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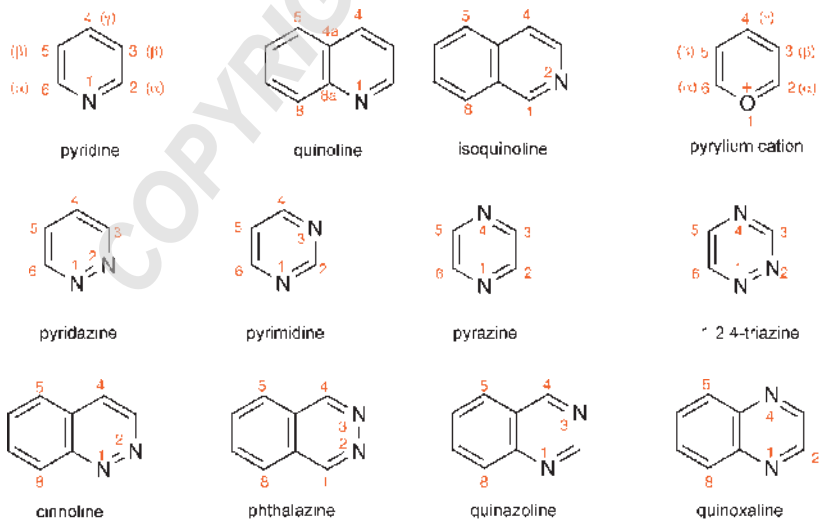
Heterocyclic Nomenclature

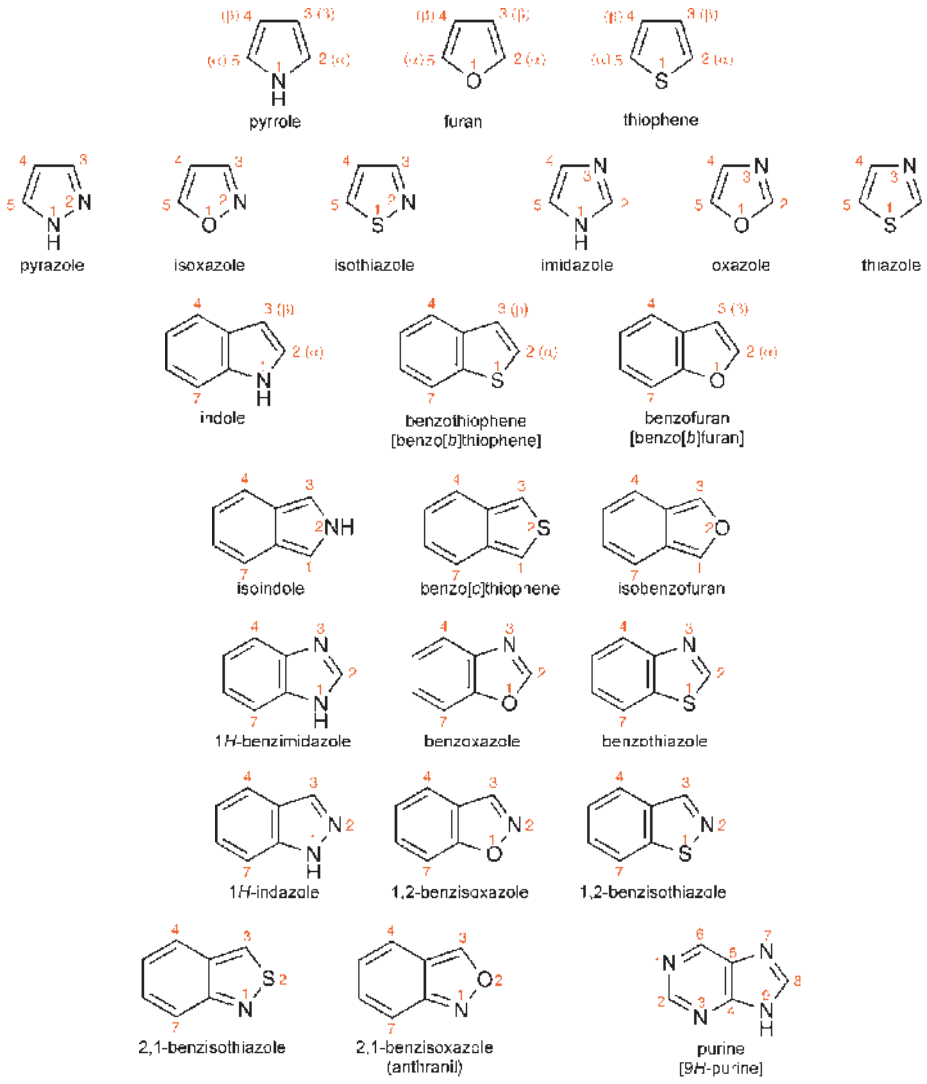
A selection of the structures, names and standard numbering of the more common heteroaromatic systems and some common non-aromatic heterocycles are given here as a necessary prelude to the discussions which follow in subsequent chapters. The aromatic heterocycles have been grouped into those with six-membered rings and those with five-membered rings. The names of six-membered aromatic heterocycles that contain nitrogen generally end in 'ine', though note that 'purine' is the name for a very important bicyclic system which has both a six- and a five-membered nitrogen-containing heterocycle. Five-membered heterocycles containing nitrogen general end with 'ole'. Note the use of italic '*H*' in a name such as '9*H*-purine' to designate the location of an *N*-hydrogen in a system in which, by tautomerism, the hydrogen could reside on another nitrogen (e.g. N-7 in the case of purine). Names such 'pyridine', 'pyrrole', 'thiophene', originally trivial, are now the standard, systematic names for these heterocycles; names such as '1,2,4-triazine' for a six-membered ring with three nitrogens located as indicated by the numbers, are more logically systematic.

A device that is useful, especially in discussions of reactivity, is the designation of positions as 'α', 'β', or 'γ'. For example, the 2- *and* the 6-positions in pyridine are equivalent in reactivity terms, so to make discussion of such reactivity clearer, each of these positions is referred to as an 'α-position'. Comparable use of α and β is made in describing reactivity in five-membered systems. These useful designations are shown on some of the structures. Note that carbons at angular positions do not have a separate number, but are designated using the number of the preceding atom followed by 'a' – as illustrated (only) for quinoline. For historical reasons purine does not follow this rule.



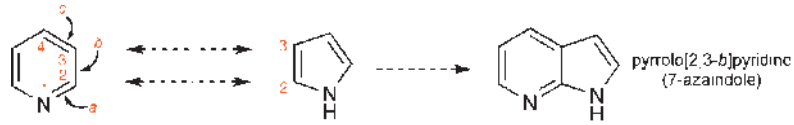
Six-membered aromatic heterocycles

Heterocyclic Chemistry 5th Edition John Joule and Keith Mills

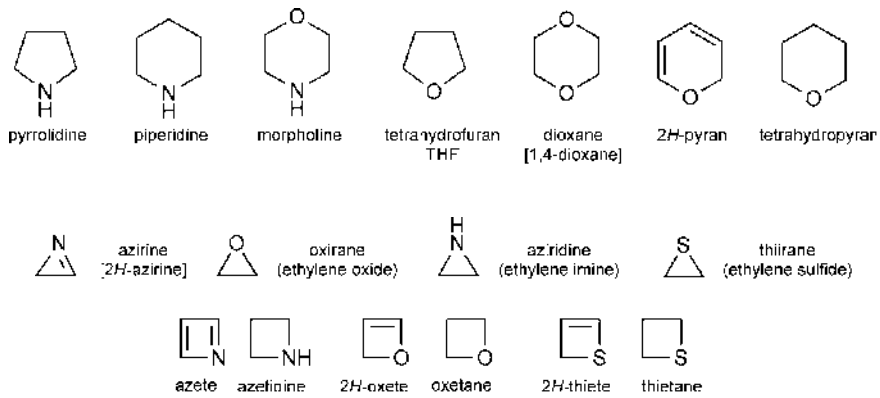


Five-membered aromatic heterocycles

A detailed discussion of the systematic rules for naming polycyclic systems in which several aromatic or heteroaromatic rings are fused together is beyond the scope of this book, however, a simple example will serve to illustrate the principle. In the name 'pyrrolo[2,3-*b*]pyridine', the numbers signify the positions of the first-named heterocycle, numbered as if it were a separate entity, which are the points of ring fusion; the italic letter, '*b*' in this case, designates the *side* of the second-named heterocycle to which the other ring is fused, the lettering deriving from the numbering of that heterocycle as a separate entity, i.e. side *a* is between atoms 1 and 2, side *b* is between atoms 2 and 3, etc. Actually, this particular heterocycle is more often referred to as '7-azaindole' – note the use of the prefix 'aza' to denote the replacement of a ring carbon by nitrogen, i.e. of C-7–H of indole by N.



The main thrust of this book concerns the aromatic heterocycles, exemplified above, however Chapter 30 explores briefly the chemistry of saturated or partially unsaturated systems, including three- and four-membered heterocycles.



Non-aromatic heterocycles