Heterocycles

Chem 6352

Heterocyclic Nomenclature (adapted from: *bruckner.chem.uconn.edu/PDFfiles/hetshort.pdf* and from Gilchrist, T. L. *Heterocyclic Chemistry*; Longman; London, 1992)

The standard method for naming heterocyclic rings is the Hantzsch-Widman nomenclature system. A heterocycle is a ring containing at least one atom that is not carbon: "hetero" means "different." Nitrogen, oxygen, and sulfur are the primary elements seen in common heterocycles. Heterocycles may be aromatic or not aromatic, but aromatic heterocycles are often called "heteroaryls."

Names in the Hantzsch-Widman system provide data relating to several categories. First, the identity of the heteroatom present in the ring is established by the use of different prefixes for each type. The three prefixes are oxa-, thia-, and aza- for oxygen, sulfur, and nitrogen, respectively. Second, numbers assigned to the atom denote heteroatom position. Third, the size of the ring and the degree of unsaturation is described by the suffix at the end.

Table. Common Hantzsch-Widman suffixes.

ring size	unsaturated ring with only O or S	unsaturated ring with N	saturated ring with only O or S	saturated ring with N
3	-irene	*-irine*	-irane	*-iridine*
4	-ete	-ete	-etane	*-etidine*
5	-ole	-ole	-olane	*-olidine*
6	-ine	-ine	-inane (-ane)	-inane (-ane)
7	-epine	-epine	-epane	-epane
8	-ocine	-ocine	-ocane	-ocane
9	-onine	-onine	-onane	-onane
10	-ecine	-ecine	-ecane	-ecane

Examples of ring naming:

Aziridine: 

This ring contains a nitrogen (prefix is aza-) and is a completely saturated three-membered ring (-iridine). Rings that contain a nitrogen require a designated suffix. When combining the prefixes and suffixes, two vowels can end up together. In this case that would be azairidine. When this happens, drop the vowel on the end of the first part.

1,2-Oxazetidine: 

This ring contains nitrogen (aza-) and oxygen (oxa-) and is a fully saturated four-membered ring (-etidine). Atom prefixes have a strict order in which they are to be listed. For the three atoms we will see, the order is oxygen followed by sulfur followed by nitrogen. So, after dropping the appropriate vowels, we get oxazetidine. Note that if there are two atom prefixes, vowels will be dropped by the earlier prefix. The numbers are placed in order of the prefixes with priority of the numbers being the same as the order of the prefixes. Oxygen is in position 1, and nitrogen is in position 2.

1,2,5-Oxadiazole: 

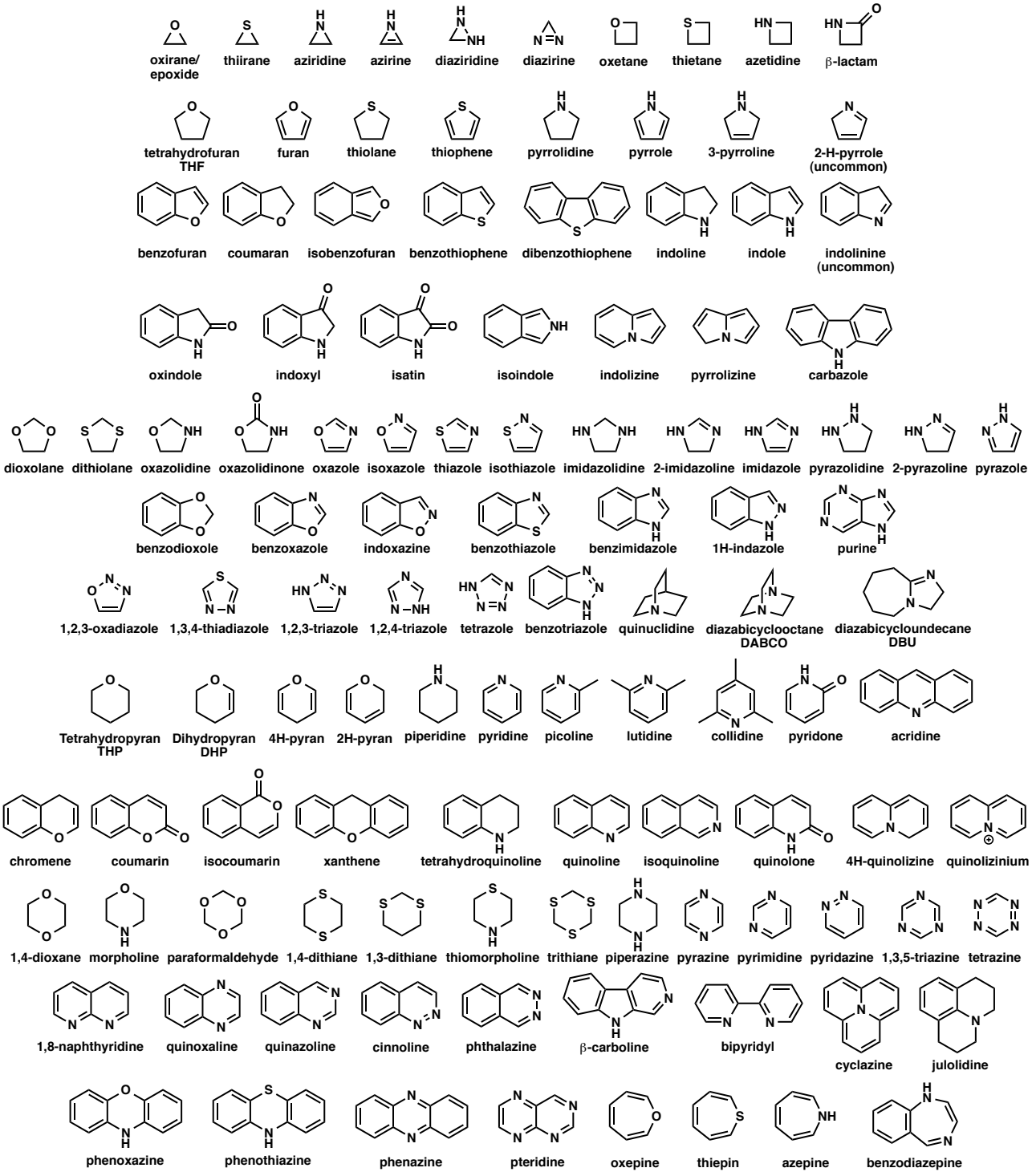
This ring has both nitrogen (aza-) and oxygen (oxa-). Unsaturated five-membered rings with nitrogen have the –ole suffix. The presence of two nitrogens requires a di- in front of aza-. Note that the 'a' in oxa- is not dropped since there are not two vowels together. Oxygen is higher priority than nitrogen, so it is in position 1 by default. The two nitrogens are therefore at positions 2 and 5.

1,3-Oxathiolane: 

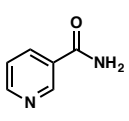
Prefixes of oxa- and thia- with a suffix of –olane initially gives oxathiolane. Oxygen takes priority in numbering to give 1,3-oxathiolane.

Not all heterocyclic rings follow the Hantzsch-Widman rules listed above, typically because they have established common names. These trivial names typically show traces of the systematic nomenclature, but do not completely follow the rules.

Heterocycles



Examples of Biologically Relevant Heterocycles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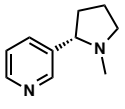
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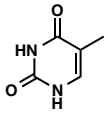
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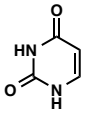
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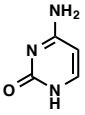
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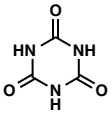
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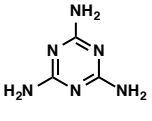
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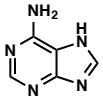
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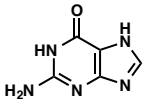
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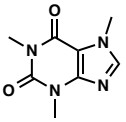
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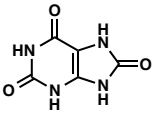
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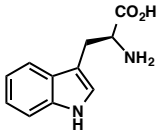
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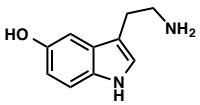
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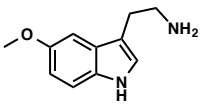
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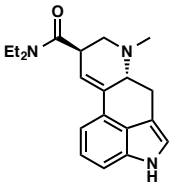
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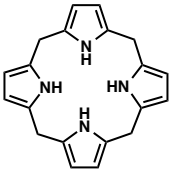
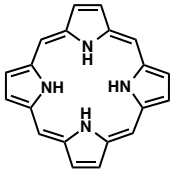
LSD


porphyrinogen


porphyrin