9.5. TYPICAL INTERATOMIC DISTANCES: ORGANIC COMPOUNDS

A combination of chemical name and linear formulation is often employed to increase the precision of the definition, e.g. NH₂—C==O in acyclic amides; C==C—C(==O)—C==O in benzoquinone. Finally, for very simple ions, the accepted conventional representation is deemed to be sufficient, e.g. in NO₃⁻, SO₄⁻, etc.

The chemical definition of substructure may be followed by brief qualifying information, concerning substitution, conformational restrictions, etc. For example: Cₛᵖ³—Cₛᵖ³: in cyclobutane (any substituent); X—C—F, (X = C, H, N, O); Cₓₓ—NH—Cₛᵖ³ (Nₛᵖ³: pyramidal). Where the generic symbol X is unqualified, it denotes any element type, including hydrogen. If the qualifying information is too extensive, then it will be given as a table footnote (see below).

The ‘Substructure’ column is designed to convey as much unambiguous information as possible within a small space. For Cₛᵖ³, we have employed the short forms Cₓ and Cₓₓ. Cₓ indicates Cₛᵖ³ whose bonds, additional to those specified in the linear formulation, are to C or H atoms only. Cₓ—OH would then represent the group of alcohols CHₓ—OH, —C—CHₓ—OH, —Cₓ—CH—OH and —Cₓ—C—OH. Cₓₓ is frequently used to restrict the secondary environment of a given bond to avoid the perturbing influence of, e.g., electronegative substituents. The symbol Cₓₓ is merely a space-saving device to indicate any Cₛᵖ³ atom and includes Cₓ as a subset.

9.5.3.3. Use of the ‘Note’ column

The ‘Note’ column refers to the footnotes collected in Appendix 1. These record additional information as follows: (a) additional details concerning the chemical definition of substructures, e.g. the omission of three- and four-membered rings; (b) statements of geometrical constraints used in obtaining the cited average, e.g. definition of planarity or pyramidality at

Fig. 9.5.3.2. Alphabetized index of ring systems referred to in the table; the numbering scheme used in assembling the bond-length data is given where necessary.

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