMETHANE	CH2CL2	255
	TETRACHLOROMETHANE	CCL4	68
METHYL ISOCYANATE		C2H3NO	
	CHLOROBENZENE	C6H5CL	389
	1,2-DICHLOROETHANE	C2H4CL2	388
	TETRACHLOROMETHANE	CCL4	88- 89
2-METHYLPYRIDINE		C6H7N	
	ACETONITRILE	C2H3N	386
	CHLOROFORM	CHCL3	245-246
	2,6-DIMETHYLPYRIDINE	C7H9N	559
	PYRIDINE	C5H5N	501

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
3-METHYLPYRIDINE		C6H7N	
	2,6-DIMETHYLPYRIDINE	C7H9N	560
	2-METHYL-5-ETHYL- PYRIDINE	C8H11N	561
	PYRIDINE	C5H5N	502-503
7-METHYLQUINOLINE		C10H9N	
	LEPIDINE	C10H9N	584
METHYLTRICHLOROSILANE		CH3CL3SI	
	SILICON TETRACHLORIDE	CL4SI	271-272
	TRIMETHYLCHLOROSILANE	C3H9CL3SI	269-270
NITROBENZENE		C6H5NO2	
	ANILINE	C6H7N	540-544
	SEC-BUTYL CHLORIDE	C4H9CL	456-460
	ETHYL IODIDE	C2H5I	401
	NITROMETHANE	CH3NO2	301
	TETRACHLOROMETHANE	CCL4	168
NITROETHANE		C2H5NO2	
	NITROMETHANE	CH3NO2	287-290
	TETRACHLOROMETHANE	CCL4	105
NITROMETHANE		CH3NO2	
	ACETONITRILE	C2H3N	281-284
	BUTYL CHLORIDE	C4H9CL	294-296
	CARBON DISULFIDE	CS2	279
	CHLOROENZENE	C6H5CL	298-300
	N,N-DIMETHYLFORMAMIDE	C3H7NO	291
	ETHYL IODIDE	C2H5I	285-286
	GLUTARONITRILE	C5H6N2	297
	NITROBENZENE	C6H5NO2	301
	NITROETHANE	C2H5NO2	287-290
	TETRACHLOROMETHANE	CCL4	69
	THIOPHENE	C4H4S	292-293
	TRICHLOROETHYLENE	C2HCL3	280

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
1-NITROPROPANE		C3H7NO2	
	CHLOROBENZENE	C6H5CL	434-435
	1,2-DIBROMOETHANE	C2H4BR2	392-394 394 R
	TETRACHLOROMETHANE	CCL4	119-120
OCTAMETHYLCYCLOTETrasiloxane		C8H24O4Si4	
	TETRACHLOROMETHANE	CCL4	181-185
PERFLUOROCYCLOBUTANE		C4F8	
	DICHLORODIFLUORO-METHANE	CCL2F2	48-54
	DICHLOROFLUOROMETHANE	CHCL2F	201
	DIFLUOROCHLOROMETHANE	CHCLF2	200
PERFLUOROHEXANE		C6F14	
	PERFLUOROTRIBUTYL-AMINE	C12F27N	514
PERFLUOROMETHYLCYCLOHEXANE		C7F14	
	HEXAFLUOROBENZENE	C6F6	506-512
PERFLUOROPROPYLENE		C3F6	
	DICHLORODIFLUORO-METHANE	CCL2F2	47
	DIFLUOROCHLOROMETHANE	CHCLF2	199
PERFLUOROTRIBUTYLAMINE		C12F27N	
	PERFLUOROHEXANE	C6F14	514
	1,1,2-TRICHLORO-1,2,2-TRIFLUOROETHANE	C2CL3F3	323
PIPERIDINE		C5H11N	
	HEXAMETHYLDISILOXANE	C6H18OSI2	504
	PYRIDINE	C5H5N	497-499
PROPIONALDEHYDE OXIME		C3H7NO	
	ACETONE OXIME	C3H7NO	421-422
	BUTYRALDEHYDE OXIME	C4H9NO	430-431
	METHYL ETHYL KETOXIME	C4H9NO	432-433

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
PROPIONITRILE		C3H5N	
	ACRYLONITRILE	C3H3N	414-415
PYRIDINE		C5H5N	
	ANILINE	C6H7N	500
	CHLOROFORM	CHCL3	237-243
	DICHLOROMETHANE	CH2CL2	267
	METHYL ETHYL KETOXIME	C4H9NO	463
	2-METHYLPYRIDINE	C6H7N	501
	3-METHYLPYRIDINE	C6H7N	502-503
	PIPERIDINE	C5H11N	497-499
	TETRACHLOROETHYLENE	C2CL4	343-347 347 R
	TETRACHLOROMETHANE	CCL4	134-143 143 R
	THIOPHENE	C4H4S	440
	TRIBROMOMETHANE	CHBR3	194-196
PYRROLIDINE		C4H9N	
	HEXAMETHYLDISILOXANE	C6H18OSI2	461-462
QUINALDINE		C10H9N	
	ISOQUINOLINE	C9H7N	583
QUINOLINE		C9H7N	
	ANILINE	C6H7N	557
	ISOQUINOLINE	C9H7N	582
SILICON TETRACHLORIDE		CL4SI	
	ACETONITRILE	C2H3N	387
	DIMETHYLDICHLORO-SILANE	C2H6CL2SI	406
	METHYLDICHLOROSILANE	CH4CL2SI	303-304
	METHYLTRICHLOROSILANE	CH3CL3SI	271-272
	TETRACHLOROMETHANE	CCL4	186-192 192 R
	TRICHLOROSILANE	CL3HSI	585
	TRIMETHYLCHLOROSILANE	C3H9CLSI	436
SULFOLANE		C4H8O2S	
	DICHLOROMETHANE	CH2CL2	266

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
SULFURYL CHLORIDE		CL2O2S	
	1,1,2,2-TETRACHLOROETHANE	C2H2CL4	359-361
1,1,1,2-TETRACHLOROETHANE		C2H2CL4	
	1,1,2,2-TETRACHLOROETHANE	C2H2CL4	358
1,1,2,2-TETRACHLOROETHANE		C2H2CL4	
	SULFURYL CHLORIDE	CL2O2S	359-361
	1,1,1,2-TETRACHLOROETHANE	C2H2CL4	358
	TETRACHLOROETHYLENE	C2CL4	333-337
TETRACHLOROETHYLENE		C2CL4	
	ACRYLONITRILE	C3H3N	341-342
	CARBON DISULFIDE	CS2	316-319 319 R
	CHLOROFORM	CHCL3	215
	1,2-DICHLOROETHANE	C2H4CL2	340
	DICHLOROMETHANE	CH2CL2	256
	PYRIDINE	C5H5N	343-347 347 R
	1,1,2,2-TETRACHLOROETHANE	C2H2CL4	333-337
	TETRACHLOROMETHANE	CCL4	77- 79 79 R
	1,1,2-TRICHLOROETHANE	C2H3CL3	338-339
	TRICHLOROETHYLENE	C2HCL3	324-332 332 R
TETRACHLOROMETHANE		CCL4	
	ACETONITRILE	C2H3N	85- 87
	ACRYLONITRILE	C3H3N	111-112
	ANILINE	C6H7N	169-174
	BROMOBENZENE	C6H5BR	152-157 157 R
	TERT-BUTYL CHLORIDE	C4H9CL	125-128
	CARBON DISULFIDE	CS2	73- 76
	CHLOROENZENE	C6H5CL	158-167 167 R
	CHLOROFORM	CHCL3	55- 61
		DICHLOROMETHANE	CH2CL2
			586-587
	1,2-DIBROMOETHANE	C2H4BR2	90- 92
	1,1-DICHLOROETHANE	C2H4CL2	93- 98
	1,2-DICHLOROETHANE	C2H4CL2	
		TRICHLOROETHYLENE	C2HCL3
			588-589

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
TETRACHLOROMETHANE	CCL4		
	DICHLOROMETHANE	CH2CL2	62- 67
		CHLOROFORM	586-587
	DIETHYLAMINE	C4H11N	130-133 133 R
	DIMETHYLAMINE	C2H7N	108-110
	N,N-DIMETHYLFORMAMIDE	C3H7NO	114-118 118 R
	DIMETHYL SULFOXIDE	C2H6OS	106-107
	ETHYL IODIDE	C2H5I	99
	HEXAFLUOROBENZENE	C6F6	144-151
	METHYLAMINE	CH5N	70- 72
	N-METHYLANILINE	C7H9N	177-180 180 R
	METHYL ETHYL KETOXIME	C4H9NO	129
	N-METHYLFORMAMIDE	C2H5NO	100-104 104 R
	METHYL IODIDE	CH3I	68
	METHYL ISOCYANATE	C2H3NO	88- 89
	NITROBENZENE	C6H5NO2	168
	NITROETHANE	C2H5NO2	105
	NITROMETHANE	CH3NO2	69
	1-NITROPROPANE	C3H7NO2	119-120
	OCTAMETHYLCYCLOTETRA- SILOXANE	C8H24O4Si4	181-185
	PYRIDINE	C5H5N	134-143 143 R
	SILICON TETRACHLORIDE	CL4SI	186-192 192 R
	TETRACHLOROETHYLENE	C2CL4	77- 79 79 R
	THIAZOLE	C3H3NS	113
	THIOPHENE	C4H4S	124
	1,1,1-TRICHLOROETHANE	C2H3CL3	82- 84
	TRICHLOROETHYLENE	C2HCL3	80- 81
		1,2-DICHLOROETHANE	C2H4CL2
			588-589
	TRIETHYLAMINE	C6H15N	175-176
	TRIMETHYLAMINE	C3H9N	121-123
1,1,1,5-TETRACHLOROPENTANE	C5H8CL4		
1,1,1,3-TETRACHLOROPROPANE	C3H4CL4		417
1,1,1,3-TETRACHLOROPROPANE	C3H4CL4		
1,1,1,5-TETRACHLOROPENTANE	C5H8CL4		417

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
TETRAMETHYLSILANE		C4H12SI	
	(BROMOMETHYL-)TRI-METHYLSILANE	C4H11BR3I	465-471
THIAZOLE		C3H3NS	
	TETRACHLOROMETHANE	CCL4	113
THIONYL CHLORIDE		CL2OS	
	BENZOYL CHLORIDE	C7H5CLO	573
THIOPHENE		C4H4S	
	N,N-DIMETHYLFORMAMIDE	C3H7NO	425
	NITROMETHANE	CH3NO2	292-293
	PYRIDINE	C5H5N	440
	TETRACHLOROMETHANE	CCL4	124
TRIBROMOMETHANE		CHBR3	
	DIMETHYL SULFOXIDE	C2H6OS	193
	PYRIDINE	C5H5N	194-196
2,3,4-TRICHLORO-1-BUTENE		C4H5CL3	
	1,3-DICHLORO-2-BUTENE	C4H6CL2	444
1,1,1-TRICHLOROETHANE		C2H3CL3	
	1,2-DICHLOROETHANE	C2H4CL2	363
	CIS-1,2-DICHLOROETHYLENE	C2H2CL2	356
	TRANS-1,2-DICHLOROETHYLENE	C2H2CL2	357
	TETRACHLOROMETHANE	CCL4	82- 84
1,1,2-TRICHLOROETHANE		C2H3CL3	
	TETRACHLOROETHYLENE	C2CL4	338-339
TRICHLOROETHYLENE		C2HCL3	
	ACETONITRILE	C2H3N	349-350
	1,2-DICHLOROETHANE	C2H4CL2	351
		TETRACHLOROMETHANE CCL4	588-589
	TRANS-1,2-DICHLOROETHYLENE	C2H2CL2	348
	DIETHYL SULFIDE	C4H10S	352
	NITROMETHANE	CH3NO2	280
	TETRACHLOROETHYLENE	C2CL4	324-332 332
	TETRACHLOROMETHANE	CCL4	80- 81
		1,2-DICHLOROETHANE C2H4CL2	588-589

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
2,2,3-TRICHLOROHEPTAFLUOROBUTANE		C4CL3F7	
	1,2-DICHLOROHEXAFLUORO-CYCLOPENTENE	C5CL2F6	439
TRICHLOROPHENYLSILANE		C6H5CL3SI	
	DICHLOROPHENYLSILANE	C6H6CL2SI	536-539 539
TRICHLOROSILANE		CL3HSI	
	METHYLDICHLOROSILANE	CH4CL2SI	382
	SILICON TETRACHLORIDE	CL4SI	585
1,1,2-TRICHLORO-1,2,2-TRIFLUOROETHANE		C2CL3F3	
	DICHLORODIFLUORO-METHANE	CCL2F2	43- 45
	PERFLUOROTRIBUTYL-AMINE	C12F27N	323
TRIETHYLAMINE		C6H15N	
	CHLOROBENZENE	C6H5CL	534-535
	CHLOROFORM	CHCL3	247
	DICHLOROMETHANE	CH2CL2	268
	DIETHYLAMINE	C4H11N	478-496 496
	ETHYLAMINE	C2H7N	412-413
	HEXAFLUOROBENZENE	C6F6	585
	TETRACHLOROMETHANE	CCL4	175-176
TRIFLUOROBROMOMETHANE		CBRF3	
	DIFLUOROCHLOROMETHANE	CHCLF2	1- 16
TRIMETHYLAMINE		C3H9N	
	N-DEUTEROMETHYLAMINE	CH3D2N	273-277
	METHYLAMINE	CH5N	312-315
	TETRACHLOROMETHANE	CCL4	121-123
TRIMETHYLCHLOROSILANE		C3H9CLSI	
	DIMETHYLDICHLORO-SILANE	C2H6CL2SI	485
	METHYLTRICHLOROSILANE	CH3CL3SI	269-270
	SILICON TETRACHLORIDE	CL4SI	436
VINYL CHLORIDE		C2H3CL	
	1,2-DICHLOROETHANE	C2H4CL2	362
	1,1-DICHLOROETHYLENE	C2H2CL2	353