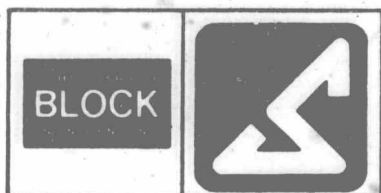


THE **SADTLER**

**STANDARD
SPECTRA**





SADTLER RESEARCH LABORATORIES, INC.

SADTLER ULTRAVIOLET (NON-POLAR) SPECTRA

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SADTLER STANDARD ULTRAVIOLET (NON-POLAR) SPECTRA

CHEMICAL CLASSES INDEX

INTRODUCTION

This index is a listing by chemical functionality of the compounds contained in the Sadtler publication of Standard Ultraviolet (Non-Polar) Spectra.

In addition to the UV (non-polar) spectrum numbers, shown in the right hand column of each page; infrared, ultraviolet (in polar solvent) and NMR spectrum numbers are included in the index to enable the location of spectra in other Sadtler publications for further reference.

The chemical class categories in the index have been devised using the Chemical Abstracts listing of "Order of Precedence" of functional groups (i.e., acids, acid derivatives, nitriles, ketones, hydrocarbons, etc.) as a basis; however a much more detailed sub-division has been formulated to permit rapid location of any particular sequence of functionality. For example, thio acids, esters, anhydrides, salts and hydrazides would be indexed by Chemical Abstracts under the corresponding acid, but separate entries have been made in this index for each of these "classes".

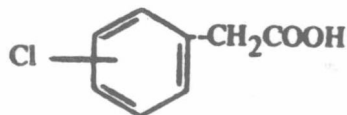
Each functional group is assigned a number in the Sadtler Chemical Classes System and coding has been performed giving precedence to low numbers first. A maximum of three functional groups may be coded for each compound (due to computer space limitations). Five columns, labelled "Functionality", serve to identify a particular compound by Chemical Classes. The first three columns indicate the types of the functional groups and the fourth column gives the total number of different groups (up to nine) which the compound contains; the fifth column number relates to the overall structure of the compound, i.e., aliphatic, aromatic, etc.

All compounds are arranged in alphabetical order under an ascending numerical order of each major functionality (column one, low number) and molecular formulae are also given for entries.

As part of this preface to the Chemical Classes Index there is a "Key to the Functional Group Notations" which describes fully what types of compounds are found in each functional group, by number.

An example will demonstrate the simplicity of coding and the ease of location of any type of compound.

If, for example, spectral and chemical characteristics point to a (chlorophenoxy) acetic acid,



all standard spectra exhibiting these same type groups will be found together in the Chemical Classes Index. The functions, cited in order of precedence, are carboxylic acid, ether and halogen (chlorine), which are coded 6 72 83. There is a total of three functional groups in this compound of aromatic nature (3). Such compounds appear in the index at 6 72 83 33 and may be found in the index as seen below.

NAME	C	H	Br	Cl	F	I	N	O	P	S	Si	M	FUNCTIONALITY		
BENZENE, P-DIETHOXY-,	10	14						2					72		1 3
BENZENE, 1,2-DIETHOXY-,	10	14						2					72		1 3
BENZENE, O-DIMETHOXY-,	8	10						2					72		1 3
BENZENE, P-DIMETHOXY-,	8	10						2					72		1 3
BENZENE, 1,2-DIPROPOXY-,	12	18						2					72		1 3
BENZENE, ETHOXY-,	8	10						1					72		1 3

If the desired compound has less than three functional groups, column 3 or both columns 2 and 3 will be devoid of entries. For a compound having more than three functional groups only those three having the highest order of precedence are indicated. The total number of functions (up to 9) is tallied in the fourth column, however.

KEY TO THE FUNCTIONAL GROUP NOTATIONS

01. Quaternary amines of any type. Nitrogen substituents may be aryl and/or alkyl (aliphatic or alicyclic, heterocyclic, etc.). Functions included in the anion of compounds having an organic cation are to be coded where possible. Ordinary amine salts are not included, but all other compounds with nitrogen bearing a charge are, e.g., hydrazonium and diazonium compounds. Nitronic acids and their salts are in this group.
06. Carboxylic acids.
07. Carboxylic acid salts. Amine salts of carboxylic acids will be included in this group.
08. Thiocarboxylic acids and derivatives excluding esters, lactones, salts, and carbamates.
10. Carboxylic acid anhydrides. Heterogenous anhydrides, bear the codes of each of the anhydride types involved, e.g. $\text{RC(=O)OSO}_2\text{R'}$ would be 10 28 —.
11. Carboxylic acid halides including haloformic and halocarbonic acids.
12. Carboxylic acid esters including carbonates. Carboxylic ortho acid esters are found in this group and in group 72, e.g.
 $\text{(CH}_3\text{O)}_3\text{C-CNH}_2$ would be coded 12 14 — and 14 72 —.
14. Carboxylic acid amides. The nitrogen and/or carboxylic acid function may be part of a ring structure (e.g. 1-benzoylpiperidine), but lactams or lactims are excluded.
15. Cyclic carboxylic acid amides, i.e., lactams and lactims; and imides.
16. Urea, guanidine, and biuret, their derivatives and salts (metal or acid), e.g., guanidine, hydrochloride. Salts of the organic acids are found in this group and under the corresponding acid groupings.
18. Nitrolic, nitrosolic, hydroxamic acids and amidine, amidoxime, azide, diimide, and hydrazide derivatives of carboxylic and thiocarboxylic acids. Salts of these functions are also included, e.g., semicarbazide, hydrochloride. Nitrogens may be part of cyclic structures, but not coannularly with the acid residue.
20. Lactones and lactides of carboxylic acids.
26. Derivatives of sulfonic, sulfinic, and sulfenic acids corresponding to those derivatives of the carboxylic acids as indicated in group 18, both linear and cyclic, including amides and imides. Derivatives of the hypothetical sulfilimine $\text{H}_2\text{S=NH}$ are also in this group.
33. Esters of acids of group 30.
41. Salts and esters of cyanic and isocyanic (fulminic) acids. Includes thio, telluro and seleno analogs.

46. Aldehydes, including thio, seleno, and telluro analogs. Carbohydrates, if aldoses, will be coded in this group and in Y3. The formyl group need not be bound to another carbon atom.
48. Aldehyde hydrazones, alkyl or aryl substituted hydrazones and salts, linear only.
50. Nitriles and isonitriles (cyanides and isocyanides) i.e., alkyl and aryl derivatives (esters) and salts of HCN and HNC. The functional group of this category need not be bound directly to another carbon atom.
52. Ketones, including thio, seleno, and telluro analogs. Carbohydrates, if ketoses, will be coded in this group and in Y3. Ketonic steroids will be found in this group and in Y5.
53. Ketone derivatives (except hydrazones), e.g., oximes, carbazones and derivatives of the oximino function ($R_2C=NOR'$), linear only. Salts and metal derivatives of the oximino function are also included.
54. Ketone hydrazones, alkyl or aryl substituted hydrazones and salts. Derivatives of the oximino function, and all other derivatives of group 53 must be linear.
56. Primary alcohols and their metal salts. Carbohydrates and sterols are cross referenced to this group. A "primary" alcohol is one in which the hydroxyl group is bound to a carbon atom that is attached to only one other carbon atom by a single bond.
57. Secondary alcohols and their metal derivatives. Carbohydrates and sterols are cross referenced to this group. A "secondary" alcohol is one in which the hydroxyl group is bound to a carbon atom which is attached to only two other carbon atoms by single bonds.
58. Tertiary alcohols and their metal derivatives. Carbohydrates and sterols are cross referenced to this group. A "tertiary" alcohol is one in which the hydroxyl group is attached to a carbon atom which is bound to three other carbon atoms.
59. Aromatic ring-hydroxylated compounds, both carbocyclic and heterocyclic and their metal derivatives, e.g., phenol, pyrimidinol, sodium naphthoxide, etc., Tautomers (enol form) of α -keto nitrogen heterocycles, if aromatic, such as 2-pyridinol, are included in this group. However, compounds such as 3,4,5,6-tetrahydro-2-pyridinol are considered as lactams and are found in group 15.
61. Thioalcohols or mercaptans and their metal derivatives. Selenium and tellurium analogs are also found in this group.
62. Thiophenol and metal derivatives with the same restrictions as imposed on group 59, including Se and Te analogs.
64. Primary amines. The amine function need not be attached to carbon, e.g., 1-amino-piperidine.
65. Secondary amines, linear and heterocyclic. Amines of the type $R-NH-X$, where X is neither alkyl nor aryl, e.g., $R-NH-NO_2$, are in this group.

66. Tertiary amines, linear and heterocyclic. Amines of the type R_2N-NO_2 , as defined in 65, are in this group. Group 66 includes aromatic nitrogen heterocycles and cyclic imines.
 70. Hydrazine and azido (triazole) compounds, linear only. 1,2-diazines are not included in this group, but are considered amines. 1-amino-piperidine and compounds of this type are also classified as amines. Although the triazole group is cyclic it cannot be part of another ring system.
 72. Ethers, acetals, and ortho esters. Such compounds may be either linear or cyclic, the oxygen not necessarily being attached to carbon. Sulfur analogs are in group 75; peroxides are in group 05. Epoxides have their own group 74.
 73. Alkenes and cycloalkenes. Those compounds exhibiting true carbon-carbon double bonds. This group does not include aromatic compounds. If the compound is a hydrocarbon and contains carbon-to-carbon unsaturation, it will also be found in group X2. This coding appears on all quinoid structures.
 75. Sulfides, polysulfides (and Se or Te analogs) and ortho esters of thiocarboxylic acids.
 76. Sulfoxides and sulfones, including Se and Te analogs.
 77. Alkynes and cycloalkynes. Those compounds exhibiting carbon-carbon triple bonds with the same restrictions imposed under group 73. These compounds also appear in X3 if hydrocarbon only.
 79. Azo and azoxy compounds, linear only, i.e., cannot be part of a ring structure, but may be attached to a ring, e.g., azobenzene or benzenediazonium sulfonic acid. Mono- or di-alkyl- or aryl-diimides are in group 79; the acyl analogs are in group 18.
 80. Nitro and Nitroso compounds.
 81. Iodoso and iodoxy compounds. Esters as $C_6H_5I(O-C-R)_2$ are coded 12 8 1 — —.
 82. Fluorine compounds.
 83. Chlorine compounds.
 84. Bromine compounds.
 85. Iodine compounds, excluding iodonium, iodoso, and iodoxy compounds.
- Code to groups following 99**
- M1. Metallo-organic compounds, regardless of functionality. Number of functions and type are still noted as a further aid to subgrouping.
 - X2. Unsaturated hydrocarbons only. Aliphatic and alicyclic hydrocarbons but not aromatic hydrocarbons are included in this group. The unsaturated aliphatic compound may, however, be attached to an aromatic hydrocarbon ring.

- X3. Aromatic hydrocarbons only. The significance of the 4th and 5th columns changes with this class. A number in the 4th column indicates the number of unfused rings, while a number in the 5th column indicates the number of fused rings, e.g., naphthalene is X3 — — 2 while biphenyl is X3 — — 2 — and binaphthyl is X3 — — — 4. The final authority on the number of rings in any given fused system will be the Ring Index (American Chemical Society, 2nd Ed. 1960 and supplements).
- X4. Aromatic-saturated aliphatic hydrocarbons only (toluene). Restrictions are imposed in the 4th and 5th columns as for X3.
- Y1. Silicon compounds. Compounds containing silicon and no functional group other than those functions listed under groups 72, 73, 74, 75, 77, 82, 83, 84, or 85. Esters of silicic acid are to be found in group 42.
- Y4. Complex molecules containing carbohydrate fragments such as glycosides, as well as carbohydrate derivatives, e.g., osazones, osones, etc.

Explanation of Column Four Under Functionality Heading

This column normally indicates the total number of functional groups in a molecule. When column 1 contains an X3 or X4 this column indicates the number of unfused rings present in the molecule.

Explanation of Column Five Under Functionality Heading

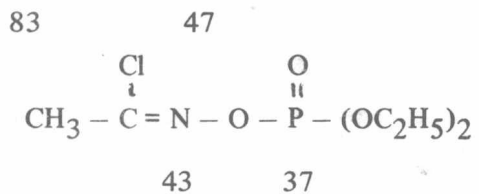
1. Alicyclic: Non-aromatic ring structures, including spiro compounds and conjugate, non-aromatic unsaturation as exhibited by cyclooctatetraene.
2. Aliphatic: Homogeneous and heterogeneous linear or branched chain compounds. Olefinic and acetylenic compounds are of this type also.
3. Aromatic: Those compounds containing one or more benzenoid rings (may be fused) and other carbocyclic molecules which exhibit a pi-electron sextet, such as azulene. Quinoid structures are not considered aromatic and will be found in this group only if attached to an aromatic ring, e.g., naphthoquinone.
4. Heterocyclic: Cyclic compounds with one or more hetero atoms but considered aromatic, e.g., dioxane and piperidine. Although pyrrole, furan, and thiophene are essentially aromatic they are classified in this group. Azido (triazole) compounds are also in this group.
5. Heterocyclic-Aromatic: Heterocyclic structures fulfilling the specifications outlined under group 3 above (with the exception of pyrrole, furan, and thiophene) are in this group. Structures which may be coded either 3 or 4 (e.g., phenylpiperidine) are included in group 5.
6. Inorganic: Any compound not containing carbon. Therefore, carbon dioxide, potassium cyanide, etc., do not fall in this category.

Note: When column 1 contains an X3 or X4 this column now indicates the number of fused rings present in the molecule.

Editorial Note

Compounds are occasionally cross-coded into groups where, by the strictest of definitions they do not belong, if such cross-coding gives additional information. Cross-coding is particularly employed when the groupings hinge on some nebulous technicality, as is the case with many heterocyclics.

Compounds having rather unusual linkages, such as the one illustrated below, are coded as the sum of their parts.



Coding: 37 43 47 4 2

SADTLER ULTRAVIOLET SPECTRA IN NON-POLAR SOLVENTS

LOCATOR

This index is based upon the wavelength locations and absorptivity of the peaks in each ultraviolet spectrum, enabling the spectroscopist to compare his own unknown spectra with the published data for evaluation or identification purposes.

The record for each spectrum consists of up to five pairs of data (maxima wavelength/absorptivity), a sixth item showing the total number of absorption peaks exhibited in the 200 - 350 $m\mu$ region (some into the visible region), followed by the spectrum serial number in this publication and the corresponding number in the Sadtler Standard Infrared publication. The last item "N" indicates that all spectra have been run in a neutral medium.

The Locator relies principally on the first five pairs of columns for its operation. The first four digits of the first column pair denote the position of the peak of maximum absorption (highest absorptivity) to the nearest 0.5 $m\mu$. The second set of four digits within the first column shows the absorptivity value (a) of that peak. To facilitate the use of the Locator with unknown compounds the absorptivity rather than the molar absorptivity has been used. The absorptivity has been calculated from:

$$a = \frac{A}{bC}$$

where a = absorptivity

A = absorbance (also known as optical density or extinction)

b = optical path length in cm

C = concentration in grams per liter

In order to convert absorptivity (a) to molar absorptivity (ϵ) simply multiply by the molecular weight of the compound.

The entries in column pairs 2 through 5 have the same designation as the first column pair and are arranged in order of descending absorptivity. If there are less than five column pairs for a spectrum entry this indicates that the compound exhibits fewer than five absorption peaks. Should all five column pairs be filled then the compound has five or more peaks in its spectrum and the total number of peaks is given in the column labelled "PEAKS".

An example of the use of the locator is shown on the following pages.

USE OF THE LOCATOR

There are two methods of locating unknown spectra for comparison. Firstly, comparing on λ values only taking the λ values of the five strongest peaks without calculating the absorptivities. This method gives a rapid preliminary screening for possible matching spectra. The second and more precise method entails the calculation of absorptivity values and more detailed searching for spectra which match on both wavelength and absorptivity values.

During the searching procedure it is advisable to look at spectra within $\pm 0.5 \mu$ if an exact match cannot be found, this allows for instrument variation.

The example shown below illustrates the composition of the Ultraviolet Locator. On the following page a worked example of an actual spectrum is illustrated.

COLUMN PAIR NO.					NO. OF PEAKS IN ENTIRE SPECTRUM					SADTLER INFRARED SERIAL NO.			
1	2	3	4	5	6	7	8	9	10	PEAKS	IR NO	UV NO	NAB
220.5	64.48	271.5	17.00	278.5	16.07	265.0	11.58			4	2988	383	N
221.0	156.0									1	1086	168	N
221.0	121.0	225.5	113.1	230.0	105.2	277.0	6.243	269.5	6.243	5	2255	297	N
221.0	93.00	265.5	76.00	209.0	72.00					3	3529	452	N
221.0	67.46	271.5	17.46	278.0	16.66	265.0	11.90			4	192	46	N
221.0	61.05	271.5	13.94	278.5	12.63	265.5	9.473			4	1863	261	N
221.5	58.00	270.0	2.450	278.0	2.250	263.0	1.850	257.0	1.350	5	2726	344	N
221.5	528.5	276.0	24.50	266.0	21.50	286.0	16.00	311.0	1.000	5	865	127	N
221.5	72.00	285.0	49.00	240.5	40.00					3	3319	426	N
221.5	174.0	293.0	13.00	299.0	12.80	283.0	12.00			4	2215	292	N
221.5	226.6	300.0	113.3	272.0	110.0	308.5	86.66	342.0	16.66	5	155	34	N
222.0	100.0	261.0	4.500	265.0	4.400	255.0	3.750	271.5	3.150	5	2655	335	N

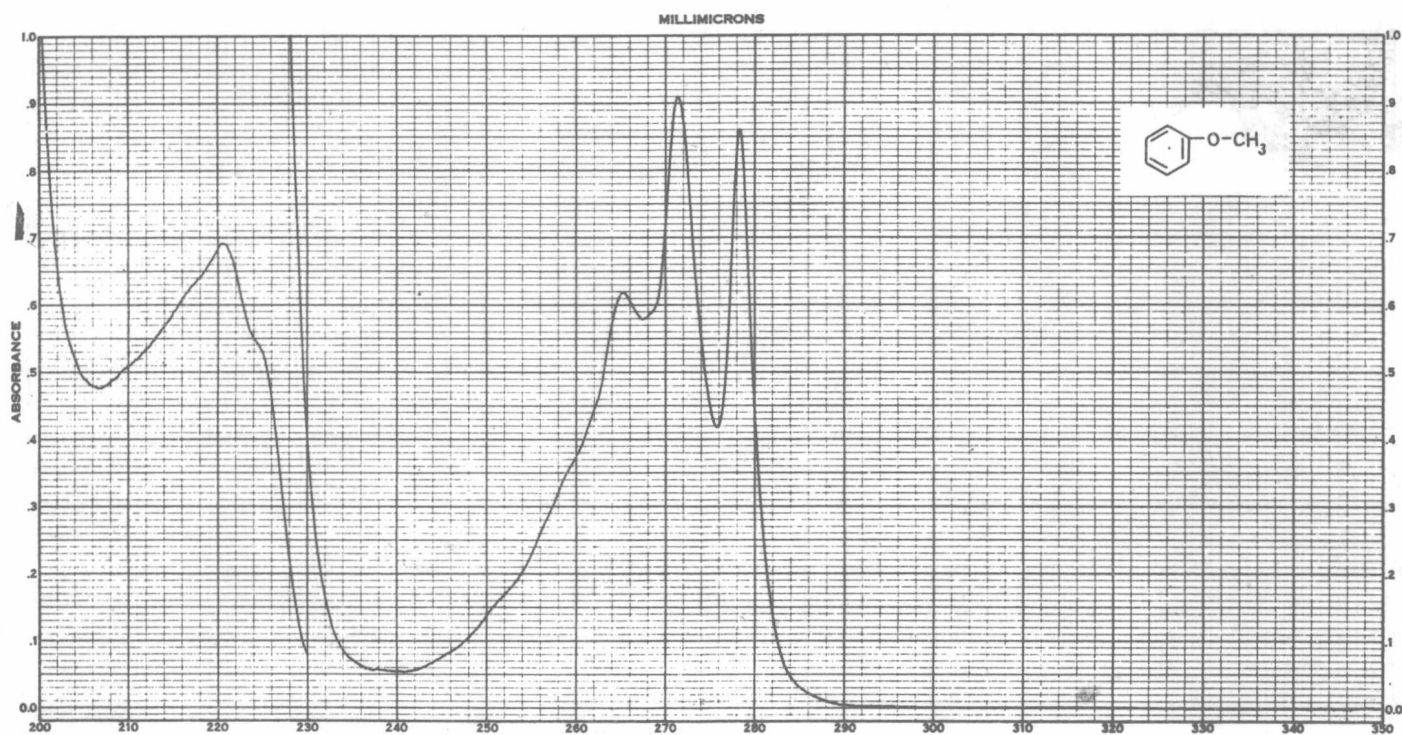
λ_{\max} - ABSORPTIVITY
FOR COLUMN PAIR NO. 1

SADTLER ULTRAVIOLET
SERIAL NO.

SOLUTION MEDIUM
NEUTRAL

EXAMPLE

1. Examine the spectrum (see illustration below) for all maxima and list them.
2. Calculate the absorptivity for each peak using the equation: $a = \frac{A}{bc}$
3. Arrange the peak data in sequence according to decreasing absorptivity, listing both the λ_{\max} and absorptivity values. This sequence will indicate which column pairs the data will fall into in the Locator.
4. Compare the data obtained from No. 3 above with the Locator, bearing in mind that the Locator is arranged according to increasing value of λ_{\max} .



Absorption Maxima

λ_{\max} (m μ)

220.5

271.5

278.5

265.0

Absorptivity

a

64.48

17.00

16.07

11.58

Column Pair No.

1

2

3

4

SADTLER ULTRAVIOLET SPECTRA IN NON-POLAR SOLVENTS

This collection of reference spectra, specifically prepared in cyclohexane solvent, has been compiled to aid spectroscopists measuring spectra in non-polar media for both identification purposes and liquid chromatography/ultraviolet detection techniques. The compounds in this publication are also found in the Sadtler Standard Ultraviolet Spectra publication, prepared in a polar solvent medium, using methanol predominantly.

The criteria used in preparing this publication are as follows:

Instrumentation

A Cary model 15 instrument was used to scan the spectra, wavelength calibration and absorbance were checked periodically using a standard potassium chromate solution. For each run the base line was set at zero absorbance with solvent in reference and sample cells. The following parameters are typical for the instrument.

Chart speed	1 $\mu\text{m/sec.}$	
Chart	200 - 350 μm (some to 500 μm)	
Scale	0 - 1 in absorbance	
Slits programmed as follows:		
350 μm - 0.13 mm	260 μm - 0.19 mm	210 μm - 0.60 mm
300 μm - 0.14 mm	240 μm - 0.22 mm	200 μm - 1.30 mm
280 μm - 0.17 mm	220 μm - 0.37 mm	

Sample Preparation

Spectral grade cyclohexane was used in all cases. Compounds of high solubility were weighed to definite concentrations, those only slightly soluble were prepared as saturated solutions without definite concentration measurement since in these few cases it was considered important to register the maxima locations and general curve shape. There is one spectrum shown for each compound, no pH adjustment was included.

When more than one concentration was necessary to bring the absorbance maxima within the absorbancy range of the instrument, the cell thickness was increased or decreased accordingly.

Chart Legend

In order to make both qualitative and quantitative aspects of the curves more evident, each chart has a legend tabulating the following information.

1. λ max - the wavelength of maximum absorption, measured to the closest 0.5 mμ.
2. Concentration *, in grams/liter; g/l.
3. a_m - molar absorptivity (also known as ϵ , the molecular extinction coefficient). This term is calculated from the equation,

$$a_m = \frac{A}{bc_m} \quad \text{where } A = \text{observed absorbancy}$$
$$c_m = \text{conc. in mol/l}$$
$$b = \text{cell thickness in cm.}$$

4. Cell thickness.

- * For saturated solutions the concentration is shown as 'Sat'd', the molar absorptivity cannot be calculated.

- NOTE: 1. a_m has been calculated to three significant figures, the limit of accuracy in reading A.
2. Due to space limitations, up to six maxima are shown on the legend although more than six may occasionally be exhibited by the compound. A maximum is interpreted as the point at which the slope of the curve changes sign (positive to negative or vice versa). Therefore, a shoulder, although quite pronounced, is not recorded. Also, as solvent cutoff, atmospheric absorption and widening slits influence the shape of the curve at shorter wavelength, no maximum is reported for a wavelength below $210 m\mu$ unless it is a pronounced peak.

Chemical Data

Each compound is shown by its Chemical Abstracts name, molecular formula, molecular weight, other physical data (when available) and the source of the sample.

Indexes

The compounds scanned for this collection were selected from the compounds in the Sadtler Standard Ultraviolet publication, consequently the indexes show the corresponding spectrum numbers of the compound in that publication and also the Sadtler Infrared and Sadtler NMR spectra publications.

The indexes comprise an Alphabetical Index, by chemical name; a Molecular Formula Index; a Numerical Index; a Chemical Class Index and a Locator Index. Further descriptions of each index are given in their introductions.

$$a_m = \frac{A}{c_m \cdot b}$$

where A = observed absorbance
 c_m = conc. in mols/l.
 b = cell thickness in cm.

SADTLER STANDARD ULTRAVIOLET (NON-POLAR) SPECTRA

ALPHABETICAL INDEX

INTRODUCTION

This index is a listing by chemical name of the compounds contained in the Sadtler publication of Standard Ultraviolet (Non-Polar) Spectra. Cross-reference and trivial names are also indexed.

The compound naming procedure used here is basically that of Chemical Abstracts, thus compounds are indexed primarily by their "parent compound" name with substituent groups and derivatives following the parent name in alphabetical sequence. This system directs the user rapidly to both the actual compound required and other similar compounds available. Cross-reference names which are generally accepted are also included in this index.

In addition to the UV (Non-Polar) spectrum numbers, shown in the right hand column of each page; infrared, ultraviolet (in polar solvents) and NMR spectrum numbers are included in the index to enable the location of spectra in other Sadtler publications for further reference.

The use of computerized equipment imposes limitations in symbolism. The alternatives used are as follows:

Deviation from standard punctuation

/	(slash)	—	Read as parenthesis, bracket, or brace
□	(lozenge)	—	Read as indication of superscripting (See last of the examples on the next page)
PR		—	Read as "prime". Therefore 2PR is read as 2'.
*	(asterisk)	—	Also read as "prime".
<		—	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.

A few examples will help to illustrate the variations to be encountered:

Chemical Abstracts System

Sadtler Index

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

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

Benz[a] anthracene-7,12-dione

BENZ/A/ANTHRACENE-7,12-DIONE

Chryseno[6,5-d] oxazole

CHRYSENO/6,5-D/OXAZOLE

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

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

or

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

Tricyclo[3.3.1.1^{3,7}] decane

TRICYCLO/3.3.1.1^{3,7}/DECANE

Note: Non-numeric prefixes to NMR spectra numbers in this index pertain to the following NMR publications:

- | | | |
|---|----|----------------------|
| V | -- | Varian spectra |
| J | -- | JEOL 60 MHz spectra |
| F | -- | JEOL F-19 spectra |
| * | -- | JEOL 100 MHz spectra |

ALPHABETICAL INDEX

NAME	PRISM	GRATING	UV	NMR	UV-NP
ABIETIC ACID, DEHYDRO-,	1545	29146	444		218
ACENAPHTHENE	875	548	272		133
ACENAPHTHENE	875	175	272	65	133
ACENAPHTHENE	7458	175	272		133
ACENAPHTHENE	7458	548	272	65	133
ACENAPHTHYLENE, 1,2-DIHYDRO-,	7458	548	272	65	133
ACENAPHTHYLENE, 1,2-DIHYDRO-,	7458	175	272		133
ACENAPHTHYLENE, 1,2-DIHYDRO-,	875	175	272	65	133
ACENAPHTHYLENE, 1,2-DIHYDRO-,	875	548	272		133
ACETAMIDE, N-/1-NAPHTHYL/-,	2164	297	571		286
ACETAMIDE, N-/2-NAPHTHYL/-,	2165	298	572	131	287
ACETANILIDE	160	49	63	5235	36
ACETANILIDE, 4*-BROMO-,	4590	416	1271	6464	500
ACETANILIDE, 4*-CHLORO-,	41888	22888	19177	13584	346
ACETANILIDE, 4*-CHLORO-,	41888	22888	19177	686	346
ACETANILIDE, 4*-FORMYL-,	1770	21336	4141		242
ACETANILIDE, 4*-FORMYL-,	1770	273	495	665	242
ACETIC ACID, BENZYL ESTER	859	167	260	10222	126
ACETIC ACID, BENZYL ESTER	859	167	260	V 530	126
ACETIC ACID, CINNAMYL ESTER	1521	254	431	682	211
ACETIC ACID, FURFURYL ESTER	1475	249	420	V 167	206
ACETIC ACID, FURFURYL ESTER	1475	249	420	10445	206
ACETIC ACID, ISOEUGENOL ESTER	2149	8235	564	130	279
ACETIC ACID, P-/2-NITROVINYL/-	3309		998		422
ACETIC ACID, PHENETHYL ESTER	3860	394	1172	V 261	475
ACETIC ACID, PHENETHYL ESTER	3860	394	1172	10618	475
ACETIC ACID, 3-PHENYLPROPYL ESTER	1650	15338	469	6697	232
ACETIC ACID, 3-PHENYLPROPYL ESTER	3862	15338	469	6697	232
ACETIC ACID, /P-CHLOROPHENOXY/-,	1590	259	457	10777	224
ACETIC ACID, /P-CHLOROPHENOXY/-,	1590	259	457	V 500	224
ACETIC ACID, /P-CHLOROPHENOXY/-,	13139	259	457	V 500	224
ACETIC ACID, /3,4-DICHLORO-	13144	33345	450	4276	221
PHENOXY/-,					
ACETIC ACID, /3,4-DICHLORO-	1571	33345	450		221
PHENOXY/-,					
ACETIC ACID, /3,4-DIMETHOXY-	506	132	176	10402	98
PHENYL/-,					
ACETIC ACID, 3,4-DIMETHOXYPHENYL-,	11174	132	176		98
ACETIC ACID, DIPHENYL-,	2112	28254	560	129	278
ACETIC ACID, DIPHENYLHYDROXY-,	1938	289	534		271
ACETIC ACID, DIPHENYLHYDROXY-,	13454	289	534	9818	271
ACETIC ACID, /2-NAPHTHYLOXY/-,	637	15061	215	6171	111
METHYL ESTER					
ACETIC ACID, PHENYL-,	1655	28241	474	117	235
ACETIC ACID, PHENYL-, METHYL ESTER	165	4764	64	19	37
ACETIC ACID, PHENYL-, PHENETHYL	1633	265	467	720	231
ESTER					
ACETIC ACID, PHENYL-, P-TOLYL ESTER	2073	15183	553	6526	277
ACETOACETIC ACID, CYCLOHEXYL ESTER	4265	28312	1221	10538	487
P-NITROPHENYLHYDRAZONE					
2*-ACETONAPHTHENE	1245	28530	371	1202	184
ACETONE, ACETONYL-,	121	15015	43	2709	23
ACETONITRILE, 3,4-DIMETHOXYPHENYL-,	431	24514	160	10267	91
ACETONITRILE, P-NITROPHENYL-,	1801	18021	503	10400	249
ACETONITRILE, P-NITROPHENYL-,	1801	18021	503	V 495	249
ACETONITRILE, PHENYL-,	2231	307	598	135	294
P-ACETOPHENETIDIDE	252	4849	102	10213	62
P-ACETOPHENETIDIDE	252	4849	102	V 267	62
ACETOPHENONE	3226	8290	953	V 192	405
ACETOPHENONE	3226	8290	953	10480	405
ACETOPHENONE, 2,4-DINITROPHENYL	1779	18020	496		243
HYDRAZONE					
ACETOPHENONE, 3*-AMINO-,	1843	28247	518	119	259
ACETOPHENONE, 4PR-/O-AMINO-	4499	28658	1252	10592	492
PHENOXY/-,					
ACETOPHENONE, 2-AZID-2*-HYDROXY-,	3513	15455	1089	7522	447
ACETOPHENONE, 2-BENZYLIDENE-,	2723	335	737	160	341
ACETOPHENONE, 4*-BROMO-,	4580	414	1267	219	499
ACETOPHENONE, 4PR-BUTOXY-3PR-	3529		1094		452
/CHLOROMETHYL/-,					
ACETOPHENONE, 2-CHLORO-,	4576	8338	1264	J 107	498
ACETOPHENONE, 2-CHLORO-,	4576	8338	1264	3174	498
ACETOPHENONE, 4*-CHLORO-,	1769	272	494	18007	241
ACETOPHENONE, 4*-CHLORO-,	1769	272	494	V 188	241
ACETOPHENONE, 4*-HYDROXY-,	3415	28289	1066	10590	438
ACETOPHENONE, 2-HYDROXY-2-PHENYL-,	2722	28561	736	9476	340
ACETOPHENONE, 4*-METHOXY-,	3883	21051	1177	10243	479
ACETOPHENONE, 4*-METHYL-,	872	174	270	10188	131
M-ACETOTOLUIDIDE	2900	351	831	10793	373
M-ACETOTOLUIDIDE, 4*-NITRO-A, A, A-	2783	15381	765	6259	353
TRIFLUORO-,					