Chemical Groups and Atom-Types

In addition to ***total*** *algebraic indices* computed for the whole molecule, a **local-fragment** formalism can be developed. In this way, the matrix representations (topologic or geometric) of the molecular structures can be transformed to considerer information related with groups or atom-types belonging to a specific molecular fragment (*F*). So, these *local-fragment matrices* are used as matrix form of the algebraic maps to compute the *local-fragment indices*. The molecular fragments employed in this software are:

- Hydrogen bond acceptors (A)
- Carbon atoms in aliphatic chains (C)
- Hydrogen bond donors (D)
- Halogens (G)
- Terminal methyl groups (M)
- Carbon atoms in aromatic portion (P)
- Heteroatoms (O, N and S in all valence states, denoted as X)