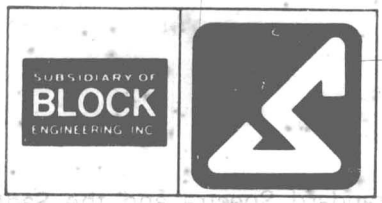
THE SADTLER STANDARD SPECTRA



SADTLER RESEARCH LABORATORIES, INC.

STANDARD GRATING SPEC-FINDER

CREATIVE CHEMISTS SINCE 1874

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SADTLER STANDARD GRATING SPECTRA SPEC-FINDER ®

The Sadtler Standard Grating Spectra Spec-Finder provides a method of rapidly locating standard reference spectra which have absorption peaks similar to an unknown spectrum. An unknown spectrum is compared with the reference spectra and the resulting information may show an exact match and therefore a positive identification of the unknown compound. Or, if an exact match is not obtained, useful pointers to the general chemical structure of the unknown compound will be found.

The Spec-Finder is created by coding the wave number location of the strongest band within each two hundred wave number interval from 3600 cm^{-1} to 2000 cm^{-1} and within each one hundred wave number interval from 2000 cm^{-1} to 400 cm^{-1}, then recording the wave number location of the strongest band in the whole spectrum. This coding procedure is performed for each spectrum in the collection of Standard Infrared Grating Spectra. The accuracy tolerance in the plotting of the band location is $\pm$ 15 cm^{-1}.

The code values for each spectrum are computer-sorted into increasing numerical sequence. Then, within a group of spectra which have the same strongest band value, the secondary sorting sequence is according to numerical ascendancy of the band codes across the 2000 cm^{-1} to 400 cm^{-1} wave number regions.

The printed page of the Spec-Finder shows the wave number value of the strongest band in the whole spectrum under the heading STRONGEST BAND. The locations of the strongest band in each interval across the spectrum are shown under the relevant heading in the WAVE NUMBER REGION.

The Sadtler chemical class codes for each compound are listed on each page to the right of the spectrum number. This information describes the chemical conformation of each compound located by the Spec-Finder method.

Note: Due to space limitations it has been necessary to abbreviate the entries in the WAVE NUMBER REGION; the abbreviations are explained as follows:

3600 cm^{-1} to 2200 cm^{-1} WAVE NUMBER REGION

A single digit in any of these columns, with a zero added represents the last two digits of the band location, e.g., a 5 in column 30 means that the strongest band is located at 3050 cm^{-1}.

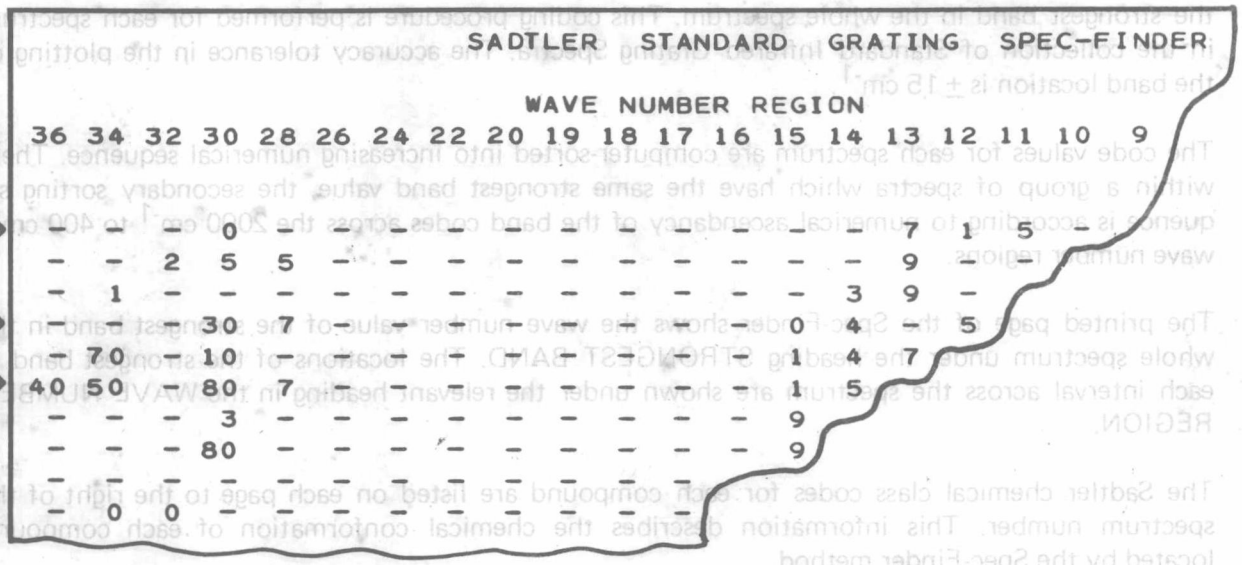
A two digit number in any of these columns represents the last two digits of a band location in the region which is one hundred less than the column heading, e.g., a 50 in column 30 means that the strongest band is located at 2950 cm^{-1}.

2000 cm^{-1} to 400 cm^{-1} WAVE NUMBER REGION

The single digit in any of these columns, with a zero added, represents the last two digits of the band location, e.g., a 7 in column 20 represents wave number 2070 cm^{-1}, a 3 in column 15 represents wave number 1530 cm^{-1}.

A dash in any column indicates the absence of any absorption band greater than 0.20 absorbance in that interval.

ILLUSTRATION OF ABBREVIATION CODES IN THE 3600 cm^{-1} TO 2200 cm^{-1} WAVE NUMBER REGION



This entry indicates a band at 3000 cm^{-1}.

This entry indicates bands at 2930 cm^{-1} and 2870 cm^{-1}.

This entry indicates bands at 3540 cm^{-1}, 3350 cm^{-1}, 2980 cm^{-1} and 2870 cm^{-1}.

HOW TO USE THE SPEC-FINDER

Step One: Code the spectrum of the unknown by selecting in sequence the one strongest band occuring in each 200 cm^{-1} region from 3600 cm^{-1} to 2000 cm^{-1} and in each 100 cm^{-1} region from 2000 cm^{-1} to 400 cm^{-1}. Signify the absence of a band in any interval by entering a dash in the relevant space on the coding slip. Remember to code the bands in the 3600 cm^{-1} to 2000 cm^{-1} according to the examples on page 1. The position of the band should be determined to the closest 10 wave numbers. Any bands having an absorbance of less than 0.20 should be ignored.

Step Two: Enter each band selected above in the appropriate space on the Sadtler Coding Slip. When no band occurs within any region, indicate this by entering a dash in the appropriate space on the coding slip.

Step Three: Select the strongest band from the bands of the unknown which have been coded; this is the band which has the greatest intensity by maximum absorption. Enter the strongest band value in the appropriate space on the coding slip.

Step Four: Match the values of the coded bands of the unknown to the values of the reference spectra in the Spec-Finder. First, turn to the pages which list all reference spectra having a strongest band the same as the spectrum of the unknown. Next, match the values of the unknown with the listed reference spectra proceeding across the page from the 2000 cm^{-1} to the 400 cm^{-1} intervals. Absence of bands in any interval is indicated by a dash in the Spec-Finder. When comparing codes allow a tolerance of $\pm$ 10 cm^{-1} in each case.

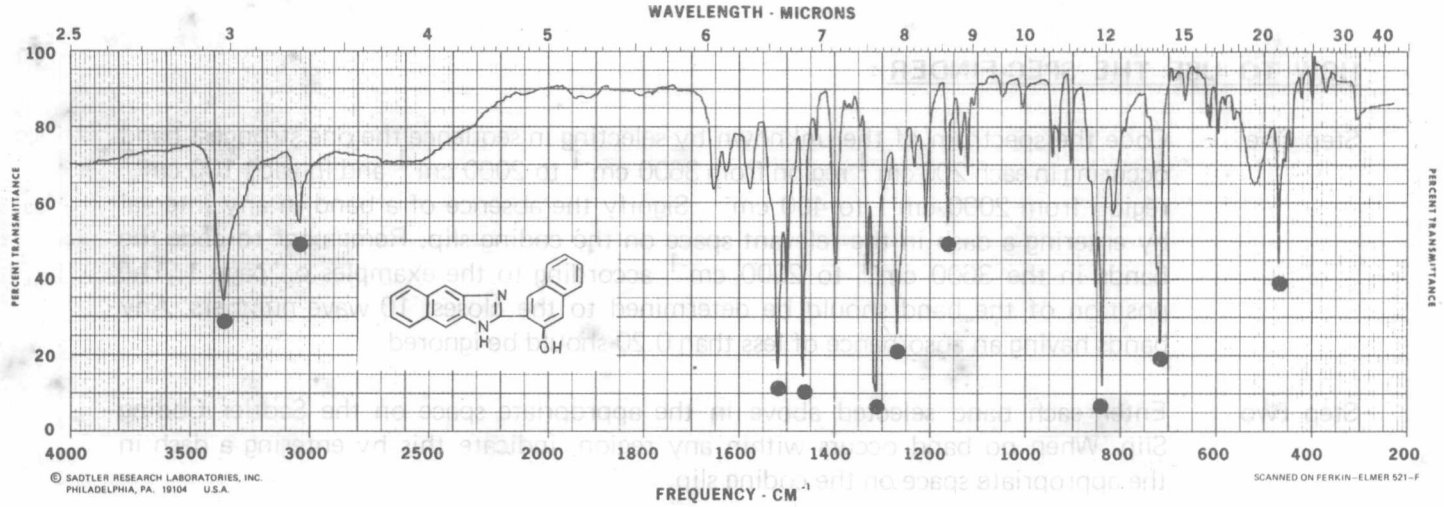
Step Five: Having found the spectra which match the coding of the unknown, check the codes under the CHEMICAL CLASS CODE which indicate the chemical conformation of the reference spectrum. This may enable some of the references to be eliminated if any chemical functionalities of the unknown are suspected. Then the remaining reference spectra numbers should be checked in the Numerical Index which gives the compound name or, better still, checked against the actual reference spectrum.

Notes

In summary, in order to avoid erroneous results, remember the following important parameters:

1. Do not code any band which has an absorbance of less than 0.20.
2. When coding any wavelength which has the first two digits 35, 33, 31, 29, 27, 25 or 23 follow the procedure shown in the example on page 1.
3. When comparing the codes of the unknown against the Spec-Finder codes allow a tolerance of $\pm$ 10 cm^{-1}.

Examples of coding and retrieval are shown on the following pages.



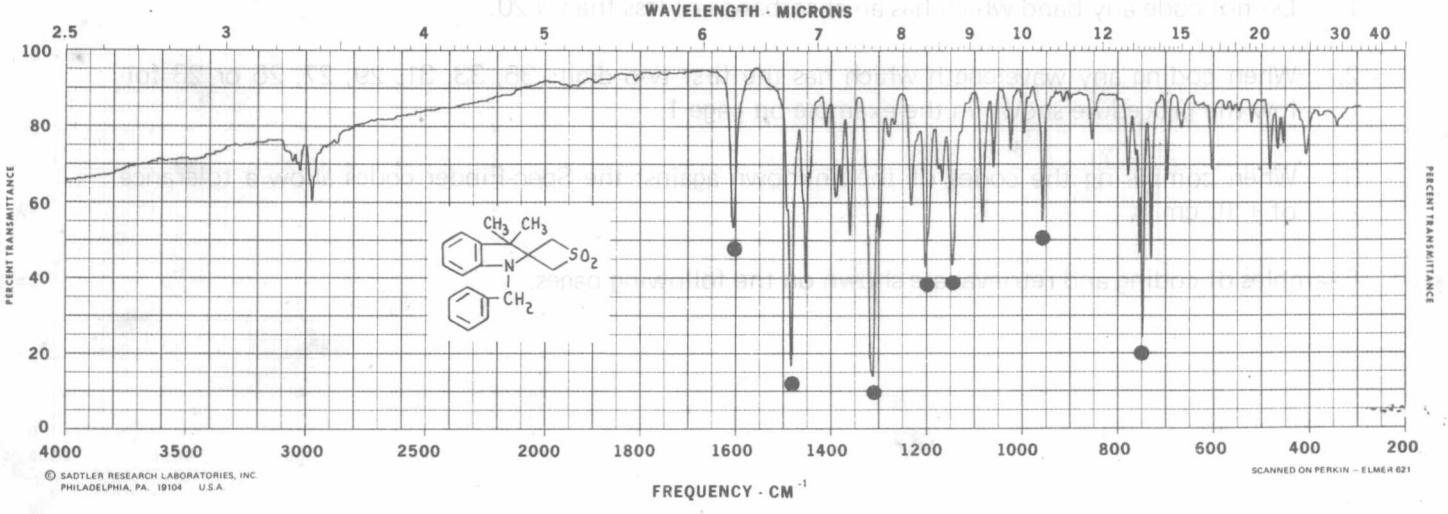
BANDS CODED: 3460 cm^{-1}, 3040 cm^{-1}, 1520 cm^{-1}, 1470 cm^{-1}, 1310 cm^{-1}, 1270 cm^{-1}, 1160 cm^{-1}, 840 cm^{-1}, 720 cm^{-1}, 470 cm^{-1}

STRONGEST BAND: 1310 cm^{-1}

BANDS CODED: 1600 cm^{-1}, 1480 cm^{-1}, 1310 cm^{-1}, 1200 cm^{-1}, 1150 cm^{-1}, 1080 cm^{-1}, 960 cm^{-1}, 750 cm^{-1}

[..... Compare this region against WAVE REGION NUMBER .....]

STRONGEST BAND: 1600 cm^{-1}



SADTLER STANDARD GRATING SPEC-FINDER

WAVE NUMBER REGION																										STRONGEST BAND	GRATING NUMBER	CHEMICAL CLASS CODE
40	38	36	34	32	30	28	26	24	22	20	19	18	17	16	15	14	13	12	11	10	9	8	7	6	5	4			
–	–	–	60	–	4	–	–	–	–	–	–	–	–	–	2	7	1	7	6	–	–	4	2	–	–	7	1310	22069 K	59 65 66 3 5
–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	3	6	1	4	5	–	3	8	6	7	–	–	1310	3275 K	59 80 83 3 3
–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	4	–	1	5	7	9	8	–	4	–	8	–	1310	21449 K	76 83 00 2 5
–	–	–	–	–	7	–	–	–	–	–	–	–	–	–	4	–	1	5	8	9	8	9	4	–	9	–	1310	21442 K	76 83 00 2 4
–	–	40	40	6	80	–	–	–	–	–	–	–	–	–	5	5	1	7	3	4	–	8	1	4	3	8	1310	22340 K	26 00 00 1 2
–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	6	3	1	2	–	3	–	–	6	–	–	–	1310	16558 K	Y7 72 00 1 5
–	–	–	10	1	1	0	8	3	–	–	–	–	–	–	6	6	1	0	–	4	–	–	–	–	–	–	1310	12411 K	63 64 66 4 5
–	–	–	–	–	9	–	–	–	–	–	–	–	–	–	6	9	1	4	8	6	8	–	5	–	–	–	1310	17446 K	08 09 00 2 5
–	–	–	–	–	8	–	–	–	–	–	–	–	–	–	7	5	1	6	0	4	–	5	3	6	–	9	1310	15595 K	24 80 83 3 3
–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	7	9	1	–	–	8	–	–	–	–	–	–	1310	7390 K	66 73 80 3 5
–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	7	9	1	5	0	–	3	9	4	–	–	–	1310	22462 K	66 80 84 3 3
–	–	–	–	80	–	–	–	–	–	–	–	–	–	–	8	1	1	2	3	1	–	–	7	1	–	–	1310	23467 K	22 52 59 6 5
–	–	–	–	8	–	–	–	–	–	–	–	–	–	–	8	6	1	6	5	1	–	4	–	0	–	–	1310	18115 K	59 84 00 2 3
–	–	–	–	–	–	–	60	6	–	–	–	–	–	–	9	4	1	4	4	9	–	9	6	–	8	–	1310	13898 K	26 69 73 3 5
–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	9	4	1	6	3	1	–	–	6	8	–	–	1310	15845 K	82 85 00 2 3
–	–	20	–	–	–	–	–	–	–	–	–	–	–	–	9	8	1	–	1	–	–	–	–	–	–	–	1310	5173 K	66 80 00 2 5
–	–	–	–	–	20	4	–	–	–	–	–	–	–	–	9	8	1	3	–	–	–	–	–	–	–	–	1310	9571 K	68 80 00 2 3
–	–	–	70	9	–	–	–	–	–	–	–	–	–	–	9	8	1	8	–	7	–	–	–	–	–	–	1310	23311 K	56 65 80 3 3
–	–	–	40	–	–	–	–	–	–	–	–	–	–	–	9	9	1	6	0	–	–	–	–	–	–	–	1310	875 K	47 48 80 3 3
–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	9	9	1	7	1	6	–	–	–	–	–	–	1310	5172 K	66 80 00 2 5
–	–	–	–	4	4	80	20	4	–	–	–	–	–	–	9	9	1	8	3	2	5	7	8	–	1	–	1310	13237 K	26 57 59 4 3
–	–	–	–	–	30	6	–	–	–	–	–	–	–	–	9	9	1	9	–	–	–	–	–	–	–	–	1310	9568 K	59 80 00 2 3
–	–	–	1	–	–	–	–	–	–	–	–	–	–	–	9	9	1	9	0	8	–	2	5	–	–	–	1310	21806 K	65 80 00 2 3
–	–	–	–	–	–	–	–	–	–	–	–	–	–	0	–	–	1	–	1	–	–	3	–	–	–	–	1310	23307 K	64 65 80 3 3
–	–	–	–	–	–	–	–	–	–	–	–	–	–	0	–	8	1	0	5	8	6	–	5	–	–	–	1310	23667 K	66 76 00 2 5
–	–	–	20	0	–	–	–	–	–	–	–	–	–	0	0	7	1	6	4	–	3	1	2	–	–	–	1310	19378 K	65 75 80 4 5
–	–	–	90	–	30	–	–	–	–	–	–	–	–	0	0	9	1	4	4	1	1	1	5	–	1	8	1310	11718 K	50 65 76 4 5
–	–	–	–	30	9	–	–	–	–	–	–	–	–	0	1	8	1	0	9	8	–	0	5	9	–	–	1310	14549 K	73 75 80 3 5
–	–	–	1	–	30	–	–	–	–	–	–	–	–	0	1	9	1	5	5	1	1	2	5	–	1	4	1310	11720 K	50 65 76 4 5
–	–	–	–	–	–	–	–	–	–	–	–	–	–	0	1	9	1	8	4	–	–	–	–	–	–	–	1310	19379 K	65 72 75 4 5
–	–	–	–	–	0	–	–	–	6	–	–	–	–	0	2	3	1	6	7	9	5	–	5	4	7	6	1310	22527 K	41 82 00 2 3
–	–	–	–	–	–	–	–	–	–	–	–	–	–	0	2	9	1	6	4	–	–	–	7	9	–	–	1310	9516 K	66 80 00 2 5
–	–	–	–	–	–	–	–	–	–	–	–	–	–	0	2	9	1	6	4	6	–	–	–	–	–	–	1310	5170 K	66 80 00 2 5
–	–	–	–	–	–	–	–	–	–	–	–	–	–	0	2	9	1	8	4	9	1	9	7	5	–	–	1310	16462 K	52 66 73 4 5
–	–	–	–	8	40	–	–	–	–	–	–	–	–	0	3	8	1	4	3	1	–	7	2	–	–	–	1310	25825 K	08 66 83 3 5
–	–	–	–	7	–	–	–	–	–	–	–	–	–	0	3	8	1	9	2	–	–	–	–	–	–	–	1310	4862 K	17 00 00 1 3
–	–	–	–	–	–	–	–	–	–	–	–	–	–	0	3	9	1	6	4	5	–	1	3	–	–	–	1310	21262 K	66 80 00 2 3
–	–	–	–	–	–	–	–	–	–	–	–	–	–	0	4	2	1	5	5	7	–	3	0	–	–	7	1310	10447 K	69 00 00 1 5

KEY TO THE FUNCTIONAL GROUP NOTATIONS

For graphic descriptions see table at end of index

01. Quaternary amines of any type, except in thiopseudourea. The function bearing the negative charge is not coded. Ordinary amine salts are not included.

02. Oxonium and sulfonium compounds. The function bearing the negative charge is not coded.

03. Quaternary amines in thiopseudourea groups. The function bearing the negative charge is not coded.

04. All other "ium" compounds other than those in groups 1, 2, or 3, e.g., phosphonium, arsonium, etc. The function bearing the negative charge is not coded.

05. Peroxides, hydroperoxides, and ozonides. Epidioxides are also included in this new group, inserted to conform to CA 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, e.g. Aniline acetate is coded both 07 – and 67 –.

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 found in this group and in group 75, e.g. $(CH_3S)_3C\text{-}C\text{-}NH_2$ would be coded 09 14 – and 14 75 --.

O

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. The identity of the halide is specified by the appropriate code (82, 83, 84 or 85).

12. Carboxylic acid esters including carbonates. Carboxylic ortho esters

O

are found in this group and in group 72, e.g. $(CH_3O)_3C\text{-}C\text{-}NH_2$ 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 (i.e. linear). Hydrosulfamines are in this group when of the form $H_2NSC(=S)NR_2$.

14. Carboxylic acid amides - linear. The nitrogen may be part of a ring structure (e.g. 1-benzoylpiperidine), but lactams or lactims are excluded.

15. Carboxylic acid amides - cyclic, 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 grouping.

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 coannularly with the acid residue.

19. Blank.

20. Lactones and lactides of carboxylic acids.

21. Blank.

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 (82, 83, 84 or 85).

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. Sulfur compounds analogous to phosphorus compounds in group 36.

28. All other carbon substituted derivatives of sulfonic, sulfinic, and sulfenic acids not previously specified.

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

30. Phosphonic and phosphinic acids and thio acids, with phosphorus bound directly to carbon. For example RPO_3H is to be found in this group but $ROPO_3H$ will be found in group 37.

31. Salts of acids of group 30.

32. Acid halides of group 30. The identity of the halide is specified by the appropriate code (82, 83, 84 or 85).

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 not previously specified.

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

37. Organic esters and salts of inorganic phosphorus acids and thio 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 benzeneboronic and methanearsonic acid, etc.

39. Organic salts and esters of acids in group 38, such as sodium benzenearsonate, methyl benzeneboronate, 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 and thio acids.

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. Blank.

46. Aldehydes and thio aldehydes. Carbohydrates, if aldoses, will be coded in this group and in Y3. The formyl group need not be bound in another carbon atom.

47. Aldehyde derivatives (excluding 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. Blank.

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. Blank.

52. Ketones and thio ketones. 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 (excluding 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 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 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 hemiacetals.

61. Thioalcohols or mercaptans and their metal derivatives.

62. Thiophenol and metal derivatives with the same restrictions as imposed on group 59.

63. All thioalcohols analogous to the compounds illustrated in group 60.

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 1°, 2°, 3°, 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-aminopiperidine 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 and thio epoxy compounds. See group 05 for epidoxy compounds; group 75 for epidithio compounds and analogs.

75. Sulfides, polysulfides and ortho esters of thiocarboxylic acids.

76. Sulfoxides and sulfones.

77. Alkynes and cycloalkynes. Those compounds exhibiting carbon-carbon triple bonds with the same restrictions imposed under group 73. These compounds also appear in X2 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 aryldiimides are in group 79; the acyl analogs are in group 18.

80. Nitro and nitroso compounds.

81. Iodoso and iodoxy compounds. Esters as $C_6H_5I(O\text{-}\overset{O}{\overset{\|}{C}}\text{-}R)_2$ 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 functional groups are present.

87. Other metallo-organic compounds such as tetraethyllead, phenylmercuric chloride, etc. Most all other functional groups take precedence, therefore C_6H_5HgOH 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. Blank.

NOTE: Selenium and Tellurium analogs may replace all sulfur-containing functions.

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/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 far as 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 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 cyclooctatraene.
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 not 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.

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

FUNCTIONAL GROUP ALPHABETICAL INDEX

The following is an alphabetical listing of many of the most commonly sought functions, with an indication of the groups in which 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.