

General terms

- D00 Inorganic
- D01 Organic
- D02 Hydrocarbon
- D03 Stereochemistry
- D04 Isotope
- D05 Bridged ring
- D06 Spiro
- D07 Tricyclic ring
- D08 ≥Tetracyclic
- D09 Elemental

Generic sub-units

- D10 Aliphatic
- D11 . Saturated
- D12 . Unsaturated
- D26 . . Acrylic
- D27 . . Allyl
- D13 Alicyclic
- D14 . Monocyclic alic
- D15 . Cyclopentadienyl
- D16 . Bicyclic alic
- D17 . Polycyclic alic
- D38 . . Adamantyl
- D39 . . Dicyclopentadien
- D18 Aromatic
- D19 . Benzene
- D20 . Naphthalene
- D21 . Polycyclic arom
- D100 . . Indenyl
- D80 . . Fluorenyl
- D22 Heterocyclic
- D23 . Monocyclic hetero
- D24 . Bicyclic hetero
- D25 . Polycyclic hetero

Ring counts

- D31 1 ring
- D32 2 rings
- D33 3 rings
- D34 4 rings
- D96 5 rings
- D97 6 rings
- D98 7 Rings
- D99 ≥8 Rings
- D73 3 membered ring
- D74 4 membered ring
- D75 5 membered ring
- D76 6 membered ring
- D77 7-9 membered
- D78 10-12 membered
- D79 ≥13 membered

Atoms in ring systems

- D40 Ring contains no C
- D41 1 N
- D42 1 O
- D43 1 S
- D36 1 Si
- D44 1 or more P
- D45 >1 N
- D46 >1 O
- D47 >1 S
- D37 1 or more Si
- D48 Other ring element

C-C unsaturation

- D50 No unsaturation
- D51 Unsaturated

- D52 . Acetylenic
- D53 . Monoolefinic
- D54 . Diolefinic
- D55 . ≥ Triolefinic
- D56 Conjugated
- D57 Nonconjugated
- D58 Terminal olefin
- D59 Internal olefin

Broad functionality types

- D60 Acid
- D61 Salt/complex
- D62 . Metallocene
- D72 . . Bridged
- D63 Ester
- D64 Acid halide
- D65 Acid anhydride
- D66 Radical
- D67 Base
- D49 Lewis acid
- D68 Metal-C bond
- D69 Halogen-C bond
- D70 Metal-halogen bond
- D71 Metal-H bond

Carbon count

- D81 1 C
- D82 2 C
- D83 3 C
- D84 4 C
- D85 5 C
- D86 6 C
- D87 7 C
- D88 8 C
- D89 9 C
- D90 10 C
- D91 11 C
- D92 12 C
- D93 13-18 C
- D94 19-24 C
- D28 25 - 30 C
- D29 31-40 C
- D30 ≥41 C

S

- F00 Sulphide -S-
- F01 Disulphide -S-S-
- F02 Tri or greater sulphide
- F03 Episulphide
- F04 Thiol
- F05 (Di)Thiocarboxylate
- F06 (Di/Tri)Thiocarbonate

N

- F07 Amine
- F08 . Monoamine
- F09 . Diamine
- F10 . ≥Tri amine
- F11 Hydrazine -N-N-
- F12 Cyano -C≡N
- F13 Azo -N=N-
- F14 Azide -N=N≡N
- F15 Imine >C=N-
- F16 Quaternary N
- F17 Amidine >N-C=N-
- F18 Guanidine
- F19 Triazinyl
- F96 Carbodiimide

- F97 Aziridine ring
- F98 Diazide
- F99 Phthalocyanine

O

- F20 Oxide
- F21 Hydroxide
- F22 Aldehyde
- F23 Ketone
- F24 Acetal
- F25 Ketene
- F26 Alcohol
- F27 . Monoalcohol
- F28 . Dihydroxy
- F29 . ≥ Trihydroxy
- F30 Phenolic
- F31 . Monophenol
- F32 . Diphenol
- F33 . ≥ Triphenol
- F34 Ether
- F35 Carboxylic acid/salt
- F36 . Monocarboxylic
- F37 . Dicarboxylic
- F38 . ≥ Tricarboxylic
- F39 Carboxylic anhydride
- F40 Carboxylic halide
- F41 Carboxylic ester
- F89 . Monocarbox ester
- F90 . Dicarbox ester
- F91 . ≥ 3 Carbox ester
- F42 Percarboxylic ester
- F43 Lactone
- F44 Carbonate
- F45 Percarbonate
- F46 Percarboxylic acid
- F47 Epoxide ring
- F48 Peroxide
- F49 Haloformate

P

- F50 Phosphine
- F51 Phosphonium

PO

- F52 Phosphite
- F53 Phosphate
- F54 Phosphonate
- F55 (Di)Thiophosphate
- F56 (Di/Tri)Thiophosphonate

SO

- F60 Sulphate, sulphuric
- F61 Sulphonyl
- F62 Sulphonic
- F63 Sulphoxide
- F64 Sulphonamide
- F65 Sulphenamide
- F66 Isothiocyanate
- F67 Thiourethane
- F68 Thiourea

NO

- F70 Carboxylic amide
- F93 . Monocarbox amide
- F94 . Dicarbox amide
- F95 . ≥ 3 Carbox amide
- F71 Lactam
- F72 Imide

- F73 Isocyanate
- F57 . Monoisocyanate
- F58 . Diisocyanate
- F59 . ≥ 3 isocyanates
- F74 Cyanate
- F75 Nitro
- F76 Hydroxylamine
- F77 Urethane
- F78 Urea
- F79 Nitroso
- F92 Oxime
- F69 Oxime ether
=C=N-O-C!
- F100 Amine oxide ≡N-O

Si

- F80 Silicate
- F81 Si-O-Si
- F82 Si-N-Si
- F83 Si-H
- F84 Si-OH
- F85 Si-Halogen
- F86 Si-C
- F87 Si-O-C
- F88 Si-Si

Acid derivatives

- E00 Diacyl
- E01 Malei-
- E02 Fumari-
- E03 Itaconi-
- E04 Citraconi-
- E05 Tetrahydrophthali-
- E06 Me tetrahydrophthali-
- E07 Nadi-
- E08 Methyl Nadi-
- E09 Chlorendi-
- E10 Oxali-
- E11 Succini-
- E12 Glutari-
- E13 Adipi-
- E14 Pimeli-
- E15 Suberi-
- E16 Azelai-
- E17 Sebaci-
- E18 Dodecanoi-
- E19 Phthali-
- E20 Isophthali-
- E21 Terephthali-
- E22 Naphthalene diacyl
- E23 Sulphoisophthali-
- E24 Hexahydrophthali-
- E25 Me hexahydrophthali-
- E26 Tetrabromophthali-
- E27 Tetrachlorophthali-
- E28 Other diacyl
- E30 Polyacyl
- E31 trimellititi-
- E32 pyromellititi-
- E33 benzphenonetetracarb
- E34 biphenyltetracarboxyli
- E36 oxydiphthali-
- E37 hexaF isoprop
diphthali-
- E35 . Other polyacyl