#### 2302687 – Heterocyclic Compounds – Part I

Lecture 1-3



# **Nomenclature of Heterocyclic Compounds Part 2**



Instructor: Dr. Tanatorn Khotavivattana Department of Chemistry, Faculty of Science, Chulalongkorn University E-mail: tanatorn.k@chula.ac.th

**Recommended Textbook:** 

Heterocyclic Chemistry, 5th Edition, J. A. Joule, K. Mills, 2010, Wiley



#### Rings with more than one heteroatom

• The order of priorities is derived from the **groups** of the Periodic System, and then within each group by **increasing atomic number**:

Group VI (O>S>Se>Te) > Group V (N>P>As) > Group IV (Si>Ge) > Group III (B)

- Each heteroatom is then given a **number** as found in the ring, with that of highest priority given position 1
- A saturated heteroatom with an extra-hydrogen attached is given priority over an unsaturated form of the same atom, as in 1H-1,3diazole
- The heteroatom prefixes follow the numbers in the priorities given
  previously
- The numbers are **grouped** together in front of the heteroatom listings (thus, 1,3-oxazole, not 1-oxa-3-azole)





Examples



Examples



**Bicyclic Compounds** share a common single/double bond: **fused rings** 

- Common case is where a benzene ring is fused to a heterocyclic ring. The name begins with the prefix "benzo"; The point of attachment is indicated by a letter that defines the "face" of the heterocycle involved. Thus, the 1,2- position on the heterocyclic ring is always the "a-face," 2,3- is the "b-face," 3,4- is the "c-face," and so on
- the final numbering always begins at a position next to the benzo group and that the heteroatoms are given the lowest numbers possible, observing the O>S>N>P rule



If **two heterocyclic rings** are fused, additional rules are required. A **parent ring** is selected, and the other ring is considered **fused on**, as was observed for benzene fusion. Some rules are as follows

- If one ring contains N, it is considered the parent
- If both rings contain N, the larger ring is the parent
- If both rings are of the same size, that with the most N atoms is the parent
- If no N is present, O has priority over S over P



•

#### **Systematic Naming of Bicyclic Compounds**

- The ring fused onto the parent has the **suffix** "o"; common names are used where possible to simplify the name
  - The **face letter** of the **parent ring** where the fusion occurs is placed in brackets preceding the name of that ring. The **position numbers** of the **fused ring** are placed inside the brackets before the face letter of the parent ring



 The proper numbers for the fused ring are those that are encountered as one goes around the ring in the same direction as going alphabetically around the faces of the parent



1,2,5-thiadiazolo[3,4-d]pyrimidine