

STANDARD SPECTRA COLLECTION

**1981-1990
SUPPLEMENTARY
MOLECULAR
FORMULA
INDEX**



*Sadtler
Division*

The publication of the physical data of the Sadtler Standard Spectra and the Sadtler Commercial Spectra is intended to be descriptive. The samples of the materials represented have come generally from other sources than our own laboratories and frequently without the donors' knowledge of their part in this publication.

On the other hand every effort is made by Sadtler Research Laboratories, a division of Bio-Rad Laboratories, Inc. to assure the reliability of the published spectra. When improved data is available or errors are called to our attention, we revise and reissue the proper replacement spectra.

SADTLER RESEARCH LABORATORIES, A DIVISION OF BIO-RAD LABORATORIES, INC. DOES NOT WARRANT MERCHANTABILITY OR FITNESS FOR ANY PARTICULAR PURPOSE, OR MAKE ANY OTHER WARRANTY OR AGREEMENT EXPRESS OR IMPLIED WITH RESPECT TO THE SPECTRA CONTAINED HEREIN. IF ANY MODEL OR SAMPLE WAS SHOWN TO BUYER, SUCH MODEL OR SAMPLE WAS USED MERELY TO ILLUSTRATE THE ARTICLE AND NOT TO REPRESENT THAT ANY SPECTRA CONTAINED HEREIN WOULD CONFORM TO THE MODEL OR SAMPLE.

COPYRIGHT NOTICE

ALL RIGHTS RESERVED

Copyright © 1990
SADTLER RESEARCH LABORATORIES
DIVISION OF BIO-RAD LABORATORIES, INC.
RESEARCHERS, Editors & Publishers
Printed in the United States of America

ISBN 0-8456-0162-8

INTRODUCTION

This 1981 - 1990 Supplementary Molecular Formula Index to Sadler Standard Spectra contains entries for all compounds newly published through 1990 in any of the collections of infrared prism, infrared grating, ultraviolet and nuclear magnetic resonance reference spectra. This publication is a continuation of the 1980 Cumulative Index series and must be used in conjunction with that publication to locate all available spectra serial numbers for a compound in the total spectra collections whether infrared, ultraviolet or nuclear magnetic resonance.

Since any spectrum published prior to 1981 is included in the 1980 Cumulative Index and spectra added in 1981 - 1990 are listed only in this supplement, it is necessary to consult *both* the 1980 Cumulative Index and this supplement in looking up a particular compound.

In this supplement the appropriately labelled columns show the serial numbers assigned to the following published spectra:

Sadtler Standard Prism Spectra 59001 - 79000
Sadtler Standard Grating Spectra 59001K - 79000K
Sadtler Standard Ultraviolet Spectra 29909UV - 42735UV
Sadtler Standard Nuclear Magnetic Resonance Spectra 32001M - 52000M

The arrangement of this Molecular Formula Index is based on the Hill system. Compounds containing carbon are listed first by the number of carbon atoms present, then by the number of hydrogen atoms, and then according to the presence and quantity of non-metallic elements following the sequence of Br, Cl, F, I, N, O, P, S and Si. Compounds containing carbon and no hydrogen are indexed at the beginning of each category according to carbon content and arranged within the category by the occurrence of the non-metallic elements listed above. Compounds which do not contain carbon are listed on the final pages of the index.

The final column in the formula table, titled M, is used to indicate the presence of other elements not otherwise specified. The presence of one of these elements in a compound is represented by its symbol (NA, K, FE, etc.). If more than one of these elements is present, they are not specified but signified by X2 (for two different elements), X3 (for three), etc.

For compounds having the same molecular formula, the further arrangement is alphabetical according to chemical name.

There are some special cases which modify the presentation of the molecular formula, they are as follows.

- (1) Inorganic acid salts of basic compounds such as amines are found under the formula of the amine alone. However the anion of "onium" compounds is included in the formula.
- (2) Compounds which contain an organic acid salt of a basic component are cross-referenced to the basic component and to the total formula of the compound.
- (3) Molecules of hydration are not included in the formula but can be ascertained from the chemical name.
- (4) In any case where the number of atoms of an element exceed the space available to list them, the highest possible integer is used. For example, for compounds containing 9 or more atoms of a halogen the representation is the maximum available of 9. Thus DECAFLUORO-o-XYLENE C₈F₁₀ is represented as C₈F₉ and 2,2,3,3,3-PENTAFLUOROPROPYL SILICATE C₁₂H₈F₂₀O₄Si is represented as C₁₂H₈F₉O₄Si.

The method of naming the chemical compounds in the Sadtler reference spectra collections closely follows the Chemical Abstracts (CA) nomenclature system which was in operation prior to the publication of the CA Ninth Collective Index. Briefly, this system assigns the parent name on the basis of a predefined priority of functionality (the Sadtler Chemical Classes Index is comparable to this priority table) and then the substituents to the parent name are listed after it in alphabetical sequence. The simple example shown below will illustrate this point. In addition to the systematized names, many cross-references to frequently used trivial names are also included in this index.

Example I

- The compound HO-CH₂-CH₂-CH₂-C≡N
could be named as (a) HYDRACRYLONITRILE
 (b) PROPIONITRILE, 3-HYDROXY-,
 (c) 1-PROPANOL, 3-CYANO-,

The index includes (a) which is a commonly-accepted name and (b) which is the systematic name but not (c) since the nitrile functionality always takes precedence over the hydroxy group in the priority table.

The infrared spectra of some compounds were run in various media or physical forms when this additional information was pertinent to spectroscopic identification, these alternative spectra are designated at the end of the name in the index entry by the following abbreviations:

Since the Sadtler indexing system is totally computerized, certain limitations are imposed in nomenclature symbolism. Deviations which appear in the printed index are as follows:

- | | | |
|----|------------|-------------------------------------------------|
| / | (slash) | - Read as parenthesis, bracket, or brace |
| < | | - Read as indication of superscripting |
| PR | | - Read as "prime". Therefore 2PR is read as 2'. |
| * | (asterisk) | - Also read as "prime". |

Lack of provision for Greek letters, super or subscripts (except as noted above) or lower case letters causes the following changes from normal notation:

- | | |
|-------|-----------------------------------------------------------------------------------------|
| A | - Read as a or α |
| B | - Read as b or β |
| G | - Read as g or γ |
| D | - Read as d or δ |
| O | - Read as o, ortho or oxygen |
| M | - Read as m or meta |
| N | - Read as normal or nitrogen |
| P | - Read as p, para or phosphorus |
| S | - Read as s (symmetrical) or sulfur |
| D & L | - Still retain their original significance when used in conjunction with carbohydrates. |

Some examples illustrating the variations to be encountered are shown below.

Chemical Abstracts System

s-Triazine, 4-amino-6-(p-bromoanilino)-1,2-dihydro-2,2-dimethyl,

Benz[a]anthracene-7,12-dione

Chryseno[6,5-d]oxazole

Spiro[cyclopropane-1,9'-fluorene], 2-acetyl,

Tricyclo[3.3.1.1^{3,7}]decane

Sadtler Index

S-TRIAZINE, 4-AMINO-6-/P-BROMOANILINO/-1,2-DIHYDRO-2,2-DIMETHYL-,

BENZ/A/ANTHRACENE-7,12-DIONE

CHRYSENO/6,5-D/OXAZOLE

SPIRO/CYCLOPROPANE-1,9PR-FLUORENE/, 2-ACETYL-,

or

SPIRO/CYCLOPROPANE-1,9*-FLUORENE/, 2-ACETYL-,

TRICYCLO/3.3.1.1#3,7/DECANE

1981-1990 SUPPLEMENTARY
MOLECULAR FORMULA INDEX

NAME	C	H	B	C	F	N	O	P	S	I	M	PRISM	GRATING	U.V.	N.M.R.	C-13
METHANESULFONYL CHLORIDE, TRI-FLUORO-,	1			1	3		2	1			72653	72653			22473	
CARBONIC ACID, DILITHIUM SALT	1					3			LI	72728	72728					
LITHIUM CARBONATE	1					3	1		LI	72728	72728					
PHOSPHONIC ACID, /TRICHLORO-METHYL/-,	1	2		3		3	1			40464	20464			33611 11971		
FORMAMIDE, SULFO-, POTASSIUM SALT	1	2				1	4	1	K	78202	78202			51149		
SULFONIC ACID, CARBAMOYL-, POTASSIUM SALT	1	2				1	4	1	K	78202	78202			51149		
MERCURY, CHLOROMETHYL-, FORMAMIDINE, 1-CHLORO-, MONOHYDRO-CHLORIDE	1	3	1			2			HG	67240	67240			40190 19552		
PHOSPHONOTHIOIC DICHLORIDE, METHYL-,	1	3		2			1	1		21804	37558P			41587 16279		
MERCURY, IODOMETHYL-, UREA, NITRO-,	1	3				1			HG	7951	44652P			35616 41754		
1H-TETRAZOLE, 5-AMINO-, METHANOL-D	1	3				3	3		D	36546	48474P	31908	30634	11228		
METHYL ALCOHOL-D	1	3					1		D	36546	48474P			35788 11949		
METHANESULFONIC ACID, SILVER SALT	1	3					1		AG	40607	20607			35788 11949		
METHANESULFONIC ACID, POTASSIUM SALT	1	3					3	1	K	67188	67188			41597 15407		
SULFURIC ACID, MONOMETHYL ESTER, SODIUM SALT, HYDRATE	1	3					4	1	NA					40154 18519		
FORMALDEHYDE, HYDRAZONE	1	4					2			17492	25710			33738		
UREA, OXALATE /2 TO 1/	1	4					2	1		44917	27917			43914		
UREA-NITRATE	1	4					2	1		9795	45405P			35627 12326		
UREA, HYDROXY-, AMMONIUM THIOCYANATE	1	4					2	2		45287	30287			33625 24474		
THIOCYANIC ACID, AMMONIUM SALT	1	4					2	1		44864	27864			41601 4745		
GUANIDINE, NITROSO-, METHANOL-D	1	4					4	1		44864	27864			41601 4745		
METHYL ALCOHOL-D	1	4						1		67417	67417			40325		
METHYLAMINE, SULFATE /2 TO 1/	1	5						1		36546	48474P			35788 11949		
HYDROXYLAMINE, N-METHYL-, HYDRO-CHLORIDE	1	5						1		36546	48474P			35788 11949		
PHOSPHONIC ACID, /AMINOMETHYL/-, MONOSODIUM SALT	1	5					1	3	1	NA	66104	66104		37937 17936		
GUANIDINE, PHOSPHATE /2 TO 1/	1	5					3			67126	67126					
GUANIDINE, SULFAMATE /1 TO 1/	1	5					3			67118	67118			20911		
GUANIDINE, MONOTHIOCYANATE	1	5					3			8323	29942	2218	51937			
GUANIDINE, THIOCYANATE	1	5					3			8323	29942	2218	51937			
SEMICARBAZIDE, THIO-, MONOHYDRO-CHLORIDE	1	5					3		1	67449	67449			40355		
GUANIDINE, 1-AMINO-3-NITRO-, METHANESULFONIC ACID, HYDRAZIDE	1	5					5	2		66547	66547			37257		
GUANIDINE, AMINO-, SULFATE /1 TO 1/, MONOHYDRATE	1	6					2	2	1	67514	67514			40401		
CARBOHYDRAZIDE, THIO-, GUANIDINE, SULFAMATE /1 TO 1/	1	6					4			78617	78617					
VALERIC ACID, 4-AMINO-4-/HYDROXY-PHENYLPHOSPHINYL/-, DISODIUM SALT	1	14					4	3	1	43010	26010		43807	20911		
							1	4	1	NA	67118	67118		68138 68138		
														40803		
ETHANE, 1,2-DIBROMOTETRACHLORO-, SULFONE, BIS/TRIBROMOMETHYL/-	2	2	6	1			2	1		64453	64453			20831		
ETHANE, 1,2-DICHLOROTETRAFLUORO-, ETHANE, 1,1,1-TRICHLORO-2,2,2-TRIFLUORO-,	2	2	2	4						78546	78546					
ACETIC ACID-D, TRIFLUORO-, METHANESULFONIC ANHYDRIDE, TRI-FLUORO-,	2	2	3	3			2		D	72897	72897			14798		
METHANESULFONIC ACID, TRIFLUORO-, TIN/2 PLUS/ SALT	2	2	6				5	2		60120	60120					
MERCURY 2 PLUS/ THIOCYANATE	2	2					6	2		72955	72955					
THIOCYANIC ACID, MERCURY/2 PLUS/ SALT	2	2					2			72721	72721					
LEAD THIOCYANATE	2	2					2			72721	72721					
OXALIC ACID, TIN/2 PLUS/ SALT	2	2					4			PB	72614	72614				
ACETIC ACID, TRIBROMO-, ETHYLENE, 1-CHLORO-1,2-DIFLUORO-,	2	1	3	1	2		2			SN	60116	60116		24091		
ACETIC ACID, DICHLORO-, SODIUM SALT	2	1	2				2			22002	21648					
2H-TETRAZOLE, 5-TRIFLUOROMETHYL/-, ETHANE, 1,1,2-TETRABROMO-,	2	1	3	3			4			76274	76274			41588 12470		
ACETAMIDINE, N+,2,2,2-TETRACHLORO-, DITHIAZOLE-3-THIONE, 3H-1,2,4-, 5-AMINO-, THIADIAZOLE-2,5-DITHIOL, 1,3,4-,	2	2	2	4			2			NA	72899	72899		45744 22582		
							2			67639	67639			40522 21995		
							3			69761	69761			42519 22080		
							4			60510	60510					
										19580	10233			6442 39708		

NAME

4

6

F

N

O

P

S

I

M

PRISM

GRATING

U.V.

N.M.R.

C-13

**1981-1990 SUPPLEMENTARY
MOLECULAR FORMULA INDEX**

NAME	C	H	Br	Cl	F	I	N	O	P	S	S:	M	PRISM	GRATING	U.V.	N.M.R.	C-13
S-TRIAZOLE, 5-NITRO-, GLYOXAL, SODIUM BISULFITE /1 TO 2/ /SALT/	2	2					4	2	2			38997 46722	17997 31722	37432	47944	5500	
FORMIC ACID, CARBAMOYL-, OXAMIC ACID, OXAMIC ACID /KBR/ TRIAZOLE-3-SULFONIC ACID, 1H-1,2,4-,	2	3					1	3				5854 5854 11350 41586	29080 29080 29080 22586	39680 39680 39680 43686	16119 16119 16119 16119		
S-TRIAZOLE-3-SULFONIC ACID THIAZIAZOLE, 1,3,4-, 2-AMINO-, TRIAZOLE-3-THIOL, 1H-1,2,4-,	2	3					1	3				41586 57711 31684 68147	22586 57711 7670 68147	31909 30635 37063	30635 9170 24359 7879		
S-TETRAZINE, 3-AMINO-, ACETIC ACID, CESIUM SALT CESIUM ACETATE	2	3					5		2			CS CS	64586 X2	64586	40810 45926 37265		
ACETIC ACID, ARSONO-, DISODIUM SALT, MONOHYDRATE ETHANESULFONIC ACID, 2-BROMO-, SODIUM SALT, MONOHYDRATE	2	3					5		2			NA	61415	61415	34304		
PHOSPHORODICHLORIDIC ACID, 2-CHLOROETHYL ESTER ACETONITRILE, AMINO-, HYDROCHLORIDE UREA, FORMYL-, K	2	4	1				3	1				67009	67009	40006	18299		
OXALOHYDROAMIC ACID AMITROLE /AMITROLE T/ AMIZOL /THE HERBICIDE/	2	4					4					48114 46492 8667 8667 8667 41602 57845 17434 37797	35114 31492 21258 21258 21258 22602 57845 48025P 16791	39781 47934 36875 36875 36875 43691 31990 37689 33600	11464 16244 6254 6254 6254 23446 33600		
S-TRIAZOLE, 3-AMINO-, TRIAZOLE-3-SULFONAMIDE, 1H-1,2,4-, 2H-TETRAZOLE-5-THIOL, 2-METHYL-, GLYCOLALDEHYDE	2	4					4	2	1						43691		
1,2-ETHANEDISULFONIC ACID, 1,2-DI-HYDROXY-, DISODIUM SALT, MONOHYDRATE GLYOXAL, CMPD WITH SODIUM BISULFITE /1 TO 2/, MONOHYDRATE	2	4					8	2				NA	37797	16791	33600		
ACETAMIDE ACETAMIDE OXAMIC ACID, HYDRAZIDE SEMIOXAMIZIDE TRIAZOLE, 4H-1,2,4-, 3,4-DIAMINO-, MONOHYDROCHLORIDE	2	5					1	1				13207 69 24467 24467 71866	15005 15005 4732 4732 71866	3451 3451 37021 37021	4280 4280		
ETHYL ALCOHOL-D TRIAZATRIPHOSPHORINE, 1,3,5,2,4,6-, 2,2-DIMETHYL-4,4,6,6-TETRACHLORO-, PSEUDOURA, 2-METHYL-, SULFATE /2 TO 1/	2	6	4				3	1	3			D	64479 62674	64479 62674	37194 35304		
PSEUDOURA, 2-METHYL-2-THIO-, MONO-HYDROIODIDE PSEUDOURA, 2-METHYL-2-THIO-, MONO-P-TOLUENESULFONATE	2	6					2		1			67182	67182	40149	18515		
UREA, AMINO-, OXALIC ACID, DIHYDRAZIDE OXAMIDOXIME GUANIDINE, MONOTHIOCYANATE GUANIDINE, THIOCYANATE	2	6					4	1				69246	69246	42023	21196		
S-TETRAZINE-3/2H/-THIONE, TETRA-HYDRO-, AMIDINO DISULFIDE, DIHYDROCHLORIDE DISULFIDE, AMIDINO, DIHYDROCHLORIDE FORMAMIDINE, 1,1-DITHIODI-, DI-HYDROCHLORIDE	2	6					4	2				60164	60164	32891	12149		
TRIAZOLE, 4H-1,2,4-, 3-AMINO-5-HYDRAZINO-, DIHYDROCHLORIDE METHANESULFONIC ACID, CALCIUM SALT LEAD, BIS(METHYLTHIO)-, PLUMBANE, BIS(METHYLTHIO)-, BORANE, CMPD WITH DIMETHYLAMINE /1 TO 1/	2	6					6	2				77064 37796 68321 8323 8323 71729	77064 16790 68321 29942 29942 71729	37351 38073	50058 26625		
DIMETHYLAMINE DIMETHYLAMINE, CMPD WITH BORANE /1 TO 1/ ETHYLAMINE, SULFATE /2 TO 1/ ACETALDEHYDE-AMMONIA ETHANOL, 1-AMINO-, GUANIDINE, METHYL-, MONOHYDRO-CHLORIDE ISOSEMICARBAZIDE, 3-METHYL-3-THIO-, MONOHYDROIODIDE BIGUANIDE BIGUANIDE, SULFATE, HYDRATE, /1.1.1/ PHOSPHONIC ACID, DIMETHYL ESTER BORON FLUORIDE, CMPD WITH METHANOL /1 TO 2/	2	7					1	1				1140 67219 5776 5776 68832 73449	41323P 67219 33658 33658 68832 73449	39669 40176	15604 19540 6813 6813 41412		
	2	7					1	1					72754 72754	72754	45630		
	2	7					3		1						15604 6813 6813 18644		
	2	7					3		1								
	2	7					5										
	2	7					5										
	2	8					3	1	2			B	61328 72645	61328 72645	6652 5820		

1981-1990 SUPPLEMENTARY
MOLECULAR FORMULA INDEX

NAME	C	H	B	F	I	N	O	P	S	Si	M	PRISM	GRATING	U.V.	N.M.R.	C-13
METHANOL, CMPD WITH BORON FLUORIDE /2 TO 1/	2	8		3		2					B	72645	72645		5820	
DIAZADIPHOSPHETIDINEDIIDE, 1,3,2,4-, 1,3-DIMETHYL-2,2,2,4,4,4,4-OCTAFLUORO-2,2,4,4-TETRAHYDRO-, DI-HYDROGEN	2	8		8		2		2				71188	71188		44180	22659
PHOSPHINIC ACID, /AMINOMETHYL/-METHYL-	2	8				1	2	1				74034	74034		46996	26264
PHOSPHONIC ACID, //METHYLAMINO/-METHYL/-	2	8				1	3	1				74036	74036		46998	26265
HYDRAZINE, 1,1-DIMETHYL-, MONO-HYDROCHLORIDE	2	8				2						54898	54898		41607	7383
HYDRAZINE, ETHYL-, OXALATE /1 TO 1/ AMMONIUM OXALATE, MONOHYDRATE	2	8				2	2	4				72528	72528		45452	24437
OXALIC ACID, DIAMMONIUM SALT, MONOHYDRATE	2	8				2	4					64475	64475		37191	37191
PHOSPHONIC ACID, /GUANIDIINO-METHYL/- SESQUIHYDRATE	2	8				3	3	1				62797	62797			
UREA, OXALATE /2 TO 1/	2	8				4	2					44917	27917			43914
BIACARABMIC ACID, DIHYDRAZIDE	2	8				6	2					69402	69402			
BISEMICARBAZIDE, 4,4--	2	8				6	2					69402	69402			
METHYL PYROPHOSPHATE	2	8				7	2					31698	7682		33582	
PHOSPHINIC ACID, BIS/AMINOMETHYL/- MONOHYDROCHLORIDE	2	9				2	2	1				65567	65567			17745
BORANE, CMPD WITH DIMETHYLAMINE 1 TO 1	2	10				1					B	72754	72754		45630	22530
DIMETHYLAMINE, CMPD WITH BORANE /1 TO 1/	2	10				1					B	72754	72754		45630	22530
METHYLAMINE, SULFATE /2 TO 1/	2	10				2						67186	67186		40152	18517
GUANIDINE, PHOSPHATE /2 TO 1/	2	13				6	4	1				67126	67126			
PROPANE, 1,1,2,2,3-PENTAFLUOROTRICHLORO-	3		3	5								69012	69012			
ACRYLOYL CHLORIDE, TRICHLORO-, PROpane, 1,1,1,3,3-PENTACHLOROTRIFLUORO-	3		4			1						68078	68078			
PROPANE, 2,2-DIFLUOROHEXACHLORO-, PROPIONYL CHLORIDE, PENTACHLORO-, ACRYLOYL CHLORIDE, 3,3-DICHLORO-, ACRYLIC ACID, TRICHLORO-, CARBONIC ACID, CYCLIC VINYLENE ESTER	3		5	3								67726	67726			
VINYLENE CARBONATE	3		6	2								67725	67725			
MESOXALIC ACID, HYDRATE	3		6				1					65879	65879			
MALONIC ACID, DIHYDROXY-, CALCIUM SALT, TRIHYDRATE	3		1	3		1						68091	68091	40761	38804	
MESOXALIC ACID, CALCIUM SALT, TRIHYDRATE	3		1	3		2						65865	65865	45711	22755	
THIAZOLE, 2-AMINO-5-BROMO-, HYDROBROMIDE	3		2			3						72847	72847		45711	22755
MELAMINE, N ₂ ,N ₄ ,N ₆ -TRICHLORO-, PROPIONIC ACID, 3,3,3-TRICHLORO-, 2,4-OXAZOLIDINEDIONE	3		3	3		6						72847	72847	47831	21922	
THIAZOLE	3		3	3		1						19915	39875P			
IMIDAZOLE, 2-NITRO-, IMIDAZOLE, 4-NITRO-, CYANURIC ACID	3		3	3		2						67308	67308			
3,5-PYPAZOLIDINEDIONE, 4-NITROSO-, S-TRIAZINE-2,4,6-TRIGLYCINE, S-TRIAZINE-2,4,6-(1H,3H,5H)-TRIONE PYRUVIC ACID, SODIUM SALT	3		3	3		1	3					32785	9780	37083	9197	
PROPIONITRILE, 2-CHLORO-, PROPIONYL CHLORIDE, 3-CHLORO-, PROPIONIC ACID, 2,3-DICHLORO-, PROPANE, 1,2,2,3-TETRACHLORO-, PROPANE, 1,1,2,3-TETRACHLORO-, ACETONITRILE, METHYLENEAMINO-, IMIDAZOLE, PENTAFLUOROPROPIONATE /1 TO 1/ SALT/	3		3	3		3	3					7027	18149	28614	35611	23040
IMIDAZOLE, TRIFLUOROACETATE /1 TO 1/ SALT/	3		4			2						7027	18149	28614	35611	23040
THIADIAZOL-5-OL, 1,2,4-, 3-/METHYLTHIO/-, THIADIAZOL-5-OL, 1,2,4-, 3-METHOXY-, 1,1-ETHANEDISULFONIC ACID, 1-AMINO-2-CYANO-, DISODIUM SALT, TRIHYDRATE	3		4			2	2	1				64091	64091	35380	36868	15537

NAME	C	H	B	F	I	N	O	P	S	Si	M	PRISM	GRATING	U.V.	N.M.R.	C-13
------	---	---	---	---	---	---	---	---	---	----	---	-------	---------	------	--------	------

**1981-1990 SUPPLEMENTARY
MOLECULAR FORMULA INDEX**

NAME	C	H	Br	Cl	F	I	N	O	P	S	Si	M	PRISM	GRATING	U.V.	N.M.R.	C-13	
5-AZACYTOSINE	3	4					4	1				61474	61474					
S-TRIAZIN-2/1H-/ONE, 4-AMINO-, TRIAZOLE, 1H-1,2,4-, 1-METHYL-	3	4					4	1				61474	61474					
3-NITRO-, 1,2-OXATHIOLAN-5-ONE, 2,2-DIOXIDE	3	4					4	2				74345	74345	41389	47282			
PROPIONIC ACID, 3-SULFO-, CYCLIC ANHYDRIDE	3	4					4	1				63292	63292					
HALONIC ACID, DIHYDROXY-, CYCLOPROPANE, BROMO-, ISOPROPENYL BROMIDE	3	4						6				72586	72586		45506	22434		
PROPENE, 2-BROMO-, 1-PROPENE, 2-BROMO-, C	3	5	1									37813	16807		33602	9166		
1-PROPENE, 2-BROMO-, C	3	5	1									13406	47541P			12231		
PROPYNYL BROMIDE	3	5	1									13406	47541P			12231		
ETHANOL, 2,2,2-TRIFLUORO-, METHANE- SULFONATE	3	5	1		3		1	3	1			2270	41848P		43491	12231		
METHANESULFONIC ACID, 2,2,2-TRI- FLUOROETHYL ESTER	3	5		3			3	1				2270	41848P		V 23	12231		
PROPARGYLAMINE, HYDROCHLORIDE	3	5					1					71756	71756		41755			
2-PROPYNYLAMINE, HYDROCHLORIDE	3	5					1					71756	71756		44717	22730		
CYCLOPROPANE, NITRO-, MALONOHYDROXAMIC ACID, MONO- POTASSIUM SALT	3	5					1	2				K	68128	68128		33612	14531	
IMIDAZOLE, 2-AMINO-, SULFATE /2 TO 1/	3	5					3					73340	73340			40793		
TRIAZOLE-3-SULFONIC ACID, 1H-1,2,4-, 5-METHYL-, THIADIAZOLE, 1,3,4-, 2-AMINO-	3	5					3	3	1			72817	72817	40373	45683	22564		
5-METHYL-, THIADIAZOLE, 1,3,4-, 2-AMINO- 5-METHYLTHIO-/-,	3	5					3		2			60940	60940		33505	13362		
S-TETRAZINE, 3-AMINO-6-METHYL-, PROPIONIC ACID, POTASSIUM SALT	3	5					5					68150	68150		40813			
GLYCERIC ACID, 3-DIHYDROGEN PHOSPHATE, BARIUM SALT, DIHYDRATE, D-, TRISELENACYCLOHEXANE, 1,3,5-.	3	5					2	7	1			K	67388	67388		40299	20339	
S-TRISELENANE	3	6										BA	67325	67325				
1-PROPANESULFONIC ACID, 3-BROMO-, SODIUM SALT	3	6	1					3	1			SE	70288	70288				
2-PROPANOL, 1,3-DIFLUORO-, 1-PROPANESULFONIC ACID, 3-IODO-, POTASSIUM SALT	3	6		2			1	3	1			K	70288	70288		42809		
SERINE, DIHYDROGEN PHOSPHATE ESTER, BARIUM SALT, DL-, B-ALANONITRILE, FUMARATE	3	6						1	6	1		NA	69374	69374		42144		
PROPINONITRILE, 3-AMINO-, FUMARATE	3	6						2				SE	70288	70288			13182	
OXAZOLIDINE, 3-NITROSO-, PYRUVALDEHYDE, DIOXIME	3	6						2	2			BA	67326	67326			22361	
GLYCINE, N-/THiocarbamoyl-/-, ACETIC ACID, /N-/HYDROXYAMIDINO-/-,	3	6						2	2	1			68150	68150				
B-ALANINE, 3-/HYDROXYIMINO-/-, GLYCINE, N-CARBAMOYL-, HYDANTOIC ACID	3	6						2	3				67388	67388				
PYRAZOL-5-OL, 3,4-DIAMINO-, SULFATE, SALT/, 1,1/	3	6						4	1				67325	67325				
TRIAZOLE-5-SULFONAMIDE, 1H-1,2,4-, 1-METHYL-, MELAMINE	3	6						4	2	1			72466	72466				
MELAMINE, PHOSPHATE /1 TO 1/ /SALT/ S-TRIAZINE, 2,4,6-TRIAMINO-, PHOS-	3	6						6					70288	70288				
PHATE /1 TO 1/ /SALT/ S-TRIAZINE, 2,4,6-TRIAMINO-, ETHER, METHYL VINYL,	3	6						6					70288	70288				
TETRAETHIOPANE, 1,2,4,6-, SILANE, PROPYLTRICHLORO-, ETHER, 2-iodoethyl Methyl,	3	7	3				1		4	1								
GLYCOLAMIDE, N-/HYDROXYMETHYL/-, SERINE, D-, ALANINE, 3-SULFO-, DL-,	3	7						1	3									
CYSTEIC ACID, DL-, PROPIONAMIDE, THIO-, 1-PROPAN-1-O-OL	3	7						1	5	1								
2-PROPAN-2-O-OL	3	7						1	5	1								
1-PROPANESULFONIC ACID, SODIUM SALT	3	7						1	5	1								
1-PROPANESULFONIC ACID, 3-HYDROXY-, MONOSODIUM SALT	3	7						4	1									
PROPYLAMINE, 3-CHLORO-, HYDRO- CHLORIDE	3	8	1				1											
PHOSPHORAMIDOTHIOIC DICHLORIDE, ISOPROPYL-, BORON FLUORIDE, CMPO WITH	3	8	2				1	1	1									
1-PROPANOL /1 TO 1/	3	8	3				1											

12-89

1981-1990 SUPPLEMENTARY
MOLECULAR FORMULA INDEX

NAME	C	H	Br	Cl	F	I	N	O	P	S	Si	M	PRISM	GRATING	U.V.	N.M.R.	C-13
1-PROPANOL, CMPS WITH BORON FLUORIDE /1 TO 1/ ALANINAMIDE, MONOHYDROBROMIDE, L-, PROPIONAMIDE, 2-AMINO-, MONOHYDROBROMIDE, L-, PROPIONIC ACID, 2,3-DIAMINO-, MONO-HYDROCHLORIDE, DL-, PROPIONIC ACID, 2,3-DIAMINO-, MONO-HYDROBROMIDE PSEUDOUREA, 2-ETHYL-2-THIO-, MONO-/P-TOLUENESULFONATE, GUANIDINE, 1,1-DIMETHYL-3-NITRO-, MALONAMIDOXIME S-TETRAZINE-3'2H/-THIONE, 6-METHYL-TETRAHYDRO-, ETHER, ETHYL METHYL, METHANE, /METHYLSULFINYL//METHYL-THIO/-, 2-PROPANOL, 1,3-DIMERCAPTO-, SULFIDE, METHYL /METHYLSULFINYL/-METHYL, SULFOXIDE, METHYL /METHYLTHIO/-METHYL, FORMALDEHYDE, DIMETHYL MERCAPTAL METHANE, BIS/METHYLTHIO/-, PROPAENERITHIOL, 1,2,3-, SULFONIUM TETRAFLUOROBORATE/1 MINUS/, TRIMETHYL-, STANNANE, IODOTRIMETHYL-, TIN, IODOTRIMETHYL-, ALANINOL, OXALATE /1 TO 1/, L-, 1-PROPANOL, 2-AMINO-, OXALATE /1 TO 1/, L-, 2-PROPANOL, 1-AMINO-, PHOSPHATE /2 TO 1/ /SALT/ TRIMETHYLAMINE, N-OXIDE, DIHYDRATE GUANIDINE, ETHYL-, MONOHYDRO-CHLORIDE PHOSPHONIC ACID, METHYL-, DIMETHYL ESTER PHOSPHORIC ACID, TRIMETHYL ESTER PHOSPHINIC ACID, /AMINOMETHYL/-ETHYL-, PHOSPHINIC ACID, METHYL//METHYL-AMINO/METHYL/-, PHOSPHONIC ACID, //ETHYLAMINO/-METHYL-, PHOSPHONIC ACID, /1-/METHYLAMINO/-ETHYL-, 1-PROPANESULFONIC ACID, 3-HYDRAZINO-, PHOSPHONIC ACID, 2-GUANIDINO-ETHYL/-, DIHYDRATE PHOSPHONIC ACID, /1,3-DIAMINO-PROPYL/-, BORON HYDRIDE-TRIMETHYLAMINE TRIMETHYLAMINE BORANE	3	8		3			1			8	72648	72648		45557	22470		
THIOPHENE, 2,5-DICHLORO-3,4-DI-NITRO-, THIOPHENE, TETRACHLORO-, ETHER, BIS/PENTACHLOROETHYL/, FURAN, 2-BROMO-3,5-DINITRO-, 2H-THIAZOLO/3,2-B/1,2,4/THIADIAZOL-2-ONE, 5-CHLORO-, MALEIC ANHYDRIDE, CHLORO-, THIOPHENE, 2-BROMO-5-CHLORO-, PYRAZOLE-3/OR 5/-CARBOXYLIC ACID, 4,5/OR 3,4/-DIBROMO-BARBITURIC ACID, 5,5-DIBROMO-, PYRAZINE, 2,6-DICHLORO-, PYRIDAZINONE, 3/2H/-, 4,5-DI-CHLORO-, THIAZOLE, 2-AMINO-5-NITRO-4-/TRI-FLUOROMETHYL/-, SUCCINIC ACID, TETRAFLUORO-, BUTYRAMIDE, 2,2,3,3,4,4,4-HEPTAFLUORO-,	4	2			2	4	1				73336	73336	40736				
	4		4		9			1			1	16580	36626	36911		10028	
	4		1	1		2	5	2			1	66809	66809				
	4		1	1		2	1	2			2	63328	63328	35938			
	4		2	2		2	2	1			2	47142	34142	22678	47988		
	4		2	2		2	3	1			2	2955	42241P		181		
	4		2	2		2	2	1			2	34612	12595	37156	45869		
	4		2	2		2	2	1			2	40985	20985	18862	43642		
	4		2	2		2	2	1			2	76988	76988	49825			
	4		2	2		2	1				2	64845	64845	35812	37509	17534	
	4		2	3		3	2	1			2	57700	57700	31900	30626		
	4		2	4		4	1				2	43109	26109		43813		
	4		2	7		1	1				2	19602	36277		33751		

NAME	C	H	Br	Cl	F	I	N	O	P	S	Si	M	PRISM	GRATING	U.V.	N.M.R.	C-13
------	---	---	----	----	---	---	---	---	---	---	----	---	-------	---------	------	--------	------

12/89

1981-1990 SUPPLEMENTARY
MOLECULAR FORMULA INDEX

NAME	C	H	Br	Cl	F	I	N	O	P	S	M	PRISM	GRATING	U+	N.M.R.	C-13
THIOPHENE, 2,5-DIODO-, DITHIOLO/4,5-D/-1,3/DITHIOLE- 2,5-DIONE, /1,3/-, DIHYDRO-, MALEIC-D2 ACID	4	2				2		2	1			58506 72968	58506 72968	32461	31291	
ACETYLENEDICARBOXYLIC ACID	4	2						4	4		D	71509 19603	71509 48111P		44488 33752	8138
CYCLOBUTENEDIONE, DIHYDROXY-, SQUARIC ACID	4	2						4	4			32814 32814	9809 9809	14941 14941	35778 35778	
OXATHIAZIN-4/3H/-ONE, 1,2,3-, 6-/BROMOMETHYL/-, POTASSIUM SALT, 2,2-DIOXIDE	4	3	1				1	4	1	K	63704	63704				
PYRAZOLE-3-OR 5-CARBOXYLIC ACID, 4-BROMO-, OXATHIAZIN-4/3H/-ONE, 1,2,3-, 5-CHLORO-6-METHYL-, POTASSIUM SALT, 2,2-DIOXIDE	4	3	1			2	2					34611	12594	37155		
OXATHIAZIN-4/3H/-ONE, 1,2,3-, 6-/CHLOROMETHYL/-, POTASSIUM SALT, 2,2-DIOXIDE	4	3	1			1	4	1	K	63703	63703	37482	36533			
PYRIMIDINE, 2-CHLORO-, PYRIMIDINE, 4-AMINO-6-CHLORO-5- NITRO-, SUCCINIC ANHYDRIDE, CHLORO-, MERCURY, CHLORO-2-THIENYL-, ACRYLIC ACID, TRICHLORO-, METHYL ESTER	4	3	1			2						1394 40597	41418P 20597	38107 38163	18656	
PROPIONIC ACID, PENIACHLORO-, METHYL ESTER	4	3	5					2				65853	65853		38792	
URACIL, 5-FLUORO-, THIAZOLE, 2-AMINO-4-/TRIFLUORO- METHYL/-,	4	3		1		2	2					43105 57702	26105 57702	21085 31901	35804 30627	
UREA, 2-THIO-1-/5-/TRIFLUORO- METHYL/-1,3,4-THIADIAZOL-2-YL/-,	4	3		3		4		2				56717	56717	31055	28961	
5-THIAZOLECARBOXYLIC ACID	4	3					1	2	1	NA	61410	61410		33972		
PYRAZINOL, SODIUM SALT	4	3					2	1		NA	67342	67342	38286	34301	20518	
BARBITURIC ACID, 2-THIO-, MONO- SODIUM SALT	4	3					2	2	1							
ALLOXAN-5-OXIME, MONOHYDRATE	4	3						3	4			37837	16830	16712	33603	
BARBITURIC ACID, 5-/HYDROXYIMINO/-, MONOHYDRATE	4	3						3	4			37837	16830	16712	33603	
BARBITURIC ACID, 5-NITROSO-, 4,6-PYRIMIDINEDIOL, 5-NITRO-, PYRIMIDINONE, 4/3H/-, 6-HYDROXY-5- NITRO-, VIOLURIC ACID, MONOHYDRATE	4	3						3	4			45289 24472	30289 4737	21573 8618	43949 43504	
BARBITURIC ACID, 5-NITRO-, FURAN, 2-AMINO-3,5-DINITRO-, 2-FURANAMINE, 3,5-DINITRO-, URACIL, 6-AMINO-5-NITROSO-, MONO- SODIUM SALT	4	3						3	4			24472 63327	4737 63327	8618 61310	17117 35937	
OXATHIAZIN-4/3H/-ONE, 1,2,3-, 6-/AZIDOMETHYL/-, POTASSIUM SALT, 2,2-DIOXIDE	4	3						4	4	1	K	63709	63709		36538	
FUMARIC ACID, MONOSODIUM SALT	4	3							4			NA	67226	67226	39552	40181
MALEIC ACID, MONOSODIUM SALT, TRI- HYDRATE	4	3							4			NA	67152	67152	39550	40125
OXATHIAZIN-4/3H/-ONE, 1,2,3-, 5-CHLORO-6-METHYL-, 2,2-DIOXIDE	4	4	1				1	4	1			63710	63710	35262	36539	
PYRIDAZINE, 3-AMINO-6-CHLORO-, PYRIMIDINE, 4-AMINO-6-CHLORO-, 4-PYRIMIDINOL, 2-AMINO-6-CHLORO-, MONOHYDRATE	4	4	1				3					57943 64557	57943 64557	32045	30783	
PYRAZINE, COMPLEX WITH MERCURY /II/ CHLORIDE	4	4	2					2			HG	21375	36366	36922		
ACRYLIC ACID, 3,3-DICHLORO-, METHYL ESTER	4	4	2						2			68070	68070		40741	
PROPIONIC ACID, 2,3,3,3-TETRA- CHLORO-, METHYL ESTER	4	4	4						2			68069	68069		40740	
PROPIONIC ACID, 2,2,3,3-TETRA- CHLORO-, METHYL ESTER	4	4	4						2			65852	65852		38791	
AS-TRIAZINE-3,5/2H,4H/-DIONE, 6- /FLUOROMETHYL/-,	4	4		1			3	2				33548	11539	37102		
THIADIAZOLE, 1,3,4-, 2-/METHYL- AMINO/-5-/TRIFLUOROMETHYL/-, ETHER, BIS/2,2,2-TRIFLUOROETHYL/, SUCCINIMIDE, N-HYDROXY-, THALLIUM SALT	4	4		3			3		1			61169	61169	33947	34140	
OXATHIAZIN-4/3H/-ONE, 1,2,3-, 6-METHYL-, POTASSIUM SALT, 2,2-DIOXIDE	4	4					1	4	1	K	63702	63702	37481	36532		
OXATHIAZIN-4/3H/-ONE, 1,2,3-, 6-/HYDROXYMETHYL/-, 3-POTASSIUM SALT, 2,2-DIOXIDE	4	4					1	5	1	K	63708	63708	37486	36537	20625	
1,3-DIAZINE	4	4						2				2121	36767	561	33550	9003

NAME	C	H	Br	Cl	F	I	N	O	P	S	M	PRISM	GRATING	U+	N.M.R.	C-13
------	---	---	----	----	---	---	---	---	---	---	---	-------	---------	----	--------	------

1981-1990 SUPPLEMENTARY
MOLECULAR FORMULA INDEX

NAME	C	H	Br	I	F	N	O	P	S	M	PRISM	GRATING	U.V.	N.M.R.	C-13
METADIAZINE	4	4				2					2121	36767	561	33550	9003
MAZINE	4	4				2					2121	36767	561	33550	9003
PYRAZINE, COMPLEX WITH MERCURY /II/ CHLORIDE	4	4				2					21375	36366	36922		
PYRIMIDINE	4	4				2					2121	36767	561	33550	9003
FORMAMIDE, N-/2-THIAZOLYL/-,	4	4				2	1				78893	78893		51831	
PYRAZOLE-3/ OR 5/-CARBOXYLIC ACID	4	4				2	2				34610	12593	37154		
4,6-PYRIMIDINEDIOL	4	4				2	2				22916	33221	17318	47835	17078
PYRROLE, 3-NITRO-	4	4				2	2				59289	59289	32908	32204	21986
THIADIAZOLE-5-CARBOXYLIC ACID, 1,2,3-, 4-METHYL-, GLYOXYLIC ACID, CYANO-, METHYL ESTER, OXIME	4	4				2	2	1			66395	66395	36605	39170	20646
2-PYRIMIDINETHIOL, MONOHYDROCHLORIDE	4	4				2	3				69680	69680	39040	42442	
CYTOSINE, 5-NITRO-, PYRIMIDINONE, 2/H/-, 4-AMINO-5-NITRO-	4	4				2	3	1			72414	72414	40232	45342	22320
PROPIOLIC ACID, METHYL ESTER	4	4					2				65878	65878		38817	18038
FURANONE, 2/-SH/-, 5-HYDROXY-, FURANONE, 2/-SH/-, 4-HYDROXY-, SUCCINIC ACID, DISODIUM SALT, HEXAHYDRATE	4	4					3				68251	68251	40895	45947	
MALEIC ACID, HYDROXY-, TARTARIC ACID, MESO-, CALCIUM SALT 1 TO 1/, TRIHYDRATE	4	4					5				67306	67306			
TARTARIC ACID, MONOPOTASSIUM MONOSODIUM SALT, TETRAHYDRATE	4	4					6				CA 67268	67268			
DITHIOLE-3-THIONE, 3H-1,2-, 5-MERCAPTO-4-METHYL-, ISOXAZOLE, 3-AMINO-4-BROMO-5-METHYL-, CARBONIC ACID, CYCLIC /BROMO-METHYL/ETHYLENE ESTER	4	4						4			48468	35468		49948	
1,3-DIOXOLAN-2-ONE, 4/-BROMOMETHYL/-, ISOTHIOCYANIC ACID, 2,3-DIBROMO-PROPYL ESTER	4	5	1			2	1				73699	73699	40940	46670	
PYRIMIDINE, 4-CHLORO-5,6-DIAMINO-, PYRIMIDINE, 2-CHLORO-4,5-DIAMINO-, CYCLOPROPANECARBONYL CHLORIDE	4	5	1				3				71546	71546		44525	
ACRYLIC ACID, 3-CHLORO-, METHYL ESTER, CIS-, CARBONIC ACID, CYCLIC/CHLORO-METHYL/ETHYLENE ESTER	4	5	1				3				40601	20601		43592	3664
1,3-DIOXOLAN-2-ONE, 4/-CHLOROMETHYL/-, PROPIONIC ACID, 2,3,3-TRICHLORO-, METHYL ESTER	4	5	1				3				40601	20601		43592	3664
PROPIONIC ACID, 2,2,3-TRICHLORO-, METHYL ESTER	4	5	3				2				68063	68063		40734	
PROPIONIC ACID, 3,3,3-TRICHLORO-, METHYL ESTER	4	5	3				2				68056	68056		40728	
FORMIC ACID, ISOTHIOCYANATO-, ETHYL ESTER	4	5				1	2	1			72595	72595		45515	
2-THIOPHENESULFONAMIDE	4	5				1	2	2			57725	57725	31921	30649	20192
MALEIC ACID	4	5				1	3				43014	26014	38219	15021	
2,4-OXAZOLIDINEDIONE, 5-METHYL-, ASPARTIC ACID, DISODIUM SALT	4	5				1	3				71451	71451		44431	
THIAZOLE, 4-METHYL-, URACIL, 6-AMINO-2-THIO-, HYDRATE	4	5				1	4				67677	67677		40560	20946
PYRAZOLE-4-CARBOXYLIC ACID, 3-AMINO-	4	5				3	1	1			76954	76954		49793	
4,6-PYRIMIDINEDITHIOL, 2-AMINO-, METHACRYLIC ACID, SODIUM SALT	4	5				3	2				24147	7982	8458	33787	17101
SUCCINIC ACID, MONOSODIUM SALT	4	5					4				18903	48081P	6138	37693	
TARTARIC ACID, MONOPOTASSIUM SALT	4	5					6								
PROPYONYL BROMIDE, 2-BROMO-2-METHYL-, BUTANE, 1,2,3,4-TETRABROMO-, MESO-, ACETOACETAMIDE, 2-CHLORO-, CARBAMIC ACID, CHLOROACETYL-, METHYL ESTER	4	6	2				1				K 67711	67711		40592	18624
PROPIONIC ACID, 3,3-DICHLORO-, METHYL ESTER	4	6	2				2				74946	74946		24727	24488
OXAZOLIDINE, 2-/TRICHLOROMETHYL/-, BUTYRONITRILE, 4-/TRICHLOROSIYL/-, TRIAZATRIPHOSPHORINE, 1,3,5,2,4,6-, 2-METHYL-2-PROPADIENYL-4,6,6-TETRA-CHLORO-, CROTONONITRILE, 3-AMINO-, PYRAZOLE, 3/ OR 5/-METHYL-, IMIDAZOLE-4-METHANOL, MONOHYDRO-CHLORIDE	4	6	3			1	1				23522	48343P		33875	
PYRAZOLE-1-METHANOL	4	6	3			2	1				20238	48161P	6779	33765	9077
	4	6	4			2	1				67137	67137		40113	18483
	4	6	4			3	3	1			74692	74692		41568	47584

1981-1990 SUPPLEMENTARY
MOLECULAR FORMULA INDEX

NAME	C	H	Br	Cl	F	I	N	O	P	S	Si	M	PRISM	GRATING	U.V.	N.M.R.	C-13
2-PYRAZOLIN-5-ONE, 4-METHYL-, ACETIC ACID, DIAZO-, ETHYL ESTER	4	6					2	1				41519	22519		43683	10945	
MALEAMIDE	4	6					2	2				17518	48031P		37690	12377	
IMIDAZOLE, 2-/METHYLTHIO/-.	4	6					2	2		1		67151	67151	37701	40124	18493	
IMIDAZOLE, 2-/METHYLTHIO/-, MONO- HYDROIODIDE	4	6					2	1		1		62053	62053		34793	11025	
ISOTHIAZOLE, 5-AMINO-3-METHYL-, HYDROCHLORIDE	4	6					2	1				57122	57122	31468	30106	14533	
2-IMIDAZOLINE-2-CARBAMONITRILE	4	6					4					73719	73719		46689		
4-PYRIMIDINOL, 2,6-DIAMINO-, 4-PYRIMIDINOL, 2,6-DIAMINO-, MONO- HYDRATE	4	6					4	1				4583	33952	20834	43494	20456	
4-PYRIMIDINOL, 5,6-DIAMINO-, SULFATE THIADIAZOLE-5-CARBOXAMIDOXIME,	4	6					4	1				40603	20603	18102	43594		
1,2,3-, 4-METHYL-, URACIL, 5,6-DIAMINO-, 2-PYRIMIDINETHIOL, 4,5-DIAMINO-, PYRIMIDINE, 2,4-DIAMINO-1,6-OI- HYDRO-6-IMINO-5-NITRO-, PYRIMIDINE, 5-NITRO-2,4,6-TRI- AMINO-, S-TRIAZOLO/4,3-A/-S-TRIAZINE, 3,5,7-TRIAMINO-, ACETIC ACID, MERCAPTO-, ACETATE	4	6					4	1		1		26887	2633		39737	19611	
ACETIC ACID, CAOMIUM SALT, DI- HYDRATE	4	6					4	1				66437	66437		39212	18166	
ACETIC ACID, LEAD/2 PLUS/ SALT, TRIHYDRATE	4	6					6	2				77866	77866		50820		
OXALIC ACID, DIMETHYL ESTER	4	6					8					72548	72548	40279			
DICARBONIC ACID, DIMETHYL ESTER	4	6										CD	78730	78730	51670		
URANIUM, BIS/ACETATO/DIOXO-, URANIUM OXYACETATE	4	6										70683	70683		41749	24365	
URANYL ACETATE	4	6										PB	60072	60072		12141	
TARTARIC ACID, D-, TARTARIC ACID, D-/MINUS/-,	4	6										5171	18452	36843	6031	6628	
COPPER ACETATE ARSENITE	4	6										75286	75286		48284		
CUPRIC ACETOARSENITE	4	6										U	63399	63399	36290	18883	
DICOPPER, /ACETATO/TRIMETA- ARSENITO-, PARIS GREEN	4	6										U	63399	63399	36290	18883	
TETRACOPPER, BIS/ACETATO/HEXA- METAARSENITO-, 1-BUTENE, 4-BROMO-, 2-BUTENE, 2-BROMO-, BUTANE, 4-BROMO-1,2-EPOXY-, S- /MINUS/-,	4	7	1									U	63399	63399	36290	18883	
BUTYRIC ACID, 4-BROMO-, 2-BUTENE, 1-CHLORO-, CYCLOPROPANE, /CHLOROMETHYL/-, OXAZOLIDINE, 5-/CHLOROMETHYL/- IMINO-, METHANOL, CHLORO-, PROPIONATE	4	7	1									U	63399	63399	36290	18883	
PROPIONIC ACID, CHLOROMETHYL ESTER	4	7	1									U	63399	63399	36290	18883	
PROPIONIC ACID, 3-CHLORO-2-METHYL-, PROPANE, 2-METHYL-1,1,2-TRICHLOORO-, 2-PROPANOL, 2-METHYL-1,1,1-TRI- CHLORO-, HYDRATED	4	7	1									U	63399	63399	36290	18883	
PROPARGYLAMINE, N-METHYL-, 2-PROPYNYLAMINE, N-METHYL-, ISOCYANIC ACID, ISOPROPYL ESTER	4	7										U	63399	63399	36290	18883	
ACETOACETAMIDE	4	7										U	63399	63399	36290	18883	
CYCLOPROPANE, /NITROMETHYL/-, 2-PYRROLIDINONE, 4-HYDROXY-, /RS/-,	4	7										U	63399	63399	36290	18883	
4-THIAZOLIDINECARBOXYLIC ACID, L-, ALANINE, N-FORMYL-, DL-, ALANINE, N-FORMYL-, L-, OXAMIC ACID, ETHYL ESTER	4	7										U	63399	63399	36290	18883	
SUCCINAMIC ACID	4	7										U	63399	63399	36290	18883	
2-THIAZOLIDINESELOWNE, 3-METHYL-, ISOTHIOCYANIC ACID, PROPYL ESTER	4	7										U	63399	63399	36290	18883	
THIATRIAZIN-3/4H-/ONE, 2H-1,2,4,6-, 5-METHOXY-2-METHYL-, 1,1-DIOXIDE	4	7										U	63399	63399	36290	18883	
PSEUDOURREA, 1-CYANO-2,3-DIMETHYL- 2-THIO-, THIADIAZOLE, 1,3,4-, 2-/ETHYL-	4	7										U	63399	63399	36290	18883	
THIADIAZOLE, 1,3,4-, 2-/ETHYL- AMINO/-, THIADIAZOLE, 1,3,4-, 2-/ETHYL- AMINO/-, HYDROCHLORIDE	4	7										U	63399	63399	36290	18883	

NAME	C	H	Br	Cl	F	I	N	O	P	S	Si	M	PRISM	GRATING	U.V.	N.M.R.	C-13
------	---	---	----	----	---	---	---	---	---	---	----	---	-------	---------	------	--------	------

12/89

**1981-1990 SUPPLEMENTARY
MOLECULAR FORMULA INDEX**

NAME	C	H	Br	Cl	F	I	N	J	P	S	Si	M	PRISM	GRATING	U.V.	N.M.R.	C-13
THIADIAZOLE, 1,3,4-, 2-AMINO-5-ETHYLTHIO/-	4	7					3		2			63147	63147	34971	36135	15346	
PYRIMIDINE, 2,4,6-TRIAMINO-/-	4	7					5					20516	10405	6943	35664	23095	
PYRIMIDOINE, 4,5,6-TRIAMINO-/-	4	7					5					22915	18810	17653	39726		
SULFATE, HYDRATE																	
S-TETRAZINE, 3-AMINO-6-ETHYL-/-	4	7					5		1			68149	68149	40812	35595		
4-PYRIMIDINOL, 2,5,6-TRIAMINO-/-	4	7					5		1			4298	33367				
SULFATE																	
4-PYRIMIDINOL, 2,5,6-TRIAMINO-/-, MONO-HYDROCHLORIDE	4	7					5		1			69562	69562	38960			
PYRIMIDINONE, 4/3H/-, 2,5,6-TRI-AMINO-/-, MONOHYDROCHLORIDE	4	7					5		1			69562	69562	38960			
DAMIDO																	
MALEIMIDE, DIAMINO-/-, DIOXIME	4	7					5		2			70942	70942	39581	43428		
XANTHIC ACID, PROPYL-/-, POTASSIUM SALT	4	7					5		1	2	K	7348	44433P	35612	12300		
CARBONIC ACID, DITHIO-/-, O-ISOPROPYL ESTER, SODIUM SALT	4	7							1	2	NA	67170	67170	40140	18505		
ISOBUTYRIC ACID, POTASSIUM SALT	4	7								2	K	67167	67167	40137	18503		
BUTYRIC ACID, 2-HYDROXY-/-, MONO-SODIUM SALT, DL-/-	4	7								3	NA	67162	67162	40132			
TETRASELENACYCLOOCTANE, 1,3,5,7-/-	4	8										SE	70286	70286			
TETRASELENOCAKE, 1,3,5,7-/-	4	8										SE	70286	70286			
PROPIONAMIDE, 2-BROMO-2-METHYL-/-	4	8	1				1		1			67705	67705	40586	18622		
GLYCINE, N-//DICHLOROMETHYL-/-, HYDROXYPHOSPHINYL-METHYL-/-	4	8	2				1		4	1		65572	65572				
1-PROPANESULFONAMIDE, 2-HYDROXY-N-METHYL-/-, 3,3,3-TRICHLORO-/-, DL-/-	4	8	3				1		3	1		61802	61802	34572	15127		
2-IMIDAZOLIDINESEOLONE, 1-METHYL-/-	4	8							2			SE	61647	61647	34464	15094	
2-IMIDAZOLINE, 2-METHYL-/-	4	8							2			19909	39874P	6599	41584	14471	
PROPIONITRILE, 2-AMINO-2-METHYL-/-	4	8							2			71119	71119	44115	22641		
UREA, CYCLOPROPYL-/-	4	8							2	1		73690	73690	46661	26107		
CARBAMIC ACID, /1-AMINOETHYL-IDEENE/-, METHYL ESTER	4	8							2	2		76418	76418	49345			
OXAZOLIDINE, 5-METHYL-3-NITROSO-/-	4	8							2	2		76062	76062	49025			
VINYLMINE, N,N-DIMETHYL-2-NITRO-/-	4	8							2	2		73603	73603	46579			
ACETIMIDIC ACID, N-CARBAMOLOYLOXY-/-THIO-/-, METHYL ESTER	4	8							2	2	1	43317	26317	20167	43824		
PROPIONAMIDE, 3-MERCAPTO-/-, THIO-CARBAMATE	4	8							2	2	1	64303	64303	37069			
ACETAMIDE, 2,2--DITHIOBIS-/-	4	8							2	2	2	75215	75215	48215			
CROTONAMIDE, 3-AMINOTHIO-/-	4	8							2	1		69552	69552	42316	21401		
PSEUDOUREA, 2-ALLYL-2-THIO-/-, MONO-HYDROBROMIDE	4	8							2	1		69252	69252	42029	21200		
TRIAZOLE, 4H-1,2,4-, 4-AMINO-3,5-DIMETHYL-/-	4	8							4			73353	73353	46339			
TRIAZOLE, 1H-1,2,4-, 3-AMINO-1-METHYL-5-/METHYLTHIO-/-	4	8							4		1	75094	75094	41741	48094	26585	
S-TETRAZINE, 3,6-BIS(METHYLTHIO)-/-, 1,2-DIHYDRO-/-	4	8							4		2	63440	63440	36314	15390		
2-PROPANOHE, 1-METHOXY-/-, CARBONIC ACID, ETHYL METHYL ESTER	4	8								2		72697	72697	21676	22499		
1,4-OXATHIANE, 4,4-DIOXIDE	4	8							3		1	66731	66731	39504	18417		
THIOPHEN-3-OL, TETRAHYDRO-/-, 1,1-DIOXIDE	4	8							3		1	77167	77167	50151			
P-DIOXANE-2,3-DIOL	4	8							3		1	61443	61443	16672			
TETRAOXACYCLOOCTANE, 1,3,5,7-/-	4	8								4		46220	31220	43975	24353		
TETROXOCANE, 1,3,5,7-/-	4	8								4		67298	67298	40228	19577		
ACETIC ACID, /METHYLSULFONYL/-, METHYL ESTER	4	8								4	1	67298	67298	40228	19577		
1,4-BUTANEDISULFONIC ACID, 1,4--DIHYDROXY-/-, DISODIUM SALT	4	8								8	2	NA	67264	67264	40209		
TETRAETHIACYCLOOCTANE, 1,3,5,7-/-	4	8										70289	70289	42810	21650		
TETRAETHIOTOCANE, 1,3,5,7-/-	4	8										70289	70289	42810	21650		
GLYCINE, N-//CHLOROMETHYL HYDROXY-/-, PHOSPHINYL-METHYL-/-	4	9	1				1		4	1		70956	70956	43441	21833		
1-PROPANESULFONIC ACID, 2-HYDROXY-3,3,3-TRICHLORO-/-, 2-METHYLHYDRAZIDE, DL-/-	4	9	3				2		3	1				35888			
THIADIAZOLIDINE-2-ETHANESULFONYL FLUORIDE, 1,2,3-, 1,1-DIOXIDE	4	9	1				2		4	2		64447	64447	35905			
ALLYLAMINE, N-METHYL-/-	4	9								1		64474	64474	37190	15600		
CYCLOBUTYLAMINE	4	9								1		76941	76941				
CYCLOPROPANE-METHYLAMINE	4	9								1		75961	75961	48931			
ISOBUTYRALDEHYDE, OXIME	4	9								1		15392	29991	29912	4173	2107	
MORPHOLINE, HYDROGEN TETRAFLUOROBORATE/-, MITUS.	4	9								1	1	64942	64942	37600	20839		
ISOCYANIC ACID, TRIMETHYLSILYL ESTER	4	9								1	1	61444	61444	45942			
SILANE, ISOCYANATOTRIMETHYL-	4	9								1	2	1	61444	61444	45942		
3-THIOPHENAMINE, TETRAHYDRO-/-, 1,1-DIOXIDE	4	9												16673			

1981-1990 SUPPLEMENTARY
MOLECULAR FORMULA INDEX

NAME	C	H	Br	O	F	I	N	O	P	S	Si	M	PRISM	GRATING	IR	N.M.R.	C-13
BUTYRIC ACID, 4-AMINO-3-HYDROXY-, DL-,	4	9					1	3				42258	23258		43740	7038	
ACETAMIDE, N,N-DIMETHYLTHIO-,	4	9					1		1			46517	31517	29921	19223	5163	
CARBONIC ACID, DITHIO-, S,S-DI-METHYL ESTER, SEMICARBAZONE	4	9					3	1	2			59949	59949		32737	12572	
SEMICARBAZIDE, 1-BIS/METHYLTHIO/-METHYLENE/-,	4	9					3	1	2			59949	59949		32737	12572	
S-TRIAZINE-2/1H-/THIONE, 5-METHYL-TETRAHYDRO-,	4	9					3		1			67508	67508		40395		
1-BUTANESULFONAMIDE, 4-BROMO-, PHOSPHOROCHLORIDIC ACID, DIETHYL ESTER	4	10	1				1	2	1			72162	72162		45100	22120	
PHOSPHORAMIDOTHIOIC DICHLORIDE, DI-ETHYL-,	4	10		1				3	1			1468	33805		37659	12219	
SILANE, DICHLORODIETHYL-, TRIAZATRIPHORINE, 1,3,5,2,4,6-, 2-METHYL-2-PROPYL-4,4,6,6-TETRACHLORO-, BORON FLUORIDE, CMPD WITH ETHYL ETHER /1 TO 1/	4	10		2			1		1			64858	64858		37522		
DIAZADIPHOSPHETIDINE, 1,3,2,4-, 1,3-DIETHYL-2,2,4,4,4-HEXAFLUORO-2,2,4,4-TETRAHYDRO-,	4	10		6			2		2			71186	71186		44178		
DIAZADIPHOSPHETIDINE, 1,3,2,4-, 1,1'-ETHYLENEBIS/2,2,2,4,4,4-HEXAFLUORO-3-METHYL-2,2,4,4-TETRAHYDRO-,	4	10		9			4		4			71184	71184		44176		
PHOSPHONIC ACID, /2-PYRROLIDINYL/-, GLYCINE, N-/HYDROXYMETHYLPHOSPHINYL/-METHYL/-, BUTYRIC ACID, 4-AMINO-4-PHOSPHONO-, PIPERAZINE, CITRATE /3 TO 2/, HYDRATED	4	10					1	5	1			68908	68908		41477		
PIPERAZINE, DIHYDROCHLORIDE, HYDRATE	4	10					2					67385	67385		40802	20661	
PIPERAZINE, DL-MALATE /1 TO 1/	4	10					2					67370	67370		40285	20326	
1-PROPANESULFONIC ACID, 3-AMIDINO-THIO/-, PSEUDOURA, 2-/3-SULFOPROPYL-	4	10					2	3	2			29190	5187		33813	19109	
2-THIO-, HYDRAZINE, ETHYL-, OXALATE /1 TO 1/	4	10					2	4				72528	72528		45452	24437	
BUTYRIC ACID, 2-AMINO-4- HYDROXY-SULFAMOYL/-, DIAZAPHOSPHORINANE-2-THIONE, 1,3,5-, 5-/AMINOMETHYL/-, 5-OXIDE	4	10					2	5				62390	62390				
DIAZAPHOSPHORINAN-2-ONE, 1,3,5-, 5-/AMINOMETHYL/-, 5-OXIDE	4	10					3	1	1	1		76566	76566		49465		
2-IMIDAZOLINE, 2-/1-METHYL-HYDRAZINO/-, MONOHYDROBROMIDE	4	10					4					73382	73382		46368		
GUANIDINE, I-NITRO-3-PROPYL-, SUCCINAMIDOXIME	4	10					4	2				69191	69191		41776	21150	
UREA, OXALATE /2 TO 1/	4	10					4	2				68322	68322		40961		
S-TETRAZINE-3/2H-/THIONE, 6,6-OI-METHYLtetrahydro-, AMMONIUM REINECKATE, HYDRATE	4	10					4	6				44917	27917		43914		
CHROMATE 1 MINUS/, DIAMMINETETRA-KIS ISOTHIOCYANATO/-, AMMONIUM-, HYDRATE	4	10					4		1			71731	71731		44693		
REINECKE SALT, HYDRATE	4	10					7		4			60158	60158				
BORON FLUORIDE, CMPD WITH ETHYL ETHER /1 TO 1/	4	10						1				72783	72783		19919	22545	
ETHER, METHYL PROPYL, 1-PROPANOL, 3-METHOXY-, ETHANOL, 2,2*-DITHIODI-, ETHANOL, 2,2*-SULFINYLDI-, ERYTHRITOL, MESO-, ETHYLENE GLYCOL, BIS-METHANE-SULFONATE/	4	10						2	2			61450	61450		41760	45873	
METHANESULFONIC ACID, ETHYLENE ESTER	4	10						3	1			64792	64792		34320	13184	
LEAD, BIS/ACETATO/TETRAHYDROXYTRI-, LEAD SUBACETATE	4	10						4	2			61330	61330		37458	17502	
PLUMBANE, BIS/ACETATO/TETRAHYDROXY-TRI-, DITHIASTANNOLANE, 1,3,2-, 2,2-DI-METHYL-, METHANE, DITHIOBIS,/METHYLTHIO/-, TETRAETHIOCTANE, 2,4,5,7-, BUTYLAMINE, HYDROGEN HEXAFLUOROPHOSPHATE/1 MINUS/	4	10						6	2			77340	77340		34256	20517	
BUTYLAMINE, TERT-, HYDROCHLORIDE	4	11						1				46321	31321		47917	5088	
ISOPROPYLAMINE, N-METHYL-, OXALATE /1 TO 1/	4	11							1			63664	63664		36498	15510	
1-BUTANOL, 2-AMINO-, D-,	4	11						1	1			72834	72834		45698	22752	

NAME

C H Br O F I N O P S Si M PRISM GRATING IR N.M.R. C-13

1981-1990 SUPPLEMENTARY
MOLECULAR FORMULA INDEX

NAME	C	H	Cl	N	O	S	P	I	PRISM	PLATIN		NMR	IR
ETHANOL, 2-DIMETHYLAMINO-, TARTRATE 2:1/ SALT/	4	11			1	1			77037	77037		50033	
ETHANOL, 2,2'-IMINODI-, HYDRO- CHLORIDE	4	11			1	2			72729	72729		45605	22513
1-PROPANOL, 2-AMINO-2-METHYL-, HYDROGEN SULFATE	4	11			1	4	1		69762	69762		42520	21556
3-THIOPHENESULFONIC ACID, TETRA- HYDRO-, AMMONIUM SALT, 1,1-DIOXIDE	4	11			1	5	2		30553	6540		35735	10-61
GLYCINE, N,N-BIS-PHOSPHONOMETHYL-, ETHANETHIOL, 2-DIMETHYLAMINO-, HYDROCHLORIDE	4	11			1	8	2		76952	76952		49791	
FORMIMIDIC ACID, N-METHYLSULFON- YL-, 2,2-DIMETHYLHYDRAZIDE	4	11			1		1		22404	33606		33784	15661
GERMANE, TETRAMETHYL-, AMMONIUM FLUORIDE, TETRAMETHYL-, PENTAHYDRATE	4	12			1	1			GE	76962	76962	5183	
AMMONIUM HEXAFLUOROPHOSPHATE,	4	12			6	1	1		64451	64451		37183	15995
TETRAMETHYL-, PHOSPHINIC ACID, 2-ETHYLAMINO-/ METHYL METHYL-, PHOSPHONIC ACID, 2-PROPYLAMINO-/ METHYL -, PHOSPHONIC ACID, 1-AMINO-2-METHYL- PROPYL -, DIETHYLAMINE, 2,2*-DISELENO-, DI-	4	12			1	2	1		30794	6769		35740	24465
HYDROCHLORIDE									74043	74043		47004	26270
ETHYLAMINE, 2,2*-OXYBIS-, DIHYDRO- CHLORIDE	4	12			2	1			72696	72696		45587	22498
MALIC ACID, DIAMMONIUM SALT	4	12			2	5			67729	67729		40608	18631
SUCCINIC ACID, HYDROXY-, DIAMMONIUM SALT	4	12			2	5			67729	67729		40608	18631
PSEUDOUREA, 2-METHYL-, SULFATE 2 TO 1/	4	12			4	2			67182	67182		40149	18515
ETHYLAMINE, SULFATE /2 TO 1	4	14			2				67219	67219		40176	19540
DISILAZANE, 1,1,3,3-TETRAMETHYL-,	4	15			1		2		61416	61416		34305	18881
2H-PYRAN-2-ONE, 3,4,5,6-TETRACHLORO-, 2,4-PENTADIENOIC ACID, 2,3,4,5,5-PENTA- CHLORO-, CIS-	5	1	4			2			57553	57553	31779		
2,4-PENTADIENOIC ACID, 2,3,4,5,5-PENTA- CHLORO-, TRANS-	5	1	5			2			57552	57552	31778	30489	11158
THIADIAZOLO[3,4-B]PYRIDINE, 1,2,5-, 6-BROMO-, THIADIAZOLO[3,4-C]PYRIDINE, 1,2,5-, 7-AMINO-4,6-DICHLORO-, 4-ISOXAZOLECARBONITRILE, 5-AMINO- 3-TRICHLOROMETHYL-, THIADIAZOLE, 1,3,4-, 2-AMINO- 5-HEPTAFLUOROPROPYL-, BICYCLO[2.1.0]PENTANE-2,3,5-TRIONE, 1,6-OXYDROXY-, PYRIDINE, 3-BROMO-4-NITRO-, 1-OXIDE	5	2	1		3	1			70987	70987		43472	
IMIDAZO[2,1-B]THIAZOLE, 6-CHLORO-, XANTHINE, 8-CHLORO-, THEMOYL CHLORIDE	5	2	2		4	1			70986	70986		43471	
2-THIOPHENECARBONYL CHLORIDE -PYRIDINOL, 3,5-DICHLORO-, PYRIDINE, 2-AMINO-3,4,5-TRICHLORO-, PYRIDINE, 2,6-DIFLUORO-, PURINE, 2-IODO-, PURINE, 6-IODO-, 9H-PURINE, 2-IODO-, PYRAZOLE-3,5-DICARBOXYLIC ACID, 3-POTASSIUM SALT	5	3	1		2	3			74661	74661		49237	
5-PYRIMIDINECARBONITRILE, 4-HYDROXY-, OXADIAZOLO[3,4-B]PYRIDINE, 1,2,5-, 1-OXIDE	5	3	1		2	1			69259	69259	38771	42036	
PYRIDONE, 4-IMID-, 3,5-DINITRO-, 2-FURAMIDE, 5-BROMO-, 5-TRIAZINE-2-ACETONITRILE, 4,6-DI- AMINO-A,A-DIBROMO-, PYRIMIDINE, 5-CHLORO-2- IODO- METHYL SULFONYL-, PYRIMIDINE, 5-CHLORO-2- IODO- METHYL THIO-, 2-PYRIDINOL, 5-CHLORO-, PYRAZOLE-3-CARBOXONITRILE, 4-CHLORO- 1-METHYL-	5	4	1		1	2	2	K	72927	72927	32453	31283	
									72596	72596		45771	22785
									56941	56941		39666	13802
									56994	56994		37457	10281
									39735	39735		40300	22442
									173	173		45516	
									36003	36003		45771	
									64181	64181		31337	29589
									64181	64181		40149	20705
									76211	76211		49158	
									76213	76213		49160	
									78553	78553		51499	
									63875	63875		35297	36688
									68415	68415		48331	
									75754	75754		48735	