PRODUCT NUMBERING SYSTEM:

Format: 1 2 3 4 - 5 - 6 7

1,2,3,4 defines the class of material
5 defines the mix of monovalent atoms:
H, F, Cl, Br, I
6,7 is the product number [00 - 99]
Pick the highest number from each group.

CLASS OF MATERIAL

First digit (1) defines the polyvalent atoms

1 = Carbon only
2 = Carbon and oxygen
3 = Carbon and Nitrogen
4 = Carbon, Nitrogen, and Oxygen
5 = Carbon and other
6 = Carbon, Oxygen + other(s)
7 = Carbon, Nitrogen + other(s)
8 = Carbon, Nitrogen, Oxygen + other(s)
9 = Organometallic, C-M or O-M-O
M = Inorganic (no monovalent non-metals bonded to C)

Second digit (2) defines dominant structural element

0 = non-carbonaceous
1 = alkanes
2 = cycloalkanes
3 = alkenes
4 = cycloalkenes
5 = Alkynes
6 = Aromatics
7 = Aryl alkanes*
8 = Aryl trifluoromethyl*
9 = Aryl alkenes/Alkynes*
H = Heterocyclic (4 or more atoms/ring)

Third & Fourth digit (3,4) defines functional groups

(If 1st digit = 9 or M then 3rd & 4th digits correspond to highest Atomic Number of metal)

00 No functional group

CARBON, OXYGEN: C_nO

01 Primary alcohols, R-OH
02 Secondary alcohols, R_2CH-OH
03 Tertiary alcohols, R_3C-OH
04 diols HO-(R)-OH
05 polyols $(OH)_n$
06 Hemiacetal, $R_2C(OH)OR'$
07 ethers, C-O-C
08 polyethers, acetals, ketals
09 epoxides
10 cyclic ethers
11 crown ethers
12 carbohydrates
13 Hypohalites, (halohydrin), ROX
14 Peroxides, ROOX / Oxonium, R_3O^+
15 Aldehydes, -HC=O, and their hydrates
16 Acid halides, -XC=O
17 ketones, R_2-C=O, and their hydrates
18 diketones / polycarbonyl
19 Ketenes, -C=C=O
20 Hydroxy ketones
21 Carboxylic acids, -COOH
22 Carboxylates, $-COO^- M^+$, $-COO^= NH_4^+$
23 Esters, -COOR
24 Unsaturated esters (acrylates, methacrylates, etc)
25 Lactones, -CO-O-
26 Anhydrides, R-CO-O-CO-R
27 Peroxyacids/peroxyesters, RC=OOOR'
28 Carbonates/ortho ester, $(RO)_2C$=O
29 Hydroxy acid / ester; / Keto-acid / ester

CARBON & NITROGEN, C_nN

30 Primary amines, $-NH_2$, and salts
31 Secondary amines, -NH- and salts
32 Tertiary amines, >N- and salts
33 Ammonium R_4N^+
34 Aziridines
35 Imines, C=NR
36 Enamines / ketenamines
37 Nitrile -CN/ Isonitrile $-N^+C^-$
38
39 Hydrazine / Hydrazone
40 Azo (Diazene) -N=N-
41 Amidine / Guanidine
42 Azide
43 Purines

CARBON, NITROGEN & OXYGEN, C_nNO

45 Nitroso / nitroxide
46 Cyanohydrin / Acyl cyanide
47 Oximes / Hydroxylamines and salts
48 Amide / Lactam / Amino ketones
49 Cyanate -O-CN/ Isocyanate -N=C=O
50 Nitrones / Nitrile oxides / amine oxides
52 Nitrosamine / Diazene oxide (Azoxy)
53 Ureas, N-C=O-N / Uracils
54 Nitro
55 Nitro amines / amides / nitriles
56 Carbamic acid / Carbamates / hydrazides
Amino alcohols / ketones / ethers
57 Amino acids & salts
58 Amino acid derivatives (esters, amides, amide/esters, silylated, etc.)
59 Nucleosides

C &/or N &/or O + OTHER NON-METALS

60 Organoboron / organic borates / Lewis adducts / organic borate salts
61 Thiols /Thiophenols
62 Sulphenyl, sulfinyl, sulfonyl halides
63 Sulfonyloxy / Sulfone
64 Sulfonates / Sulfates
65 Sulfinate / Sulfoxide
66 Sulfides, disulfides, polysulfides
67 Thiocarbonyl / Thiocarboxy / Thioamide / Thiourea / S+ -COOH
68 Thiocyanate -S-CN / Isothiocyanate -
69 Sulfonamide / Sulfonimide / amino-sulfur. Ammonium sulfur acid salts
70 S + other heteroatom heterocyclics
71 Sulfur halides, eg RSF_5
72 Phosphines, PR_3
73 Halophosphines, $PR_{3-n}X_n$
74 Phosphites /Phosphine oxides
75 Phosphates, PO_4R_2
76 Phosphonium
77 Phosphonate
78 Phosphorus ylide / Phosphorane
79 Phosphazenes / phosphoramide
80 Silanes
81 Halosilane, Si-X
82 Silanol, Si-OH
83 Alkoxy silane, Si-OR
84 Aryloxysilane
85 Siloxane, -Si-O-Si-
86 Silane ester
87 Amino silanes
88 Silazane
89 amido, imino, and ketoximino silanes
90 Other silanes
91-97 Reserved
98 Polymers

MONOVALENT ATOMS

Fifth character defines monovalent substituents as follows:

0 = no H, F, Cl, Br, or I
1 = H
2 = F
3 = F, H
4 = Cl
5 = Cl, H
6 = Cl, F
7 = Cl, F, H
8 = Br
9 = Br, H
A = Br, F
B = Br, F, H
C = Br, Cl
D = Br, Cl, H
E = Br, Cl, F
F = Br, Cl, F, H
G = I
H = I, H
J = I, F
K = I, F, H
L = I, Cl
M = I, Cl, H
N = I, Cl, F
P = I, Cl, F, H
R = I, Br
S = I, Br, H
T = I, Br, F
U = I, Br, F, H
V = I, Br, Cl
W = I, Br, Cl, H
X = I, Br, Cl, F
Y = I, Br, Cl, F, H

EXAMPLES

Trifluoromethane: CHF_3
Contains only carbon, therefore 1st digit = 1
It is an alkane, therefore 2nd digit = 1
No functional gps, therefore 3rd & 4th digits = 00
Monovalent atoms are H,F therefore 5th digit = 3
Product number starts with 1100-3-

Hexafluoroisopropanol: $(CF_3)_2CHOH$
Contains C & O, therefore 1st digit = 2
Alkyl compound, therefore 2nd digit = 1
Secondary alcohol, therefore 3rd & 4th digit = 02
Monovalent atoms are H,F therefore 5th digit = 3
Product number starts with 2102-3-

4-Bromo-2-fluoroaniline
Contains C & N, therefore 1st digit = 3
Aromatic compound, therefore 2nd digit = 6
Primary amine, therefore 3rd & 4th digits = 30
Monovalent ats. are H, Br, F therefore 5th digit = B
Product number starts with 3630-B-

Cesium fluoride, CsF
Inorganic, therefore 1st character = M
Non-carbonaceous, therefore 2nd digit = 0
Atomic number of Cesium = 3rd & 4th digit = 55
Monovalent atoms is F therefore 5th digit = 2
Product number starts with M055-2-

A neat little system, once you get the hang of it!

* C_{Alk} not bonded to polyvalent atom other than C