SADTLER
INFRARED PRISM
COLLECTION

1980
CUMULATIVE
SPEC—FINDER
INDEX

STANDARD
SPECTRA

INFRARED PRISM COLLECTION

1980 CUMULATIVE SPEC-FINDER® INDEX

STANDARD SPECTRA

Sadtler Research Laboratories

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 repre-
sented have come generally from other sources than our own laboratories and fre-
quently 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.

STANDARD INFRARED PRISM SPEC-FINDER®

The Prism Spec-Finder® is an index which contains data obtained by coding the band locations of all spectra in the Sadtler Standard Infrared Prism Collection. Each spectrum is coded first by the location of its major band, and then by the major band within each micron region. The data is systematically arranged by major band location. Spectral data for all compounds which have the same major band location are grouped together in this index. An unknown spectrum can be rapidly identified by coding its absorption bands in the same way and matching it against the Spec-Finder® data.

The spectral data is presented in a numerical format which is arranged systematically according to the location of its major band. In addition to the major band, each spectrum is also coded by the strongest band within each micron region from two (2 μ) to fourteen (14 μ) microns.

HOW TO USE THE SPEC-FINDER®

1.   **THE FIRST STEP** -- code the spectrum of the unknown. This is done by selecting in sequence the one strongest band occuring in each full micron region, proceeding from 2 to 14. The position of the one band selected in each full micron region is determined to the closest 1/10th of a micron. A band occuring on the line dividing two full micron regions is coded as a zero value of the higher valued region.

2.   **THE SECOND STEP** --

(a)   Each band selected as shown is entered to the closest 1/10th micron in the appropriate space on the Sadtler Coding Slip. Where no band occurs within a full micron region, this fact is indicated by entering a dash in the appropriate space on the Sadtler Coding Slip.

(b)   Where two or more bands of apparently equal intensity occur within any one full micron region, the alternates are usually indicated on the Sadtler Coding Slip. However, it is only necessary to indicate one, because the Spec-Finder® includes all possible codings of major 1/10th micron bands occuring in any of the full micron regions. Thus, one compound may have two or more entries in the Spec-Finder®.

(c)   Doubtful bands are also equally indicated on the Sadtler Coding Slip. Doubtful bands are those having about or somewhat more than 60% transmittance. It should be realized that Sadtler Standard Spectra are generally run with the strongest band between 20% and 0% transmittance, and rarely are there envelopes of the strongest bands. Under these circumstances, bands of more than 60% transmittance have generally not been coded for inclusion in the Spec-Finder®. In some cases where such bands are significant, bands of more than 60% transmittance have been coded. However, when a spectrum of an unknown is coded, allowance should be made for variations in technique which may cause more or fewer bands to appear significant than was the case when the Sadtler Standard Spectrum was coded for inclusion in the Spec-Finder®.

3.   **THE THIRD STEP** -- Select the one strongest band from the bands of the unknown which have been coded. This strongest band is the band which has the greatest intensity by maximum absorption. The position at which this strongest band occurs is recorded separately on the Sadtler Coding Slip, as the strongest band code number. The strongest band is coded using as a whole number the full micron region in which it is present and as a decimal number the 1/10th micron region at which the band occurs. This strongest band code is entered on the Sadtler Coding Slip in the upper right hand corner. Only one strongest band of any possible two or more apparently equally strong bands need be selected because the Spec-Finder® includes all possible strongest band codes of the reference spectra which might be selected as having the indicated strongest band.

4.   **THE FOURTH STEP** -- Match the code of the coded bands of the unknown to the codes of the reference spectra in the Spec-Finder®. First turn to the pages which list all reference spectra having a strongest band corresponding to the spectrum of the unknown. Next, match the code of the unknown numerically with the listed reference spectra proceeding across the page from the 5 full micron region to the 14 full micron region. Match the occurences of the bands by the 1/10th micron values as well as by the absence of absorption bands in the full micron regions. Bands occuring on the line dividing full micron regions have the value 0. Absence of bands in full micron regions are indicated by the dashes or by the absence of entries in appropriate full micron regions of the codes of the reference spectra in the Spec-Finder®.

5.   **THE FINAL STEP** -- Having found the index number (or numbers) of the closest matching reference data, compare the unknown with the reference spectra in the collection. The Prism Numerical Index will also give the chemical name of each reference located.

In the Spec-Finder®, all bands in each full micron region from 5 to 14 microns are arranged in increasing numerical sequence with dashes preceding 0's, which are followed by 1's, then 2's, etc. **IT IS IMPORTANT TO REMEMBER THAT ALL DASHES (5 - 14) AND BLANK SPACES (2 - 4) IN ANY COLUMN IN THE SPEC-FINDER® INDICATE NO BAND IN THAT MICRON REGION WITH MORE THAN 60% TRANSMITTANCE.**

The bands in the 3 and 4 micron regions are coded but not numerically indexed, due to mulls and hydrocarbon groupings which absorb in the 3 micron region, and due to the lack of any appreciable number of codifiable bands in the 4 micron region. Hence, in the interpretation of any spectra, bands occuring in either of the above regions should be disregarded unless these bands are the strongest in the entire spectrum.

It will also be observed that, within any one "strongest band" grouping of the Spec-Finder®, spectra having 2.7, 2.8, or 2.9 micron bands of 60% transmittance or less, are listed separately following those not having such bands. Since the presence of water in any sample could give a codifiable band in any one of the above three regions, it is well to compare the unknown with both locations in the Spec-Finder®.

It is well to remember that although the Spec-Finder® is highly mechanized, we must still use our training in locating a spectrum. One should look for a spectrum as coded in values of plus or minus 1/10th of a micron. That is, if the strongest band is coded 8.0, and cannot be found under that listing, one should look under 7.9 and 8.1 microns. The same procedure holds for the less intense bands.

Having found the number of the Sadtler Standard Spectrum in the Spec-Finder®, the unknown should be compared with the Sadtler Standard Spectrum to verify the identification or assist in showing variations or impurities. In the Sadtler Standard Spectra, we have endeavored to run the spectrum so that the strongest band shows a transmittance in the 20% - 0% range. Accordingly, for the best results when using the Spec-Finder®, we would suggest that the spectrum of any unknown should be run so that the transmittance of its strongest band will fall in this same range. It should be remembered, that by changing the thickness of the sample, the ratio of the various bands may change. Also, in preparing the Spec-Finder® we may or may not have included a band as codeable when the transmittance of the band was more than 60%. Finally, there may be a codeable impurity in the standard as well as in the unknown.

ii

The "Chemical Class" columns of the Spec-Finder® are included as an aid in characterizing the chemical nature of the unknown compound. Each code number corresponds to a different chemical functionality and may be used to eliminate certain references in comparing band locations if any chemical characteristics of the unknown are available. Chemical functionalities corresponding to code numbers are listed in the preface sections which follow.

The two examples on the following sheets illustrate the actual use of the Standard Spec-Finder®.

SADTLER STANDARD SPECTRA
SPEC FINDER 1980

2	3	4	5	6	7	8	9	10	11	12	13	14	STRONGEST BAND	CHEMICAL CLASS	INDEX NUMBER
0	4	-	8		5						9		5.8	46 73 2 1	31986
0	4	-	8		5		0						5.8	52 72 2 1	31775
0	4	-	8		5		0						5.8	52 72 2 1	31776
0	-	-	8		5		3	9	9			4	5.8	15 66 72 4 5	19008
0	4	-	8		5	0				8			5.8	6 1 3	29357
0	-	-	8		5	1							5.8	15 66 2 4	19299
0	1	-	8		5	2			9				5.8	15 73 2 5	34922
0	-	-	8		5	3					9		5.8	15 84 2 4	2172
0	1	-	8		5	3			9	1		1	5.8	15 73 2 5	37389
0	-	-	8		5	4			4		8		5.8	15 48 59 5 5	31552
0	4	-	8		5	4	0						5.8	52 72 2 1	31772
0	3	-	8		5	4	6					0	5.8	12 73 2 1	38695
0	-	-	8		5	8		2	4		2	5	5.8	15 48 72 4 5	31550
0	5	-	8		5	0		8					5.8	15 66 72 3 4	36922
0	4	-	8		5	1							5.8	52 72 2 1	31777
0	3	-	8		5	5	4	7	9				5.8	15 1 4	48086
0	2	-	8		5	5	6		9	1			5.8	15 66 2 4	31949
0	3	-	8		5	6				7			5.8	15 58 2 4	15661
0	4	-	8		5	7		7					5.8	12 1 1	14610
0	-	-	8		5	8	2	3			1	3	5.8	12 52 2 3	31572
0	-	-	8		6								5.8	15 66 2 5	10435
0	-	-	8		6								5.8	52 1 3	29236
0	-	-	8		6							1	5.8	15 71 2 5	44686
0	-	-	8		6							1	5.8	15 71 83 3 5	41043
0	-	-	8		6				2	9	9	1	5.8	15 71 72 3 5	41781
0	-	-	8		6			4					5.8	15 50 66 3 5	48379
0	4	-	8		6			4					5.8	15 66 2 5	41035
0	-	-	8		6			4			7		5.8	15 50 66 3 5	48389
0	-	-	8		6			5			8	0	5.8	15 65 66 3 5	48497
0	-	-	8		6			7		5			5.8	73 82 2 2	30862
0	8	5	8		6			7		5			5.8	73 82 2 2	30862
0	-	-	8		6		0	4	2	2		2	5.8	15 71 2 5	41041
0	3	-	8		6		0	4	7		2	2	5.8	6 73 2 1	29243
0	4	-	8		6	0		6					5.8	6 1 1	46433
0	4	-	8		6	0		6					5.8	6 1 2	31692
0	4	-	8		6	0	3	1					5.8	15 66 72 3 5	19006
0	0	-	8		6	1				9	7		5.8	12 65 73 4 5	41786
0	-	-	8		6	1	0				3	2	5.8	15 76 2 5	55529 ←
0	4	-	8		6	1	8	6			3		5.8	6 52 2 1	9618
0	1	-	8		6	2						2	5.8	15 50 2 5	50812
0	4	-	8		6	2					2	2	5.8	52 1 3	32396
0	0	-	8		6	3				9	7		5.8	12 65 73 4 5	41786
0	4	-	8		6	3		3			6		5.8	15 50 66 3 5	48380
0	4	-	8		6	3		6	2			8	5.8	6 75 2 1	52428 ←
0	3	-	8		6	3		6	3			9	5.8	6 83 2 2	22376
0	-	-	8		6	3	4	0	3	8			5.8	8 9 15 4 4	47362
0	-	-	8		6	4							5.8	15 84 2 4	7619
0	5	-	8		6	4		7	1	4	9	9	5.8	6 75 2 2	24539
0	-	-	8		6	5							5.8	15 48 73 4 5	31537
0	-	-	8		6	5						0	5.8	15 48 73 4 5	31536
0	1	-	8		6	5	5				9	2	5.8	15 59 71 4 5	41040
0	4	-	8		6	5	7	0					5.8	6 12 73 3 1	54817
0	4	-	8		6	6							5.8	15 75 2 4	46838
0	-	-	8		6	6					8	3	5.8	12 64 2 3	27519
0	1	-	8		6	6	4				7		5.8	15 1 4	21374
0	3	-	8		6	6	6			4	1		5.8	15 52 2 4	15286
0	2	-	8		6	7							5.8	12 15 66 4 4	50072
0	-	-	8		6	7	0			6	8		5.8	12 15 26 3 5	52172
0	4	-	8		6	7	4	4		4			5.8	52 1 1	17177
0	4	-	8		6	7	6						5.8	12 1 2	51388
0	4	-	8		6	7	7						5.8	12 52 2 2	50315
0	-	-	8		6	8						2	5.8	15 75 2 5	46834
0	-	-	8		6	9			2		0	1	5.8	15 71 83 3 5	41042
0	4	-	8		6	9		1			2	4	5.8	15 66 2 5	36918
0	-	-	8		6	9	2		2			0	5.8	15 71 83 3 5	42161
0	-	-	8		6	9	2		4		1	2	5.8	15 71 2 5	41044
0	-	-	8		7								5.8	15 73 2 4	52124
0	4	-	8		7								5.8	6 1 1	29292
0	4	-	8		7						3		5.8	6 50 2 3	41279
0	-	-	8		7						8		5.8	15 65 2 5	48521
0	-	-	8		7						8		5.8	15 66 2 5	10445
0	4	-	8		7			9	8				5.8	6 1 2	76
0	3	-	8		7	0							5.8	6 1 2	33049
0	4	-	8		7	1						1	5.8	6 52 73 3 1	28387
0	-	-	8		7	1						2	5.8	6 73 75 3 4	32398

SAMPLES OF CODING PROCEDURE
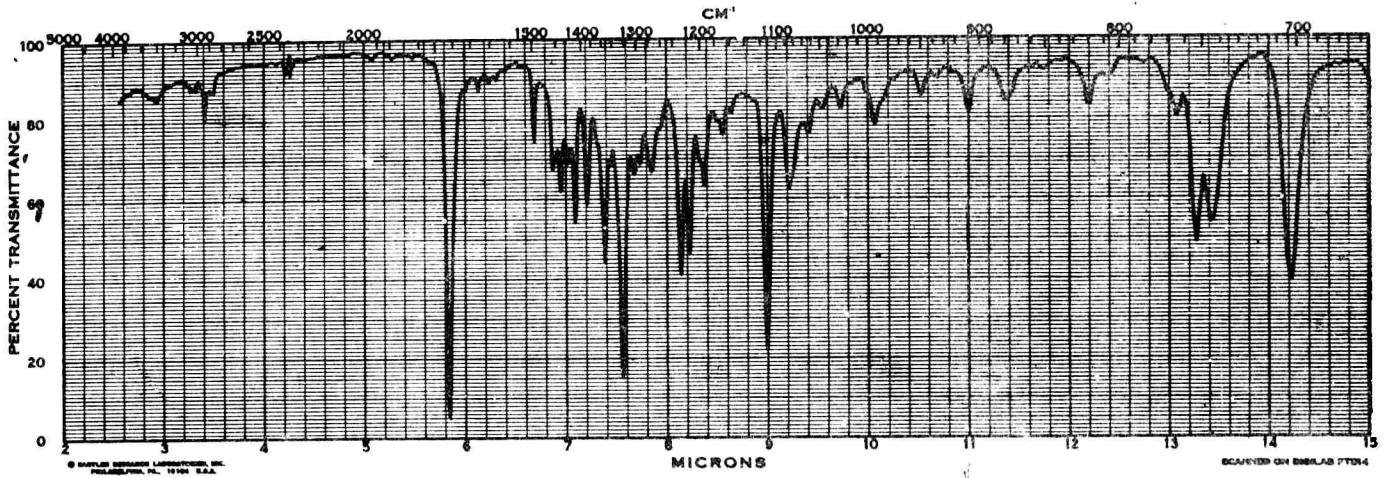
STANDARD PRISM SPEC-FINDER CODING SLIP
2 to 14 MICRON SEQUENCE

This coding matches
reference number
55529 opposite.
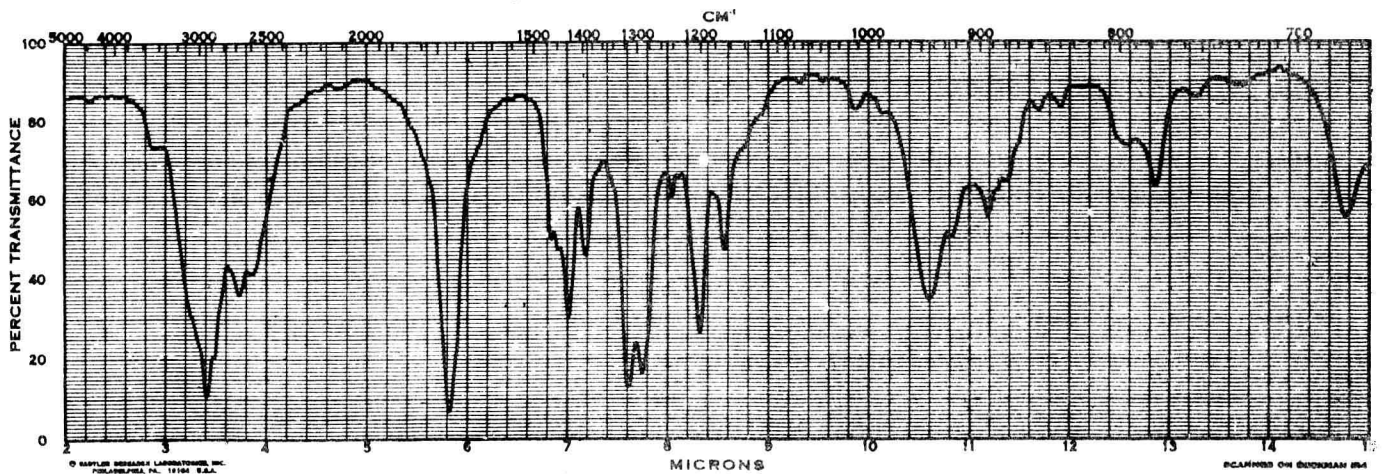
STANDARD PRISM SPEC-FINDER CODING SLIP
2 to 14 MICRON SEQUENCE

This coding matches
reference number
52428 opposite.

KEY TO THE CHEMICAL CLASS 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.

02. Oxonium and sulfonium compounds (and their selenium or tellurium analogs), except thiopseudourea compounds. Functions included in the anion of compounds having an organic cation are coded where possible.

03. Compounds with alkyl or aryl thiopseudourea. Functions included in the anion of compounds having an organic cation are coded where possible.

04. All other "ium" compounds other than those in groups 1,2, or 3, e.g., phosphonium, arsonium, etc. Functions included in the anion of compounds having an organic cation are coded where possible.

05. Peroxides, hydroperoxides, and ozonides. Epidioxides are also included in this new group inserted to conform to Chemical Abstracts practice. These substances were previously in group 78.

06. Carboxylic acids.

07. Carboxylic acid salts. Amine salts of carboxylic acids will be included in this group and also cross referenced under the appropriate amine salt classification, 67, 68, or 69. Aniline acetate is coded both 07 – – and 67 – –.

08. Thiocarboxylic acids and derivatives excluding esters, lactones, salts, and carbamates.

09. Esters, lactones, and salts of acids in group 8. Xanthates and trithiocarbonates are to be found in this group. Thiocarboxylic ortho acid esters are to be found in this group and in group 75, e.g. $(CH_3S)_3C-\underset{\underset{O}{\|}}{C}-NH_2$ would be coded 09 14 – and 14 75 –.

10. Carboxylic acid anhydrides. Heterogenous anhydrides, bear the codes of each of the anhydride types involved, e.g. $RC(=O)OSO_2R'$ 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.

$(CH_3O)_3C-\underset{\underset{O}{\|}}{C}-NH_2$ would be coded 12 14 – and 14 72 –.

13. Carbamic and carbazic acids and their derivatives, including thiocarbamates, the only restriction being that the nitrogen and the acid residue must not be coannular. Hydrosulfamines are in this group when of the form $H_2NSC(=S)NR_2$.

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.

17. Thiourea, pseudourea and their derivatives, other than those in group 03.

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 co-annularly with the acid residue.

19. Not assigned.

20. Lactones and lactides of carboxylic acids.

21. Not assigned.

22. Sulfonic, sulfinic, and sulfenic acids with carbon bound directly to sulfur, as in methanesulfonic acid. Compounds having carbon bonded to sulfur acids through oxygen are collected in group 29.

23. Salts of acids of group 22, e.g. sodium benzenesulfonate. Amine salts of inorganic acids, e.g., aniline sulfate will not be found in this group but salts such as aniline p-toluenesulfonate are coded both 23 – – and 67 – –.

24. Sulfonic, sulfinic, sulfenic acid halides, in which carbon is bound directly to sulfur. The identity of the halogen is specified by the appropriate code.

25. Esters of acids of group 22.

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 $H_2S=NH$ are also in this group.

27. Not assigned.

28. All other carbon substituted derivatives of sulfonic, sulfinic, and sulfenic acids.

29. Organic esters and salts of inorganic sulfur acids. Inorganic salts are in group 44 only.

30. Phosphonic and phosphinic acids with phosphorus bound directly to carbon. Includes sulfur analogs of oxygen-containing phosphorus acids. For example RPO_2H is to be found in this group but $ROPO_2H$ will be found in group 37.

31. Salts of acids of group 30. Includes sulfur analogs of oxygen-containing phosphorus acids.

32. Acid halides of group 30.

33. Esters of acids of group 30.

34. Derivatives of acids of group 30, analogous to the derivatives of carboxylic acids as indicated in group 18, however, both linear and cyclic, amides and imides are included.

35. All other derivatives of acids in group 30.

36. Organic derivatives of phosphine, phosphorane, phosphine oxide, and phosphine sulfide.

37. Organic esters and salts of inorganic phosphorus acids, including sulfur analogs of oxygen containing phosphorus acids. Inorganic salts are in group 44 only.

38. All other acids with carbon bound to the central atom of the acid function, such as benzene-boronic and methanearsonic acid, etc.

39. Organic salts and esters of acids in group 38, such as sodium benzenearonate, methyl benzene-boronate, and aniline benzeneboronate. The latter compound is coded 39 − − and 67 − −.

40. All other derivatives of acids in group 38.

41. Salts and esters of cyanic and isocyanic (fulminic) acids. Includes thio, telluro and seleno analogs.

42. Organic esters of inorganic acids such as propyl silicate, butyl nitrite, etc., excluding sulfur and phosphorus acids.

43. All other organic derivatives of inorganic acids (including sulfur and phosphorus acids), such as $RNHNHSO_3H$. Salts such as aniline hydrochloride are not cross referenced to the inorganic acid function.

44. All inorganic compounds such as $POCl_3$, P_2O_5, SO_3, etc. All compounds in this group are coded 44 only.

45. Not assigned.

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.

47. Aldehyde derivatives (except hydrazones) e.g., oximes, carbazones, and derivatives of the oximino function (RCH=NOR). Salts and metal derivatives of the oximino function are also included. Derivatives of the oximino function, and all other derivatives of group 46 must be linear.

48. Aldehyde hydrazones, alkyl or aryl substituted hydrazones and salts, linear only.

49. Not assigned.

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.

51. Not assigned.

viii

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.

55. Carbonyls: Substances in which carbon is multiply bound to oxygen, but excluding carboxylic acids and their derivatives, aldehydes, ketones, ketenes, and oxonium compounds. An example is $Ni(CO)_4$.

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 a-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 lactims and are found in group 15.

60. All other hydroxy compounds and their metal salts, e.g., hydroxy group attached to a hetero atom, as in R_2NOH, or R_3SiOH, or attached to the 2-position of 1,3-heteroatomic, nonaromatic compounds, as in m-dioxan-2-ol. Also in this group are carbonyl hydrates, such as chloral hydrate, carbocyclic and linear enols and heimiacetals.

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.

63. All thioalcohols analogous to the compounds illustrated in group 60, including Se and Te analogs.

64. Primary amines. The amine function need not be attached to carbon, e.g., 1-aminopiperidine.

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. Imines, if linear, are in group 71.

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.

67. Primary amine **salts, including** salts of both organic and inorganic acids. For polyaminic compounds, **salts are assumed to form** in the order 1º, 2º, 3º, and are coded accordingly. Salts of **organic acids are also** coded in group 7. Therefore, aniline acetate will be coded both 07 – – and 67 – –. **Amine salts** of inorganic acids are not cross referenced.

68. Secondary amine salts, in the manner as illustrated under group 67.

69. Tertiary amine salts, in the manner as illustrated under group 67.

70. Hydrazine and azido (triazo) 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 triazo group is cyclic it cannot be part of another ring system.

71. Imines, anils, and Schiff bases, linear only. The imine function cannot be part of a ring structure as this is considered an amine.

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.

74. Epoxy compounds, including S, Se, and Te analogs. See group 05 for epidoxy compounds; group 75 for epidithio compounds and analogs.

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.

78. Non-metallic oxides, such as amine oxides or nitrones, but excluding substances in groups 36 and 81.

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 benzeneazosulfonic 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 $C_6HI(O-\overset{\overset{O}{\|}}{C}-R)_2$ are coded 12 81 – –.

82. Fluorine compounds.

83. Chlorine compounds.

84. Bromine compounds.

85. Iodine compounds, excluding iodonium, iodoso, and iodoxy compounds.

86. Metallo-organic coordination compounds, including "ocenes". Any compound of this type is also grouped under M1, even though other function groups are present.

87. Other metallo-organic compounds such as tetraethyllead, phenylmercuric chloride, etc. N.B. Most all other functional groups take precedence, therefore, $C_6H_5H_gOH$ is coded 60 87 −. All compounds in this group are also coded M1.

88. Organic molecular complexes (urea complexes, hydrocarbon picrates, styphnates, etc.). This group is not cross-coded according to the non-hydrocarbon fragment of the molecule. Cross-referenced into this group are oxygen-ether dihalides, e.g., dioxane dibromide, coded both 72 84 88 and 88 − −.

89. Perchloryl compounds; those with the −ClO$_3$ group.

90-99. Not assigned.

Code to groups following 99

D1. Deuterated compounds, regardless of other functionality.

M1. Metallo-organic compounds, regardless of functionality. Number of functions and type are still noted as a further aid to subgrouping.

R1. Stable free radicals. No other function is coded for compounds of this group.

X1. Saturated hydrocarbons only.

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.

Y2. Boron compounds, with similar restrictions as imposed under Y1.

Y3. Pure carbohydrates.

Y4. Complex molecules containing carbohydrate fragments such as glycosides, as well as carbohydrate derivatives, e.g., osazones, osones, etc.

Y5. Steroids.

Y6. Antibiotics.

Y7. Sydnones.

Explanation of Column Four Under Functionality Heading

This column normally indicates the total number of different 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.
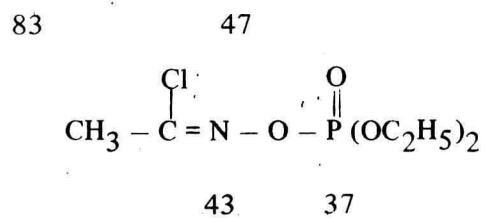
Explanation of Column Five Under Functionality Heading

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 (triazo) 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 techniciality, 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.

$$83 \qquad\qquad 47$$

$$CH_3 - \overset{\overset{\displaystyle Cl}{|}}{C} = N - O - \overset{\overset{\displaystyle O}{\|}}{P}(OC_2H_5)_2$$

$$43 \qquad\quad 37$$

Coding: 37 43 47 83

ALPHABETICAL INDEX OF CHEMICAL CLASS FUNCTIONAL GROUPS

The following is an alphabetical listing of many of the most commonly sought functions, with an indication of the groups in wich they will be found. Coding numbers within commas are to be considered as a unit, regardless of the number of digits. Two examples to illustrate the point:

A.   Amides, salts.   14, 15, 26, 34, 40

Compounds which are salts of amides will be found in each of these separate groups, depending entirely on the nature of the acid of which the amide has been formed.

B.   Acid halides, phosphorus, organic.   32 82, 32 83, 32 84, 32 85

All acid halides of organophosphorus acids, e.g., phenylphosphonyl dichloride, are in group 32, but the nature of the halogen must also be noted to obtain a complete and correct code.

The user of this system may assume, unless it is specifically stated to the contrary, that any function not listed is included with the most similar group which is listed. As an example, telluroxides and tellurones, not in the list to follow, would fall in 76, with selenoxides and selenones.

Acetals,   72
         Carbohydrate,   Y7 (cross-referenced)
         Hemi-,   60 72
Acetylenic Function,   77
Acetylenic Hydrocarbons,   77, X2
Acetylides,   87
Acid Anhydrides, Carboxylic,   08, 10
         Inorganic,   44
         Mixed, found with group bearing lower code number
         Phosphorus, organic,   35
         Sulfur, organic,   28
         Those not listed above,   40, 41, 43
Acid Halides, Carboxylic,   11 82, 11 83, 11 84, 11 85
         Inorganic,   44
         Phosphorus, organic,   32 82, 32 83, 32 84, 32 85
         Sulfur, organic,   24 82, 24 83, 24 84, 23 85
         Those not listed above,   40, 43
Acids,   Carboxylic,   06
         Aldehydic,   06 46
         Amidic,   06 14
         Amine salts,   07, 67, 68, 69
         Amino,   06 64, 06 65, 06 66
         Anhydrides,   10
         Anilic,   06 14
         Dithio-,   08