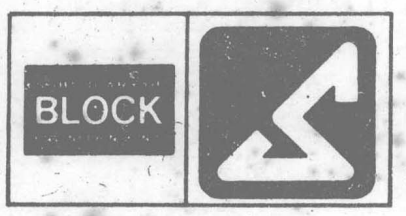
THE SADTLER STANDARD SPECTRA



SADTLER RESEARCH LABORATORIES, INC.

FLUORESCENCE SPECTRA

CREATIVE CHEMISTS SINCE 1874

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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, 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.

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This collection of spectra contains the excitation and emission spectra, measured on an Aminco-Bowman SPF spectrophotofluorometer, for 500 compounds. The purpose of the publication is to provide the analyst with a reliable source of reference fluorescence spectra for use in identifying and investigating materials.

The Aminco-Bowman SPF single beam instrument (Model 4-8202D) with a 10-280 microphotometer produces uncorrected spectra in the 200 - 800 nm scanning range utilizing a 150 watt xenon excitation source and a 1P21 photomultiplier tube. In each case the spectrum was scanned at the smallest slit width setting consistent with moderate noise levels and high resolution. If the fluorescence characteristics of a given compound where dependent on pH value, its spectra were prepared at the pH which produced maximum fluorescence. During the preparation the fluorescence characteristics were compared with the UV spectra previously published by Sadtler to ensure representative spectra.

Methods for preparing calibration curves to enable the published spectra to be "corrected" for comparison with data from other spectrofluorometers are currently being investigated in our laboratories, and comments and suggestions from users of this publication would be appreciated by our staff.

The indexes which accompany this publication are as follows:

the alphabetical index permits the contents to be located by chemical name,

the molecular formula index is arranged in increasing carbon atom number sequence,

the chemical classes index categorizes the compounds according to chemical functionalities present in the molecule,

and the numerical index lists the compounds by their fluorescence spectrum number.

The fluorescence spectrum number appears in the right hand column of each index under the title "FLUOR." and the spectrum numbers in the columns labelled PRISM, GRATING, UV and NMR refer to the spectra for compounds issued in the corresponding publications.

We acknowledge the assistance of Dr. Richard A. Passwater of the American Instrument Company in making this publication possible.

SADTLER STANDARD FLUORESCENCE SPECTRA

ALPHABETICAL INDEX

INTRODUCTION

This index is a listing by chemical name of the compounds contained in the Sadtler publication of Standard Fluorescence Spectra.

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 Fluorescence spectrum numbers, shown in the right hand column of each page; infrared, ultraviolet 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

SADTLER FLUORESCENCE SPECTRA

CHEMICAL CLASSES INDEX

NAME	C	H	Br	Cl	F	I	N	O	P	S	Si	M	FUNCTIONALITY					PRISM	GRATING	U.V.	N.M.R.	FLUOR.
CARBOXYLIC ACIDS																						
BUTYRIC ACID, 3-METHYL-2-/P-BIPHENYLYL/-,	17	18						2					6			1	3	16279		5057		402
4-HEXENOIC ACID, 2-/P-BIPHENYLYL/-,	18	18						2					6			1	3	16280	25314	5058		403
1-NAPHTHALENEACETIC ACID	12	10						2					6			1	3	5874	585	2965	3238	209
1-NAPHTHALENEACETIC ACID K	12	10						2					6			1	3	10905	585	2965	3238	209
HIPPURIC ACID, P-AMINO-,	9	10					2	3					6	14	64	3	3	11186	8202	511	10098	80
HIPPURIC ACID, P-AMINO-,	9	10					2	3					6	14	64	3	3	1819	8202	511	10098	80
ACETIC ACID, /3-CARBAMYL-2-NAPHTHYLOXY/-,	13	11					1	4					6	14	72	3	3	17208	24588	7277		431
SALICYLIC ACID, 5-SULFO-,	7	6						6		1			6	22	59	3	3	137	29551	50	16001	9
ACETIC ACID, /3-CYANO-2-NAPHTHYLOXY/-,	13	9					1	3					6	5	72	3	3	17210	24590	5434		432
1H-BENZ/E/INDENE-1-CARBOXYLIC ACID, 2,3-DIHYDRO-3-OXO-,	14	10						3					6	52		2	3	18278		5801		464
ACETIC ACID, O-HYDROXYPHENYL-,	8	8						3					6	59		2	3	17420	25680	7333	12840	443
BENZOIC ACID, 2,5-DIHYDROXY-,	7	6						4					6	59		2	3	7173	8495	2028	3210	256
BENZOIC ACID, M-HYDROXY-,	7	6						3					6	59		2	3	3247	368	967	1624	142
BENZOIC ACID, 2,3,4-TRIHYDROXY-,	7	6						5					6	59		2	3	4577	18063	1265	8668	167
CINNAMIC ACID, O-HYDROXY-,	9	8						3					6	59		2	3	17173	8719	5419	12878	428
2,3-CRESOTIC ACID	8	8						3					6	59		2	3	10590	8578	2910	3281	297
GALLIC ACID, MONOHYDRATE	7	6						5					6	59		2	3	7376	546	2090		259
GALLIC ACID, MONOHYDRATE	7	6						5					6	59		2	3	7376	546	2090	10229	258
GENTISIC ACID	7	6						4					6	59		2	3	7173	8495	2028	3210	256
HYDROCINNAMIC ACID, P-HYDROXY-,	9	10						3					6	59		2	3	9916	28042	2613	14712	288
HYDROCINNAMIC ACID, P-HYDROXY-,	9	10						3					6	59		2	3	9916	7593	2613	4450	288
1-NAPHTHOIC ACID, 2-HYDROXY-,	11	8						3					6	59		2	3	234	78	90	13433	15
1-NAPHTHOIC ACID, 2-HYDROXY-,	11	8						3					6	59		2	3	13209	78	90	13433	15
2-NAPHTHOIC ACID, 1-HYDROXY-,	11	8						3					6	59		2	3	16455	8715	5154	12735	410
PENTANOIC ACID, 4,4-BIS/4-HYDROXYPHENYL/-,	17	18						4					6	59		2	3	14559	24472	4133		354
PHLORETIC ACID	9	10						3					6	59		2	3	9916	7593	2613	4450	288
PHLORETIC ACID	9	10						3					6	59		2	3	9916	28042	2613	14712	288
PROPIONIC ACID, 3-/P-HYDROXYPHENYL/-,	9	10						3					6	59		2	3	9916	7593	2613	4450	288
PROPIONIC ACID, 3-/P-HYDROXYPHENYL/-,	9	10						3					6	59		2	3	9916	28042	2613	14712	288
B-RESORCYLIC ACID	7	6						4					6	59		2	3	17377	8722	7324	12834	438
G-RESORCYLIC ACID	7	6						4					6	59		2	3	10967	8587	2986	540	295
G-RESORCYLIC ACID	7	6						4					6	59		2	3	10967	8587	7269		299
SALICYLIC ACID, 6-HYDROXY-,	7	6						4					6	59		2	3	17123	8587		540	299
SALICYLIC ACID, 3-PHENYL-,	13	10						3					6	59		2	3	9174	15693	2382		282
SALICYLIC ACID, 5-PHENYL-,	13	10						3					6	59		2	3	9173	15692	2381		281
SALICYLIC ACID, 5-AMINO-, HYDROCHLORIDE	7	7					1	3					6	59	67	3	3	13600	8621	3580	18056	323
BENZOIC ACID, 3-METHOXY-4-HYDROXY-,	8	8						4					6	59	72	3	3	1975	8217	546	9077	105
VANILLIC ACID	8	8						4					6	59	72	3	3	1975	8217	546	9077	105
SALICYLIC ACID, 5-CHLORO-,	7	5		1				3					6	59	83	3	3	3248	18033	968	8773	143
SALICYLIC ACID, 5-CHLORO-, K	7	5		1				3					6	59	83	3	3	11599	18033	968	8773	143
ANTHRANILIC ACID	7	7					1	2					6	64		2	3	2703	330	729	3159	117
BENZOIC ACID, M-AMINO-,	7	7					1	2					6	64		2	3	6493	526	1802	2822	233
BENZOIC ACID, O-AMINO-,	7	7					1	2					6	64		2	3	2703	330	729	3159	117
BENZOIC ACID, P-AMINO-,	7	7					1	2					6	64		2	3	1542	15145	15745		91
BENZOIC ACID, P-AMINO-,	7	7					1	2					6	64		2	3	1542	15145	441	6944	91
ISOPHTHALIC ACID, 5-AMINO-,	8	7					1	4					6	64		2	3	18164	25867	5766		459
ANTHRANILIC ACID, 5-CHLORO-,	7	6		1			1	2					6	64	83	3	3	13915	471	1486	1216	186
ANTHRANILIC ACID, 5-CHLORO-,	7	6		1			1	2					6	64	83	3	3	5426	471	1486	1216	186
BENZOIC ACID, 2-AMINO-5-CHLORO-,	7	6		1			1	2					6	64	83	3	3	5426	471	1486	1216	186
BENZOIC ACID, 4-BUTYLAMINO-,	11	15					1	2					6	65		2	3	18726	8879	6034	2088	494
3-INDOLEPROPIONIC ACID K	11	11					1	2					6	65		2	5	10719	15557	1489	6802	188
BUTYRIC ACID, 4-/3-INDOLYL/-,	12	13					1	2					6	65	73	3	5	5430	28778	1488	17317	187
3-INDOLEBUTYRIC ACID	12	13					1	2					6	65	73	3	5	5430	28778	1488	17317	187
3-INDOLEPROPIONIC ACID	11	11					1	2					6	65	73	3	5	5431	15557	1489	6802	188
PROPIONIC ACID, 3-/3-INDOLYL/-,	11	11					1	2					6	65	73	3	5	5431	15557	1489	6802	188
BENZOIC ACID, M-/DIMETHYLAMINO/-,	9	11					1	2					6	66		2	3	13931	8637	3907	6164	335
CINCHONINIC ACID, 2-PHENYL-,	16	11					1	2					6	66		2	5	473	128	166	10217	30
CINCHONINIC ACID, 2-PHENYL-,	16	11					1	2					6	66		2	5	11644	128	166		30
CINCHOPHEN	16	11					1	2					6	66		2	5	11644	128	166		30
CINCHOPHEN	16	11					1	2					6	66		2	5	473	128	166	10217	30
4-QUINOLINECARBOXYLIC ACID, 2-PHENYL-,	16	11					1	2					6	66		2	5	473	128	166	10217	30
4-QUINOLINECARBOXYLIC ACID, 2-PHENYL-,	16	11					1	2					6	66		2	5	11644	128	166		30
QUININIC ACID	11	9					1	3					6	66	72	3	5	6519	18132	1812		236
QUININIC ACID	11	9					1	3					6	66	72	3	5	6519	18132	1812	10752	235
4-QUINOLINECARBOXYLIC ACID, 6-METHOXY-,	11	9					1	3					6	66	72	3	5	6519	18132	1812		236
4-QUINOLINECARBOXYLIC ACID, 6-METHOXY-,	11	9					1	3					6	66	72	3	5	6519	18132	1812	10752	235

NAME	C	H	Br	Cl	F	I	N	O	P	S	Si	M	FUNCTIONALITY					PRISM	GRATING	U.V.	N.M.R.	FLUOR.
06 CARBOXYLIC ACIDS																						
BENZCIC ACID, M-AMINO-, HYDROCHLORIDE	7	7					1	2					6	67		2	3	15272	21346	4547		372
PHTHALIC ACID, 3-AMINO-, HYDROCHLORIDE	8	7					1	4					6	67		2	3	18677	8861	6002	18802	487
ACETIC ACID, /3-CARBOXY-2-NAPHTHYLOXY/-,	13	10						5					6	72		2	3	17211	24591	5435		433
ACETIC ACID, /3,4-DIMETHOXY-PHENYL/-,	10	12						4					6	72		2	3	506	132	176	10402	32
ACETIC ACID, 3,4-DIMETHOXYPHENYL-,	10	12						4					6	72		2	3	11174	132	176		32
ACETIC ACID, M-METHOXYPHENYL-,	9	10						3					6	72		2	3	18331	10114	5833	4228	467
ACETIC ACID, P-METHOXYPHENYL-,	9	10						3					6	72		2	3	6263	8454	1727	3192	215
ACETIC ACID, 1-NAPHTHYLOXY-,	12	10						3					6	72		2	3	587C	8422	1646	10486	207
ACETIC ACID, 2-NAPHTHYLOXY-,	12	10						3					6	72		2	3	5871	504	1647	10485	208
ACETIC ACID, PHENOXY-,	8	8						3					6	72		2	3	5852	500	1637	264	206
ACETIC ACID, M-TOLYLOXY-,	9	10						3					6	72		2	3	17479	24661	5550	12854	444
BENZOIC ACID, P-ETHOXY-,	9	10						3					6	72		2	3	1623	15151	462	6972	95
BENZOIC ACID, M-/2-METHOXY/ETHOXY-,	10	12						4					6	72		2	3	2757	15376	751	7525	120
BENZOIC ACID, 3,4,5-TRIMETHOXY-,	10	12						5					6	72		2	3	8449	18223	2242	8667	272
HOMOANISIC ACID	9	10						3					6	72		2	3	6263	8454	1727	3192	215
HOMOVERATRIC ACID	10	12						4					6	72		2	3	506	132	176	10402	32
2-NAPHTHOIC ACID, 3-CARBOXYMETHOXY/-,	13	10						5					6	72		2	3	17211	24591	5435		433
ACETIC ACID, /3-FLUORO-2-NAPHTHYLOXY/-,	12	9			1			3					6	72	82	3	3	17214		7278		434
07 CARBOXYLIC ACID SALTS																						
FLUORESCEIN, SODIUM DERIVATIVE SODIUM SALT	20	10						5				NA	7	52	59	5	5	1836	18023	517		101
URANIN	20	10						5				NA	7	52	59	5	5	1836	18023	517		101
SALICYLIC ACID, SODIUM SALT	7	5						3				NA	7	59		2	3	10261	8569	2775	3233	294
SALICYLIC ACID, ZINC SALT	14	10						6				ZN	7	59		2	3	18054		5716	13009	448
SALICYLIC ACID, 4-AMINO-, CALCIUM SALT	14	12					2	6				CA	7	59	64	3	3	14719		4172	18070	358

NAME	C	H	Br	Cl	F	I	N	O	P	S	Si	M	FUNCTIONALITY					PRISM	GRATING	U.V.	N.M.R.	FLUOR.
12 ESTERS OF CARBOXYLIC ACIDS																						
ACETIC ACID, 2-NAPHTHYL ESTER	12	10						2					12			1	3	9683	15714	2571	6382	286
1-NAPHTHALENEACETIC ACID, METHYL ESTER	13	12						2					12			1	3	2961	357	852	583	130
SALICYLIC ACID, P-PHENYLPHENACYL ESTER	21	16						4					12	52	59	3	3	2885	28990	818		123
ACETIC ACID, M-HYDROXYPHENYL ESTER	8	8						3					12	59		2	3	5552	15570	1546	8589	195
BENZOIC ACID, P-HYDROXY-, BUTYL ESTER	11	14						3					12	59		2	3	5434	474	972	1214	146
BENZOIC ACID, P-HYDROXY-, BUTYL ESTER	11	14						3					12	59		2	3	5434	372	972		146
BENZOIC ACID, P-HYDROXY-, BUTYL ESTER	11	14						3					12	59		2	3	3252	474	972	1214	146
BENZOIC ACID, P-HYDROXY-, BUTYL ESTER	11	14						3					12	59		2	3	3252	372	972		146
BENZOIC ACID, P-HYDROXY-, ETHYL ESTER	9	10						3					12	59		2	3	3250	370	970	1192	145
BENZOIC ACID, P-HYDROXY-, METHYL ESTER	8	8						3					12	59		2	3	3249	369	969	1191	144
BENZOIC ACID, P-HYDROXY-, METHYL ESTER	8	8						3					12	59		2	3	18045	369	969	1191	144
BENZOIC ACID, P-HYDROXY-, METHYL ESTER, SODIUM DERIVATIVE	8	7						3				NA	12	59		2	3	18044		5713	4002	447
MENTHOL, SALICYLATE	17	24						3					12	59		2	3	1008	204	306	9725	59
RESORCINOL, ACETATE	8	8						3					12	59		2	3	5552	15570	1546	8589	195
SALICYLIC ACID, BENZYL ESTER	14	12						3					12	59		2	3	1523	256	433	719	89
SALICYLIC ACID, BENZYL ESTER	14	12						3					12	59		2	3	1523	256	433		90
SALICYLIC ACID, ETHYL ESTER	9	10						3					12	59		2	3	3870	396	1174	196	160
SALICYLIC ACID, ISOBUTYL ESTER	11	14						3					12	59		2	3	1007	203	305	724	58
SALICYLIC ACID, ISOPENTYL ESTER	12	16						2					12	59		2	3	1522	255	432	1189	88
SALICYLIC ACID, P-MENTH-3-YL ESTER	17	24						3					12	59		2	3	1008	204	306	9725	59
SALICYLIC ACID, PHENYL ESTER	13	10						3					12	59		2	3	2931	353	841	178	129
SALOL	13	10						3					12	59		2	3	2931	353	841	178	129
ANESTHESINE	9	11					1	2					12	64		2	3	3059	8286	888	1856	137
ANTHRANILIC ACID, ISOBUTYL ESTER	11	15					1	2					12	64		2	3	949	193	295	10191	55
BENZOCAINE	9	11					1	2					12	64		2	3	3059	8286	888	1856	137
BENZOIC ACID, P-AMINO-, BENZYL ESTER	14	13					1	2					12	64		2	3	18401	10138	5861	4051	475
BENZOIC ACID, P-AMINO-, BUTYL ESTER	11	15					1	2					12	64		2	3	5154	28732	1402	243	179
BENZOIC ACID, P-AMINO-, ETHYL ESTER	9	11					1	2					12	64		2	3	3059	8286	888	1856	137
BENZOIC ACID, P-AMINO-, ISOBUTYL ESTER	11	15					1	2					12	64		2	3	5155	8375	1403	3179	180
BENZOIC ACID, P-AMINO-, METHYL ESTER	8	9					1	2					12	64		2	3	5433	473	1490	585	189
5-PYRIMIDINECARBOXYLIC ACID, 4-AMINO-2-TRIFLUOROMETHYL-, ETHYL ESTER	8	8			3		3	2					12	64	66	4	5	15259	25132	4541		370
ACETIC ACID, 4-ALLYL-2-METHOXY-PHENYL ESTER	12	14						3					12	72		2	3	5257	8384	1447	3183	182
ACETIC ACID, P-METHOXYBENZYL ESTER	10	12						3					12	72		2	3	2187	8240	581	1205	106
ACETIC ACID, 2-PHENOXYETHYL ESTER	10	12						3					12	72		2	3	5256	15522	1446	6791	181
P-ANISIC ACID, METHYL ESTER	9	10						3					12	72		2	3	1936	288	533	124	104
ANISYL ALCOHOL, ACETATE	10	12						3					12	72		2	3	2187	8240	581	1205	106
BENZOIC ACID, 2,3-DIMETHOXY-, METHYL ESTER	10	12						4					12	72		2	3	2856	15384	797	11243	121
BENZOIC ACID, 2,3-DIMETHOXY-, METHYL ESTER	10	12						4					12	72		2	3	2856	15384	797		122
BENZOIC ACID, 4,4PR-OXYDI-, DIMETHYL ESTER	16	14						5					12	72		2	3	4813		1343		175
CARBONIC ACID, DIESTER WITH O-METHOXYPHENOL	15	14						5					12	72		2	3	8677	15666	2258	6868	276
EUGENOL, ACETATE	12	14						3					12	72		2	3	5257	8384	1447	3183	182
PHENOL, 4-ALLYL-2-METHOXY-, ACETATE	12	14						3					12	72		2	3	5257	8384	1447	3183	182
PHENOL, O-METHOXY-, CARBONATE	15	14						5					12	72		2	3	8677	15666	2258	6868	276
O-VERATRIC ACID, METHYL ESTER	10	12						4					12	72		2	3	2856	15384	797		122
O-VERATRIC ACID, METHYL ESTER	10	12						4					12	72		2	3	2856	15384	797	11243	121

NAME	C	H	Br	Cl	F	I	N	O	P	S	Si	M	FUNCTIONALITY					PRISM	GRATING	U.V.	N.M.R.	FLUOR.
14 CARBOXYLIC ACID AMIDES																						
ACETAMIDE, N-/6-CHRYSENYL/-,	20	15					1	1					14			1	3	13120	18322	3415		320
ACETAMIDE, N-/2-FLUORENYL/-,	15	13					1	1					14			1	3	2458	8590	4150	[illegible]8	112
ACETAMIDE, N-/2-FLUORENYL/-, K	15	13					1	1					14			1	3	14651	8590	4150	9438	112
ACETAMIDE, 2-/1-NAPHTHYL/-, K	12	11					1	1					14			1	3	10921	8583	2975	18753	298
ACETAMIDE, 2-/1-NAPHTHYL/-, K	12	11					1	1					14			1	3	10921	8583	15840		298
ACETAMIDE, N-/2-PHENYL-1-NAPHTHYL/-,	18	15					1	1					14			1	3	16498	25396	5162		411
FLUORENE, 2-ACETAMIDO-,	15	13					1	1					14			1	3	2458	8590	4150	9438	112
ACETANILIDE, 2-/P-AMINOBENZOYL/-,	15	14					2	2					14	52	64	3	3	14210	24431	3995		346
SALICYLAMIDE	7	7					1	2					14	59		2	3	3253	373	973	6740	147
2-NAPHTHANILIDE, 4PR-CHLORO-3-HYDROXY-, K	17	12		1			1	2					14	59	83	3	3	11679	32359	3259		310
NICOTINAMIDE, 6-AMINO-,	6	7					3	1					14	64	66	3	5	15313	33113	4574	18080	383
ACETAMIDE, 2-/2-PHENOXYETHOXY/-,	10	13					1	3					14	72		2	3	16892	25527	5304	12648	420
DIBENZOFURAN, 3-ACETIMIDO-,	14	11					1	2					14	72		2	5	2454	28555	639	10854	110
ACETAMIDE, N-/1-/METHYLTHIO/-2-NAPHTHYL/-,	13	13					1	1		1			14	75		2	3	16499	25397	5163	12499	412
ACETAMIDE, 2-CHLORO-N-/1-NAPHTHYL/-,	12	10		1			1	1					14	83		2	3	13628	32368	3301	18053	315
ACETAMIDE, 2-CHLORO-N-/1-NAPHTHYL/-, M	12	10		1			1	1					14	83		2	3	12145	32368	3301	18053	315
15 CYCLIC AMIDES, IMIDES, LACTAMS & LACTIMS OF CARBOXYLIC ACIDS																						
BARBITAL	8	12					2	3					15			1	4	5759	33037	5423	1173	199
BARBITURIC ACID, 5,5-DIETHYL-,	8	12					2	3					15			1	4	5759	33037	5423	1173	199
BARBITURIC ACID, 5,5-DIETHYL-,	8	10					2	3					15			1	4	17178	33037	5423	1173	199
8-AZAGUANINE	4	4					6	1					15	26	56	4	4	15301		4567		379
4H-PYRIDO/1,2-A/PYRIMIDINE-3-CARBONITRILE, 9-METHYL-4-OXO-,	10	7					3	1					15	5	66	3	5	14247	24437	4019		347
4,6-PYRIMIDINEDIOL, 2-AMINO-,	4	5					3	2					15	64		2	5	18127	8807	5743	2006	451
2-PYRAZOLIN-5-ONE, 1-/P-AMINOPHENYL/-4-/P-DIETHYLAMINOPHENYLIMINO/-3-METHYL-,	20	23					5	1					15	64	66	4	5	15855	25226	4820		393
BARBITURIC ACID, 5-BENZYLIDENE-,	11	8					2	3					15	73		2	5	6471	29237	1798	10851	231
CARBOSTYRIL	9	7					1	1					15	73		2	5	13899	21325	3792	6891	332
CARBOSTYRIL, 4-METHYL-,	10	9					1	1					15	73		2	5	8342	18221	2224	18384	270
QUINOLONE, 2/1H/-,	9	7					1	1					15	73		2	5	13899	21325	3792	6891	332
18 NITROLIC, NITROSOLIC, HYDROXAMIC ACIDS, AMIDINE, AMIDOXIME, AZIDE & HYDRAZIDE DERIVATIVES OF CARBOXYLIC & THIOCARBOXYLIC ACIDS																						
2-NAPHTHOIC ACID, 3-HYDROXY-, HYDRAZIDE	11	10					2	2					18	59		2	3	8696	15672	2269	9136	277

NAME | C | H | Br | Cl | F | I | N | O | P | S | Si | M | FUNCTIONALITY | PRISM | GRATING | U.V. | N.M.R. | FLUOR.

NAME	C	H	Br	Cl	F	I	N	O	P	S	Si	M	FUNCTIONALITY						PRISM	GRATING	U.V.	N.M.R.	FLUOR.
20 LACTONES AND LACTIDES OF CARBOXYLIC ACIDS																							
COUMARIN, 4,8-DIMETHYL-7-HYDROXY-,	11	10						3					20	59			2	5	18750	8889	6045	13644	498
COUMARIN, 7-ALLYLOXY-4-METHYL-,	13	12						3					20	72			2	5	3148	15427	919	10531	139
HERNIARIN, 4-METHYL-,	11	10						3					20	72			2	5	3161	15437	930	6636	140
22 SULFUR ACIDS																							
2-NAPHTHALENESULFONIC ACID	10	8						3		1			22				1	3	6333	29224	1742	10947	220
1,5-AMINO ACID	10	9					1	3		1			22	64			2	3	8459		2244		273
BENZENESULFONIC ACID, M-AMINO-,	6	7					1	3		1			22	64			2	3	17193	24479	5427		429
LAURENTS ACID	10	9					1	3		1			22	64			2	3	8459		2244		273
METANILIC ACID	6	7					1	3		1			22	64			2	3	17193	24479	5427		429
1,5-NAPHTHALENEDISULFONIC ACID, 2-AMINO-,	10	9					1	6		2			22	64			2	3	18697	24772	7671		491
1-NAPHTHALENESULFONIC ACID, 2-AMINO-,	10	9					1	3		1			22	64			2	3	17196	33496	7273	5139	430
1-NAPHTHALENESULFONIC ACID, 5-AMINO-,	10	9					1	3		1			22	64			2	3	8459		2244		273
1-NAPHTHYLAMINE-5-SULFONIC ACID	10	9					1	3		1			22	64			2	3	8459		2244		273
M-TOLUENESULFONIC ACID, 4-AMINO-,	7	9					1	3		1			22	64			2	3	16030	10039	4942	4420	396
BENZENESULFONIC ACID, O-/P-AMINO-ANILINO/-,	12	12					2	3		1			22	64	65		3	3	18119	8801	7544		449
DIPHENYLAMINE-2-SULFONIC ACID, 4*-AMINO-,	12	12					2	3		1			22	64	65		3	3	18119	8801	7544		449
2-DIBENZOFURANSULFONIC ACID	12	8						4		1			22	72			2	5	7073	18492	2004		254
23 SALTS OF SULFUR ACIDS																							
2-FLUORENESULFONIC ACID, POTASSIUM SALT	13	9						3		1		K	23				1	3	6730	28833	1879		242
1,3-BENZENEDISULFONIC ACID, 4,5-DIHYDROXY-, DISODIUM SALT	6	4						8		2		NA	23	59			2	3	14899	8696	4317	3262	361
1,3-BENZENEDISULFONIC ACID, 4,5-DIHYDROXY-, DISODIUM SALT	6	4						8		2		NA	23	59			2	3	14899	8696	4317	4413	361
SULFANILIC ACID, SODIUM SALT	6	6					1	3		1		NA	23	64			2	3	10260	18244	2774		293

	NAME	C	H	Br	Cl	F	I	N	O	P	S	Si	M	FUNCTIONALITY	PRISM	GRATING	U.V.	N.M.R.	FLUOR.
26	AMIDES AND IMIDES OF SULFUR ACIDS																		
	METHANESULFONAMIDE, N-2-FLUORENYL-,	14	13					1	2		1			26 1 3	6731	21106	1880		243
	BENZENESULFONAMIDE, P-AMINO-,	6	8					2	2		1			26 64 2 3	301	102	117	9685	25
	DESEPTYL	6	8					2	2		1			26 64 2 3	301	102	117	9685	25
	PRONTOSIL ALBUM	6	8					2	2		1			26 64 2 3	301	102	117	9685	25
	PRONTYLIN	6	8					2	2		1			26 64 2 3	301	102	117	9685	25
	SULFANILAMIDE	6	8					2	2		1			26 64 2 3	301	102	117	9685	25
29	ORGANIC ESTERS AND SALTS OF INORGANIC SULFUR ACIDS																		
	PHENOL, 4-AMINO-, HYDROGEN SULFATE, POTASSIUM SALT, HYDRATE	6	6					1	4		1		K	29 64 2 3	3698	15463	1131	7247	157
30	PHOSPHORUS ACIDS																		
	PHOSPHINIC ACID, /M-AMINOPHENYL/-PHENYL-,	12	12					1	2	1				30 64 2 3	2610	15365	691		114
	PHOSPHINIC ACID, BIS-/M-AMINO-PHENYL/-,	12	13					2	2	1				30 64 2 3	2612	29158	692		115
38	ALL CARBON SUBSTITUTED ACIDS NOT PREVIOUSLY CLASSIFIED																		
	M-ARSANILIC ACID, 4-HYDROXY-,	6	8					1	4				AS	38 59 64 3 3	18414		7600		477

NAME | C | H | Br | Cl | F | I | N | O | P | S | Si | M | FUNCTIONALITY | PRISM | GRATING | U.V. | N.M.R. | FLUOR.

NAME	C	H	Br	Cl	F	I	N	O	P	S	Si	M	FUNCTIONALITY					PRISM	GRATING	U.V.	N.M.R.	FLUOR.
46 ALDEHYDES																						
1-NAPHTHALDEHYDE	11	8						1					46			1	3	8444	21818	2239	11666	271
1-NAPHTHALENECARBOXALDEHYDE	11	8						1					46			1	3	8444	21818	2239	11666	271
ISOPHTHALALDEHYDE, 5-ETHOXY-4-HYDROXY-,	10	10						4					46	59	72	3	3	6301	18120	1735	6454	217
BENZALDEHYDE, 3,4-DIMETHOXY-,	9	10						3					46	72		2	3	3887	8313	1179	V 236	162
BENZALDEHYDE, 3,4-DIMETHOXY-,	9	10						3					46	72		2	3	3887	8313	1179	197	162
BENZALDEHYDE, 3,4-METHYLENEDIOXY-,	8	6						3					46	72		2	3	3885	15466	1178	10619	161
BENZALDEHYDE, 3,4-METHYLENEDIOXY-,	8	6						3					46	72		2	3	3885	15466	1178	V 187	161
HELIOTROPIN	8	6						3					46	72		2	3	3885	15466	1178	V 187	161
HELIOTROPIN	8	6						3					46	72		2	3	3885	15466	1178	10619	161
VERATRALDEHYDE	9	10						3					46	72		2	3	3887	8313	1179	197	162
VERATRALDEHYDE	9	10						3					46	72		2	3	3887	8313	1179	V 236	162
BENZALDEHYDE, 2-METHOXY-3,4-/METHYLENEDIOXY/-,	9	8						4					46	72		2	5	2626	15232	702	6001	116
PIPERONAL	8	6						3					46	72		2	5	3885	15466	1178	10619	161
PIPERONAL	8	6						3					46	72		2	5	3885	15466	1178	V 187	161
PIPERONAL, 2-METHOXY-,	9	8						4					46	72		2	5	2626	15232	702	6001	116
47 ALDEHYCE DERIVATIVES																						
SALICYLALDEHYDE, AZINE	14	12					2	2					47	59		2	3	5705	15579	1586		198
50 NITRILES AND ISONITRILES																						
BENZONITRILE	7	5					1						50			1	3	2255	312	602	138	108
BENZONITRILE, 4,4PR-ETHYLENEDI-,	16	12					2						50			1	3	4789	29052	1324		174
A,A-BI-P-TOLUNITRILE	16	12					2						50			1	3	4789	29052	1324		174
TEREPHTHALONITRILE, 2,5-DIMETHYL-,	10	8					2						50			1	3	16387	25355	5124		408
TEREPHTHALONITRILE, 2,6-DIMETHYL-,	10	8					2						50			1	3	16395	32554	7076	18087	409
M-TOLUNITRILE	8	7					1						50			1	3	2886	8268	819	168	124
O-TOLUNITRILE	8	7					1						50			1	3	2898	8271	829	174	128
P-TOLUNITRILE	8	7					1						50			1	3	2887	8269	820	169	125
ACETONITRILE, 2-/P-AMINOPHENYL/-,	8	8					2						50	64		2	3	18156	18365	5763	4984	458
5-PYRIMIDINECARBONITRILE, 4-AMINO-2-METHYL-,	6	6					4						50	64	66	3	5	18138	8811	5749	2008	454
5-PYRIMIDINECARBONITRILE, 4-AMINO-2-TRIFLUOROMETHYL-,	6	3			3		4						50	64	66	4	5	15261	25133	4543		371
PROPIONITRILE, 3-/O-CHLOROANILINO/-,	9	9		1			2						50	65	83	3	3	6458	15606	1793	6929	230
ACETONITRILE, 3,4-DIMETHOXYPHENYL-,	10	11					1	2					50	72		2	3	431	24514	160	10267	27
ACETONITRILE, /M-METHOXYPHENYL/-,	9	9					1	1					50	72		2	3	861		262	1401	48
ACETONITRILE, P-METHOXYPHENYL-,	9	9					1	1					50	72		2	3	18504	33900	5928	4141	484
P-ANISONITRILE	8	7					1	1					50	72		2	3	14300	24443	4049	18774	350
HOMOVERATRONITRILE	10	11					1	2					50	72		2	3	431	24514	160	10267	27
P-TOLUNITRILE, A,APR-OXYDI-,	16	12					2	1					50	72		2	3	4814	28337	1344		176
BENZONITRILE, P-CHLORO-,	7	4		1			1						50	83		2	3	2893	349	826	10806	127
BENZONITRILE, P-CHLORO-,	7	4		1			1						50	83		2	3	2893	349	826	V 483	127

NAME | C | H | Br | Cl | F | I | N | O | P | S | Si | M | FUNCTIONALITY | PRISM | GRATING | U.V. | N.M.R. | FLUOR.

NAME	C	H	Br	Cl	F	I	N	O	P	S	Si	M	FUNCTIONALITY					PRISM	GRATING	U.V.	N.M.R.	FLUOR.
52 KETONES																						
BENZANTHRENONE	17	10						1					52			1	3	11260	18916	3071		301
BENZANTHRONE	17	10						1					52			1	3	11260	18916	3071		301
7H-BENZ/DE/ANTHRACEN-7-ONE	17	10						1					52			1	3	11260	18916	3071		301
9-FLUORENONE	13	8						1					52			1	3	7390	28034	2095	287	261
PENTACENEQUINONE, 6,13-,	22	12						2					52			1	3	6875	29262	6981		249
2-ACETONAPHTHONE, 1-HYDROXY-,	12	10						2					52	59		2	3	7525	15630	2109	11263	262
ALIZARIN	14	8						4					52	59		2	3	15308	635	4570		380
ANTHRAQUINONE, 1,2-DIHYDROXY-,	14	8						4					52	59		2	3	15308	635	4570		380
ANTHRAQUINONE, 1,8-DIHYDROXY-,	14	8						4					52	59		2	3	14902	18454	4318		185
ANTHRAQUINONE, 1,8-DIHYDROXY-,	14	8						4					52	59		2	3	5420	18454	4318		185
ANTHRONE, 1,8-DIHYDROXY-,	14	10						3					52	59		2	3	3552		1096		149
CHRYSAZIN	14	8						4					52	59		2	3	5420	18454	4318		185
CHRYSAZIN K	14	8						4					52	59		2	3	14902	18454	4318		185
2-PROPANONE, /3-HYDROXY-4-BIPHENYLYL/-,	15	14						2					52	59		2	3	16930	25550	5332		422
ANTHRAQUINONE, 1-AMINO-4-HYDROXY-,	14	9					1	3					52	59	64	3	3	5769	21068	1610		200
XANTHEN-9-ONE, 2-/2,3-DIBROMO-PROPYL/-1-HYDROXY-,	16	12	2					3					52	59	72	4	5	18297	25897	5816		465
P-BENZOQUINONE, CMPD WITH HYDROQUINONE	12	10						4					52	59	88	3	3	5976	511	1682	17094	211
HYDROQUINONE, CMPD WITH P-BENZOQUINONE	12	10						4					52	59	88	3	3	5976	511	1682	17094	211
QUINHYDRONE	12	10						4					52	59	88	3	3	5976	511	1682	17094	211
ACETOPHENONE, 3PR-AMINO-,	8	9					1	1					52	64		2	3	1843	28247	518	119	102
ACETOPHENONE, 4PR-AMINO-,	8	9					1	1					52	64		2	3	5111	8370	1387	242	178
ANTHRAQUINONE, 1,4-DIAMINO-,	14	10					2	2					52	64		2	3	14895	24474	4314		360
ANTHRAQUINONE, 1,5-DIAMINO-,	14	10					2	2					52	64		2	3	2983	8283	858		131
PROPIOPHENONE, 4PR-AMINO-,	9	11					1	1					52	64		2	3	5775	28809	1616	10449	201
ANTHRAQUINONE, 1-AMINO-,	14	9					1	2					52	64	73	3	3	13893	8629	3787		328
ANTHRAQUINONE, 2-AMINO-,	14	9					1	2					52	64	73	3	3	13894	8630	3788		329
ANTHRAQUINONE, 1-AMINO-5-CHLORO-,	14	8		1			1	2					52	64	83	3	3	18149	25862	5758		456
ANTHRAQUINONE, 1-METHYLAMINO-,	15	11					1	2					52	65		2	3	18319	10108	5830	4221	466
9-ACRIDANONE	13	9					1	1					52	65		2	5	7560				265
9-ACRIDANONE	13	9					1	1					52	65		2	5	7560	33059	2117		263
9-ACRIDANONE	13	9					1	1					52	65		2	5	7560	33059	2117		264
ACRIDINONE, 9/10H/-,	13	9					1	1					52	65		2	5	7560				265
ACRIDINONE, 9/10H/-,	13	9					1	1					52	65		2	5	7560	33059	2117		264
ACRIDINONE, 9/10H/-,	13	9					1	1					52	65		2	5	7560	33059	2117		263
7,8-BENZOFLAVONE, 5,6-DIHYDRO-,	19	14						2					52	72	73	3	5	13730	18629	3656		327
4H-NAPHTHO/1,2-B/PYRAN-4-ONE, 5,6-DIHYDRO-2-PHENYL-,	19	14						2					52	72	73	3	5	13730	18629	3656		327
54 KETONE HYDRAZONES AND DERIVATIVES																						
KETONE, METHYL 3-PHENANTHRYL, PHENYLHYDRAZONE	22	18					2						54			1	3	13101	18602	3405		319

NAME	C	H	Br	Cl	F	I	N	O	P	S	Si	M	FUNCTIONALITY					PRISM	GRATING	U.V.	N.M.R.	FLUOR.
56 PRIMARY ALCOHOLS AND THEIR METAL SALTS																						
4-HEXEN-1-OL, 2-/P-BIPHENYLYL/-,	18	20						1					56			1	3	16289	25321	5067		4C4
BENZYL ALCOHOL, O-HYDROXY-,	7	8						2					56	59		2	3	4572	28023	1263	14698	166
SALICYL ALCOHOL	7	8						2					56	59		2	3	4572	28023	1263	14698	166
SALIGENIN	7	8						2					56	59		2	3	4572	28023	1263	14698	166
8-QUINOLINOL, 5-/HYDROXYMETHYL/-2-METHYL-,	11	11					1	2					56	59	66	3	5	16907	25536	5311		421
CONIFERYL ALCOHOL	10	12						3					56	59	72	3	3	5948		1674		21C
2-PROPEN-1-OL, 3-/4-HYDROXY-3-METHOXY/PHENYL-,	10	12						3					56	59	72	3	3	5948		1674		21C
ETHANOL, 2-ANILINO-,	8	11					1	1					56	65		2	3	8636	29800	2252	295	275
1-PROPANOL, 3-/O-TOLUINO/-,	10	15					1	1					56	65		2	3	11316		3084		303
4-INDOLEMETHANOL	9	9					1	1					56	65		2	5	14269	24439	4027		349
ETHANOL, 2,2PR-/PHENYLIMINO/DI-,	10	15					1	2					56	66		2	3	750	10843	1670	9777	8
ETHANOL, 2,2PR-/PHENYLIMINO/DI-,	10	15					1	2					56	66		2	3	750	10843	1670	8133	8
ETHANOL, 2,2PR-/PHENYLIMINO/DI-,	10	15					1	2					56	66		2	3	5923	10843	1670	9777	8
ETHANOL, 2,2PR-/PHENYLIMINO/DI-,	10	15					1	2					56	66		2	3	5923	10843	1670	8133	8
ETHANOL, 2,2PR-/PHENYLIMINO/DI-, F	10	15					1	2					56	66		2	3	135	10843	1670	9777	8
ETHANOL, 2,2PR-/PHENYLIMINO/DI-, F	10	15					1	2					56	66		2	3	135	10843	1670	8133	8
ANISYL ALCOHOL	8	10						2					56	72		2	3	6349	8462	1750	3194	222
BENZYL ALCOHOL, 3,4-DIMETHOXY-,	9	12						3					56	72		2	3	7171	15620	2027	6930	255
BENZYL ALCOHOL, P-METHOXY-,	8	10						2					56	72		2	3	6349	8462	1750	3194	222
ETHANOL, 2-/P-SEC-BUTYLPHENOXY/-,	12	18						2					56	72		2	3	249	15024	100	6663	17
ETHANOL, 2-/P-TERT-BUTYLPHENOXY/-,	12	18						2					56	72		2	3	259	15026	104	6664	19
ETHANOL, 2-PHENOXY-,	8	10						2					56	72		2	3	248	84	99	10211	16
ETHANOL, 2-PHENOXY-,	8	10						2					56	72		2	3	248	84	99	V 506	16
VERATRYL ALCOHOL	9	12						3					56	72		2	3	7171	15620	2027	6930	255
57 SECONDARY ALCOHOLS AND THEIR METAL SALTS																						
BENZYL ALCOHOL, M-AMINO-A-METHYL-,K	8	11					1	1					57	64		2	3	17221		5440	3280	229
BENZYL ALCOHOL, M-AMINO-A-METHYL-,	8	11					1	1					57	64		2	3	6453	8470	1790	3280	229
BENZYL ALCOHOL, M-AMINO-A-METHYL-,	8	11					1	1					57	64		2	3	6452	8470	1790	3280	229
QUINIDINE, TRIHYDRATE	20	24					2	2					57	66	72	4	5	5993	18113	1686	16545	213
QUININE, TRIHYDRATE	20	24					2	2					57	66	72	4	5	5993	18113	1686	16545	213
4-QUINOLINEMETHANOL, 6-METHOXY-A-/5-VINYL-2-QUINUCLIDINYL/-, TRIHYDRATE	20	24					2	2					57	66	72	4	5	5993	18113	1686	16545	213

NAME | C | H | Br | Cl | F | I | N | O | P | S | Si | M | FUNCTIONALITY | PRISM | GRATING | U.V. | N.M.R. | FLUOR.

NAME	C	H	Br	Cl	F	I	N	O	P	S	Si	M	FUNCTIONALITY					PRISM	GRATING	U.V.	N.M.R.	FLUOR
59 PHENOLS AND THEIR METAL SALTS																						
ANTHRATRIOL, 1,2,10-,	14	10						3					59			1	3	18451	25927	5899		480
BENZENE, O-DIHYDROXY-,	6	6						2					59			1	3	268	29687	108	17034	21
BENZENE, O-DIHYDROXY-,	6	6						2					59			1	3	268	29687	108	V 124	21
BENZENE, P-DIHYDROXY-,	6	6						2					59			1	3	153	47	60	10350	10
BENZENE, P-DIHYDROXY-,	6	6						2					59			1	3	13206	47	60	10350	10
P-BENZENEDIOL	6	6						2					59			1	3	13206	47	60	10350	10
P-BENZENEDIOL	6	6						2					59			1	3	153	47	60	10350	10
BENZENETRIOL, 1,2,3-,	6	6						3					59			1	3	8766	8542	2278	3225	278
BIPHENOL, O,O*-,	12	10						2					59			1	3	1154	15118	343	6529	70
BIPHENOL, P,P*-, 2,2*-DI-TERT-BUTYL-6,6*-DIMETHYL-,	22	30						2					59			1	3	13941	15765	3812	7945	337
BIPHENYLDIOL, 2,2*-,	12	10						2					59			1	3	1154	15118	343	6529	70
BISPHENOL A	15	16						2					59			1	3	1070	216	325	18669	64
CARBOLIC ACID	6	6						1					59			1	3	843	165	258	3152	47
CARVACROL	10	14						1					59			1	3	2470	325	653	684	113
M-CRESOL, 6-TERT-BUTYL-,	11	16						1					59			1	3	257	89	103	525	18
M-CRESOL, 4,5-DIAMYL-,	17	28						1					59			1	3	1230		367		77
M-CRESOL, 4,6-DI-TERT-BUTYL-,	15	24						1					59			1	3	262	4896	106	10197	20
M-CRESOL, 5-ETHYL-,	9	12						1					59			1	3	8805	8128	2282	3226	68
M-CRESOL, 5-ETHYL-,	9	12						1					59			1	3	1147	8128	2282	3226	68
M-CRESOL, 6-ISOPROPYL-,	10	14						1					59			1	3	1916	286	531	V 270	103
M-CRESOL, 6-ISOPROPYL-,	10	14						1					59			1	3	1916	286	531	14605	103
O-CRESOL, 6-ALLYL-,	10	12						1					59			1	3	18129	32462	5744	18405	452
O-CRESOL, 4,4*-BIS/6-TERT-BUTYL-,	22	30						2					59			1	3	13941	15765	3812	7945	337
O-CRESOL, 4-TERT-BUTYL-,	11	16						1					59			1	3	1061	8118	322	527	63
O-CRESOL, 6-TERT-BUTYL-,	11	16						1					59			1	3	1234	8131	370	673	79
O-CRESOL, 5,5PR-ETHYNYLENEDI-,	16	14						2					59			1	3	15022	25085	4400		365
P-CRESOL	7	8						1					59			1	3	33	8005	15	9491	3
P-CRESOL, 2-ALLYL-,	10	12						1					59			1	3	18143	8815	5754	13082	455
P-CRESOL, 2,6-DI-TERT-BUTYL-,	15	24						1					59			1	3	540	18002	9777	526	38
P-CRESOL, 2,6-DI-TERT-BUTYL-,	15	24						1					59			1	3	283	18002	9777	526	22
P-CRESOL, 2-/A-METHYLBENZYL/-,	15	16						1					59			1	3	1231	15121	368	6616	78
P-CRESOL, 2-/1,1,3,3-TETRAMETHYL-BUTYL/-,	15	24						1					59			1	3	545	15057	191	6460	39
P-CUMENOL	9	12						1					59			1	3	1073	15303	326	6685	65
2-P-CYMENOL	10	14						1					59			1	3	2470	325	653	684	113
3-P-CYMENOL	10	14						1					59			1	3	1916	286	531	14605	103
3-P-CYMENOL	10	14						1					59			1	3	1916	286	531	V 270	103
DURENOL	10	14						1					59			1	3	486	15165	172	6015	31
HEMIMELLITENOL	9	12						1					59			1	3	296		116	6013	24
HYDROQUINOL	6	6						2					59			1	3	153	47	60	10350	10
HYDROQUINOL	6	6						2					59			1	3	13206	47	60	10350	10
HYDROQUINONE	6	6						2					59			1	3	13206	47	60	10350	10
HYDROQUINONE	6	6						2					59			1	3	153	47	60	10350	10
HYDROQUINONE, 2,5-DI-TERT-PENTYL-,	16	26						2					59			1	3	3230	15442	957	6922	141
HYDROQUINONE, METHYL-,	7	8						2					59			1	3	707	18404	232	9249	40
ISOPSEUDOCUMENOL	9	12						1					59			1	3	1382	18410	406	8659	86
MESITOL	9	12						1					59			1	3	295	8029	115	8657	23
1,3-NAPHTHALENEDIOL	10	8						2					59			1	3	6360	519	1752		224
1,3-NAPHTHALENEDIOL	10	8						2					59			1	3	6360	519	1752	6835	223
1,6-NAPHTHALENEDIOL	10	8						2					59			1	3	994	15293	301	6943	57
2,3-NAPHTHALENEDIOL	10	8						2					59			1	3	6759	8486	1889	3207	244
1-NAPHTHOL	10	8						1					59			1	3	7204	8004	2045	5	2
1-NAPHTHOL	10	8						1					59			1	3	30	8004	2045	5	2
2-NAPHTHOL	10	8						1					59			1	3	18	8001	2551	3230	1
2-NAPHTHOL K	10	8						1					59			1	3	9639	8001	2551	3230	1
PHENOL	6	6						1					59			1	3	843	165	258	3152	47
PHENOL, 2-ALLYL-3,5,6-TRIMETHYL-,	12	16						1					59			1	3	18359	24679	5848		470
PHENOL, 2,4-BIS/1-METHYLBUTYL/-,	16	26						1					59			1	3	984	198	299		56
PHENOL, M-BUTYL-,	10	14						1					59			1	3	16264	25310	5046	12311	401
PHENOL, P-TERT-BUTYL-,	10	14						1					59			1	3	522	133	179	47	34
PHENOL, P-TERT-BUTYL-,	10	14						1					59			1	3	8111	133	179	47	34
PHENOL, P-TERT-BUTYL-,	10	14						1					59			1	3	8111	133	179	J 132	34
PHENOL, 2-TERT-BUTYL-6-ISOPROPYL-,	13	20						1					59			1	3	1016	15105	310	6615	61
PHENOL, O-CYCLOHEXYL-,	12	16						1					59			1	3	17169	21389	5417	8595	427
PHENOL, 4,4PR-CYCLOPENTYLIDENEDI-,	17	18						2					59			1	3	18433	25923	5885		478
PHENOL, 2,2PP-DI-,	12	10						2					59			1	3	1154	15118	343	6529	70
PHENOL, 2,6-DIISOPROPYL-,	12	18						1					59			1	3	11625	18580	3227	6439	308
PHENOL, 2,6-DIISOPROPYL-,	12	18						1					59			1	3	11625	18580	3227		309
PHENOL, 3,5-DIMETHYL-,	8	10						1					59			1	3	8080	15646	349	83	73
PHENOL, 3,5-DIMETHYL-,	8	10						1					59			1	3	1183	15646	349	83	73
PHENOL, P-ISOPROPYL-,	9	12						1					59			1	3	1073	15303	326	6685	65
PHENOL, 4,4PP-ISOPROPYLIDENEDI-,	15	16						2					59			1	3	1070	216	325	18669	64
PHENOL, P-/1-METHYLBUTYL/-,	11	16						1					59			1	3	6554	32045	1819		237
PHENOL, M-PHENYL-,	12	10						1					59			1	3	5832	28813	1629	262	205
PHENOL, O-PHENYL- K	12	10						1					59			1	3	1192	15309	341	6528	67
PHENOL, O-PHENYL- S	12	10						1					59			1	3	1146	15309	341	6528	67
PHENOL, 2,3,5,6-TETRAMETHYL-,	10	14						1					59			1	3	486	15165	172	6015	31

NAME	C	H	Br	Cl	F	I	N	O	P	S	Si	M	FUNCTIONALITY				PRISM	GRATING	U.V.	N.M.R.	FLUOR.
59 PHENOLS AND THEIR METAL SALTS																					
PHENOL, P-/1,1,3,3-TETRAMETHYL-BUTYL/-,	14	22						1					59			1 3	4459	28654	1242	10681	164
PHENOL, P-/1,1,3,3-TETRAMETHYL-BUTYL/-,	14	22						1					59			1 3	4459	28654	1242	V 315	164
PHENOL, 2,3,5-TRIMETHYL-,	9	12						1					59			1 3	1382	18410	406	8659	86
PHENOL, 2,4,6-TRIMETHYL-,	9	12						1					59			1 3	295	8029	115	8657	23
PHENOL, 3,4,5-TRIMETHYL-,	9	12						1					59			1 3	296		116	6013	24
PYROCATECHOL	6	6						2					59			1 3	268	29687	108	17034	21
PYROCATECHOL	6	6						2					59			1 3	268	29687	108	V 124	21
PYROCATECHOL, 4-TERT-BUTYL-,	10	14						2					59			1 3	3060	8287	889	3169	138
PYROGALLOL	6	6						3					59			1 3	8766	8542	2278	3225	278
QUINOL	6	6						2					59			1 3	13206	47	60	10350	10
QUINOL	6	6						2					59			1 3	153	47	60	10350	10
RESORCINOL, 4-HEXYL-,	12	18						2					59			1 3	8339	10856	2223	3219	269
THYMOL	10	14						1					59			1 3	1916	286	531	14605	103
THYMOL	10	14						1					59			1 3	1916	286	531	V 270	103
P-TOLUHYDROQUINONE	7	8						2					59			1 3	707	18404	232	9249	40
2,4-XYLENOL	8	10						1					59			1 3	521	15054	178	6016	33
2,4-XYLENOL, 6-TERT-BUTYL-,	12	18						1					59			1 3	537	135	189	307	37
3,4-XYLENOL	8	10						1					59			1 3	3819	393	1162	193	74
3,4-XYLENOL	8	10						1					59			1 3	1184	393	1162	193	74
3,5-XYLENOL	8	10						1					59			1 3	1183	15646	349	83	73
3,5-XYLENOL	8	10						1					59			1 3	8080	15646	349	83	73
ANTHRADIOL, 1,4-DIAMINO-9,10-,	14	12					2	2					59	64		2 3	15434	32550	4615		387
2-NAPHTHOL, 8-AMINO-,	10	9					1	1					59	64		2 3	5441	8394	1494		190
PHENOL, O-AMINO-,	6	7					1	1					59	64		2 3	6764	21112	1894	1176	245
PHENOL, P-AMINO-,	6	7					1	1					59	64		2 3	712	158	236	717	43
2-PYRIDINOL, 6-AMINO-,	5	6					2	1					59	64	66	3 5	18413	10140	7599	2025	476
PHENOL, P-ANILINO-,	12	11					1	1					59	65		2 3	16035	33886	4944		397
P-CRESOL, 3-/DIMETHYLAMINO/-,	9	13					1	1					59	66		2 3	13932	15764	3808	6165	336
PHENOL, M-DIMETHYLAMINO-,	8	11					1	1					59	66		2 3	5444	29748	1496	255	192
O-TOLUIDINE, N,N-DIMETHYL-5-HYDROXY-,	9	13					1	1					59	66		2 3	13932	15764	3808	6165	336
CARBOSTYRIL	9	7					1	1					59	66		2 5	13899	21325	3792	6891	332
CARBOSTYRIL, 4-METHYL-,	10	9					1	1					59	66		2 5	8342	18221	2224	18384	270
3-PYRIDINOL	5	5					1	1					59	66		2 5	17490	32455	5554	9092	446
3-PYRIDINOL	5	5					1	1					59	66		2 5	17490	32455	5554	V 428	446
2-QUINOLINOL	9	7					1	1					59	66		2 5	13899	21325	3792	6891	332
2-QUINOXALINOL, 3-ISOBUTYL-,	12	14					2	1					59	66		2 5	6884	18487	1924		252
2-QUINOXALINOL, 3-ISOBUTYL-,	12	14					2	1					59	66		2 5	6884	18487	1924	11018	251
2-QUINOXALINOL, 3-ISOPROPYL-,	11	12					2	1					59	66		2 5	6885	18142	1925		253
2-QUINOXALINOL, 3-PROPYL-,	11	12					2	1					59	66		2 5	6883	18141	1923		250
THIENO/3,2-C/QUINOLIN-6-OL, 2,3-DIHYDRO-4-METHYL-,	12	11					1	1		1			59	66	75	3 5	16622	25430	7097		415
PHENOL, P-AMINO-, HYDROCHLORIDE	6	7					1	1					59	67		2 3	15635	643	4692	5096	391
PHENOL, P-AMINO-, SULFATE	6	7					1	1					59	67		2 3	5443	8395	1495		191
PHENOL, P-/2-AMINOETHYL/-, HYDROCHLORIDE	8	11					1	1					59	67		2 3	10274	8571	2779	3239	295
PHENOL, 2,4-DIAMINO-, DIHYDROCHLORIDE	6	8					2	1					59	67		2 3	6766	8488	1896		247
TYRAMINE, HYDROCHLORIDE	8	11					1	1					59	67		2 3	10274	8571	2779	3239	295
PHENOL, P-/METHYLAMINO/-, SULFATE /SALT/ /2TO1/	7	9					1	1					59	68		2 3	8426	29287	2235	12570	246
PHENOL, P-/METHYLAMINO/-, SULFATE /SALT/ /2TO1/	14	18					2	2					59	68		2 3	6765	8487	1895	3208	246
PHENOL, P-/METHYLAMINO/-, SULFATE /SALT/ /2TO1/	7	9					1	1					59	68		2 3	6765	8487	1895	3208	246
5-INDANOL, 6-/2-METHYL-1-PIPERIDYL-METHYL/-, HYDROCHLORIDE	16	23					1	1					59	69		2 5	16784	25496	7156		418
2-NAPHTHOL, 3-/1-PIPERIDYLMETHYL/-, HYDROCHLORIDE	16	19					1	1					59	69		2 5	16798	25503	7167		419
PIPERIDINE, 1-/5-ETHYL-2-HYDROXY-4-METHYLBENZYL/-, HYDROCHLORIDE	15	23					1	1					59	69		2 5	16770	25485	7147		417
PIPERIDINE, 1-/5-HYDROXY-6-INDANYL-METHYL/-2-METHYL-, HYDROCHLORIDE	16	23					1	1					59	69		2 5	16784	25496	7156		418
PIPERIDINE, 1-/2-HYDROXY-3-NAPHTHYLMETHYL/-, HYDROCHLORIDE	16	19					1	1					59	69		2 5	16798	25503	7167		419
2,5-XYLENOL, 4-ETHYL-A2-/1-PIPERIDYL/-, HYDROCHLORIDE	15	23					1	1					59	69		2 5	16770	25485	7147		417
GUAIACOL	7	8						2					59	72		2 3	90	8013	36	3149	7
PHENOL, P-BUTOXY-,	10	14						2					59	72		2 3	18720	33903	6030	2086	493
PHENOL, 2,6-DI-TERT-BUTYL-4-ETHOXY-,	16	26						2					59	72		2 3	525	15056	181	6458	35
PHENOL, 2,6-DI-TERT-BUTYL-4-METHOXY-,	15	24						2					59	72		2 3	526	15276	182	6459	36
PHENOL, M-ETHOXY-,	8	10						2					59	72		2 3	5980	29758	1683	267	212
PHENOL, O-ETHOXY-,	8	10						2					59	72		2 3	2889	29722	822	170	126
PHENOL, P-ETHOXY-,	8	10						2					59	72		2 3	85	24508	35	12	6
PHENOL, O-METHOXY-,	7	8						2					59	72		2 3	90	8013	36	3149	7