

## APPENDIX

# ■ NOMENCLATURE OF HETEROCYCLIC COMPOUNDS

IN AN EFFORT to systematize the naming of heterocyclic compounds, a system has been devised which permits the accurate and intelligible conveyance of information from one chemist to another.<sup>1</sup>

For monocyclic rings, the proper nomenclature is derived by combining an appropriate prefix and suffix to a given stem according to the following rules.

(a) The size of the ring is denoted by the appropriate stem selected from Table A-1.

(b) The nature of the hetero atom is denoted by such prefixes as oxa, thia, or aza for oxygen, sulfur, or nitrogen, respectively. Multiplicity of the same hetero atom is designated by an additional prefix such as di- or tri-, etc. When two or more different hetero atoms are present, they are named in the order O > S > N, for example, oxaza and thiaza.

TABLE A-1 ▪

*Stems and Suffix for Three- to Ten-Membered Monocyclic Heterocycles*

Ring size	Stem	Stem and suffix			
		Rings containing nitrogen		Rings without nitrogen	
		Unsaturated <sup>a</sup>	Saturated	Unsaturated <sup>a</sup>	Saturated
3	-ir-	-irine	-iridine	-irene	-irane
4	-et-	-ete	-etidine	-ete	-etane
5	-ol-	-ole	-olidine	-ole	-olane
6	-in-	-ine	<sup>b</sup>	-in	-ane
7	-ep-	-epine	<sup>b</sup>	-epin	-epane
8	-oc-	-ocine	<sup>b</sup>	-ocin	-ocane
9	-on-	-onine	<sup>b</sup>	-onin	-onane
10	-ec-	-ecine	<sup>b</sup>	-ecin	-ecane

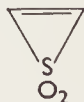
<sup>a</sup> Corresponding to the maximum number of double bonds, excluding cumulative double bonds.

<sup>b</sup> Expressed by prefixing "perhydro" to the name of the corresponding unsaturated compound.

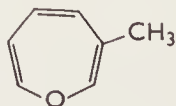
(c) The degree of unsaturation is specified in the suffix as given in Table A-1. It is important to note that the suffix is slightly modified when nitrogen is absent from the heterocyclic ring.

(d) The numbering of the ring begins with the hetero atom of highest priority and proceeds around the ring so as to give other hetero atoms or substituents the lowest numbers possible.

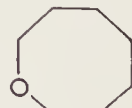
These rules may be illustrated by the following examples.



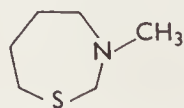
thiirene 1,1-dioxide



3-methyloxepin



oxocane

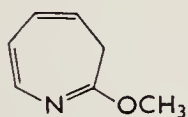
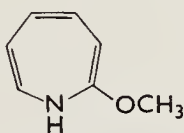
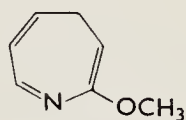
3-methylhexahydro  
1,3-thiazepine

thiete

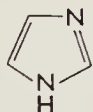


1,2-oxathiolane

When a name applies equally to two or more isomeric parent ring systems with the maximum number of noncumulative double bonds, and when the name can be made specific by indicating the position of one or more hydrogen atoms in the structure, this is accomplished by modifying the name with a locant followed by italic capital *H* for each of these hydrogen atoms. Such symbols ordinarily precede the name.

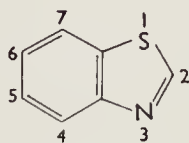
2-methoxy-3*H*-azepine2-methoxy-1*H*-azepine2-methoxy-4*H*-azepine

Many of the common heterocyclic ring systems have acquired trivial names which are retained in systematic nomenclature. The majority of these have been discussed throughout this text.

imidazole  
(1,3-diazole)pyridazine  
(1,2-diazine)tetrahydrofuran  
(oxolane)

*Polycyclic systems* are named according to the following rules<sup>1,2</sup>:

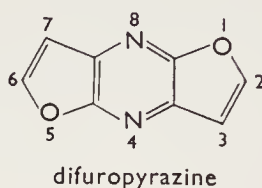
(e) The name of the hetero ring is chosen as the parent compound and the name of the fused ring is attached as a prefix. For example,



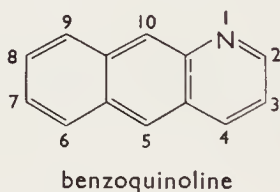
benzothiazole

(f) In selecting the parent ring when two or more hetero rings are present, a nitrogen-containing ring is given precedence over an oxygen-containing ring (and oxygen over sulfur). However, in

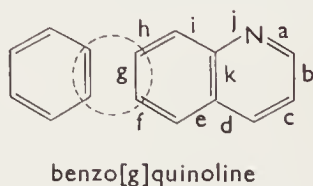
numbering the polycyclic compound, an oxygen hetero atom, if such is present, is given the lowest number consistent with rule (i) (see p. 391).



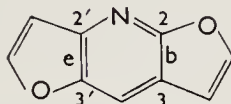
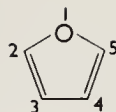
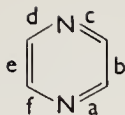
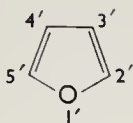
(g) Preference is given to the largest hetero ring system which has a simple name. The example that follows is therefore called benzoquinoline rather than naphthopyridine.



(h) The structure given to illustrate rule (g) above is not fully identified by the name benzoquinoline, for it is necessary to indicate in the name the position of the ring junction. To do this, the sides of the parent ring (quinoline) are lettered a, b, c, etc., starting with the 1,2-bond; the benzo grouping is found fused to bond g, and this is so indicated in the name.

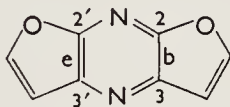


In the example given in rule (f) above, there is a further complication, because the position of the ring junction has to be specified for each of three rings. The following breakdown of the structure with appropriate numbering and lettering will serve to illustrate how this is done.



difuro[2,3-b:2',3'-e]pyrazine

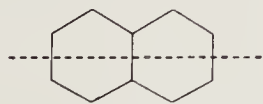
Note that the isomeric structure would have to be named as follows; the individual numbering of the parent ring and the subsidiary ring(s) follow the same order through the points of fusion, as in meshing gears.



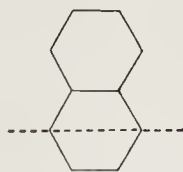
difuro[2,3-b:3',2'-e]pyrazine

(i) In numbering the periphery of a polycyclic compound, the written structure must first be oriented according to certain rules.

a. The greatest number of rings must lie along a horizontal axis.

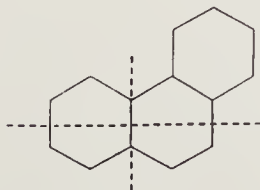


correct orientation

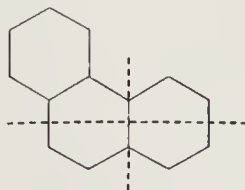


incorrect orientation

b. Of the other rings present, a maximum must lie uppermost to the right above the horizontal axis.

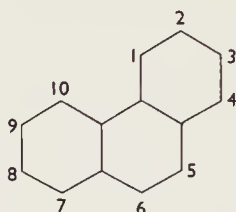


correct orientation

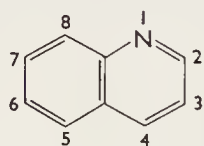


incorrect orientation

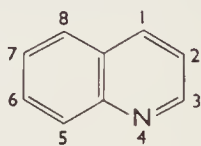
Numbering starts with the uppermost ring farthest to the right and proceeds in a clockwise direction, omitting the ring junctions.



Other things being the same, the orientation of the rings should be such as to lead to the lowest possible number for the hetero atoms.

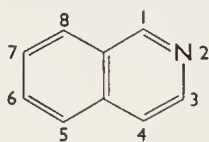


correct orientation

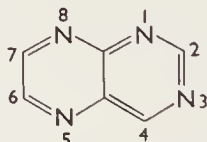


incorrect orientation

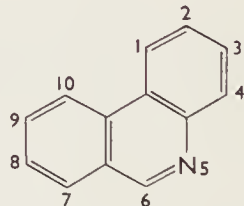
A few commonly encountered examples follow:



isoquinoline



pteridine



phenanthridine

### References and Notes

(1) *J. Am. Chem. Soc.*, **82**, 5566 (1960).

(2) (a) A. M. Patterson, L. T. Capell, and D. F. Walker, *The Ring Index*, 2nd ed., 1959; (b) J. D. Roberts and M. C. Caserio, *Basic Principles of Organic Chemistry*, W. A. Benjamin, Inc., New York, 1964, pp. 972-4.

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