Special Topics of IUPAC Nomenclature of Organic Compounds

Nature makes complex compounds regardless of how difficult they are to name. The IUPAC "blue book" describing how to name organic compounds contains over 500 pages. Our short descriptions barely scratch the surface of nomenclature, and very few chemists have a deep understanding of the complexity of the nomenclature conventions.

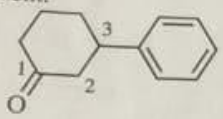
The purpose of this addendum to the IUPAC Nomenclature summary is to describe three areas of naming compounds beyond the basics. They are: 1. Nomenclature of Bicyclic Compounds; 2. Replacement Nomenclature of Heteroatoms; and 3. Stereochemical Designations (R and S, E and Z, the Cahn-Ingold-Prelog system).

SPECIAL TOPIC 1. Nomenclature of Bicyclic Compounds

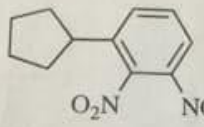
"Bicyclic" compounds are those that contain two rings. There are four possible arrangements of two rings that depend on how many atoms are shared by the two rings. The first arrangement in which the rings do not share any atoms does not use any special nomenclature, but the other types require a method to designate how the rings are put together. Once the ring system is named, then functional groups and substituents follow the standard rules described in the Summary document.

Type 1. Two rings with no common atoms

These follow the standard rules of choosing one parent ring system and describing the other ring as a substituent.



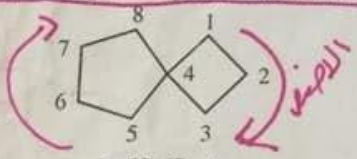
ketone is the highest priority functional group, phenyl is substituent
⟹ 3-phenylcyclohexan-1-one ("1" could be omitted here)



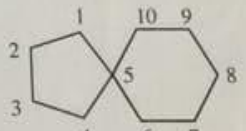
benzene is the parent ring system as it is larger than cyclopentane and it has three substituents
⟹ 1-cyclopentyl-2,3-dinitrobenzene

Type 2. Two rings with one common atom – spiro ring system

The ring system in spiro compounds is indicated by the word "spiro" (instead of "cyclo"), followed by brackets indicating how many atoms are contained in each path around the rings, ending with the alkane name describing how many carbons are in the ring systems including the spiro carbon. (If any atoms are not carbons, see Special Topic 2.) Numbering follows the smaller path first, passing through the sprio carbon and around the second ring.

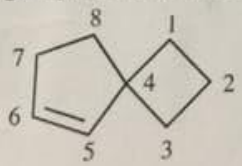


spiro[3.4]octane

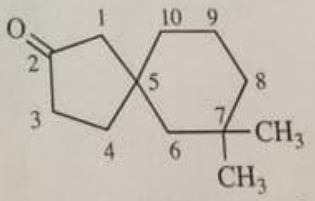


spiro[4.5]decane

Substituents and functional groups are indicated in the usual ways. Spiro ring systems are always numbered smaller before larger, and numbered in such a way as to give the highest priority functional group the lower position number.



spiro[3.4]oct-5-ene



7,7-dimethylspiro[4.5]decan-2-one

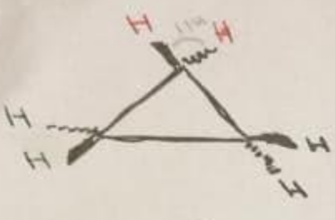
Cyclopropane

3 CH2 → heat of combustion

6 - CH

27.7 Kcal/mol total ring strain

CH2



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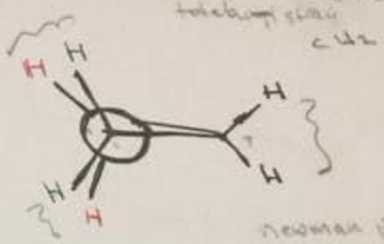
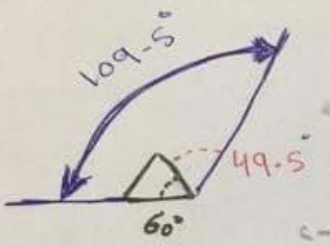
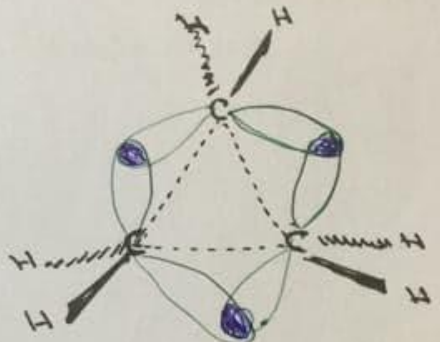


نلاحظ في cyclopropane له درجة عالية من الشد الالتوائي

torsional strain يعود الى عدد كبير من تجاذب eclipsing interaction





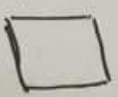
Ring strain = 27.5 Kcal/mol

angle strain

التوتر الزاوي الكبير angular strain في سايكلوبروبان يرجع الى الاواصر المنحنية bent bonds

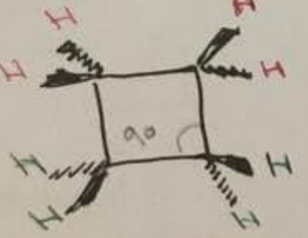
cyclobutane

planar



توتر زاوي عالي وتوتر التوائي عالي في المستوي الافتراضي

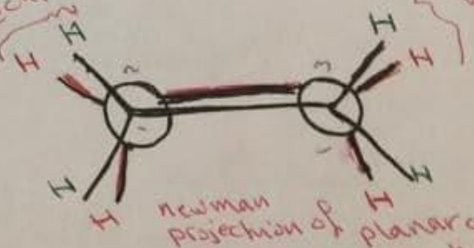
26.3 Kcal/mol



4 CH2 = a

8 - CH

≡



cyclobutane تمتلك ثمانية H...H eclipsing interaction في التركيب المستوي

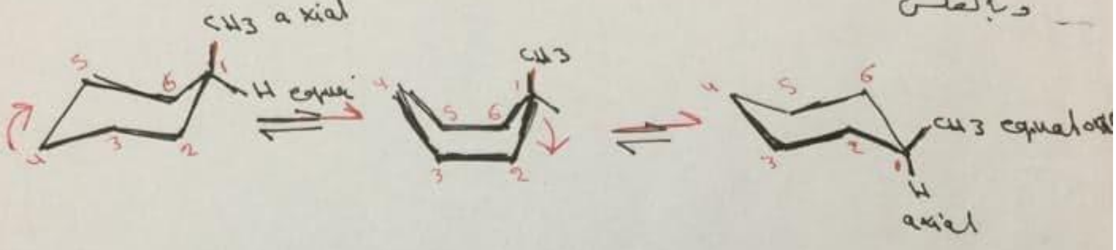
planar

Cyclohexane — monosubstituted cyclohexanes

المعوض على حلقة سايكلوهكسان بوضعية chair-conf اما شغل موقع axil او الequatorial . في درجة حرارة الغرفة RT هناك صيغتي chair

في حالة التوازن chair-chair-interconversion وتصاستبدل axial ← لequal

وبالعكس



chair-chair-interconversion

كله الي منهم هو الاقل طاقة ؟

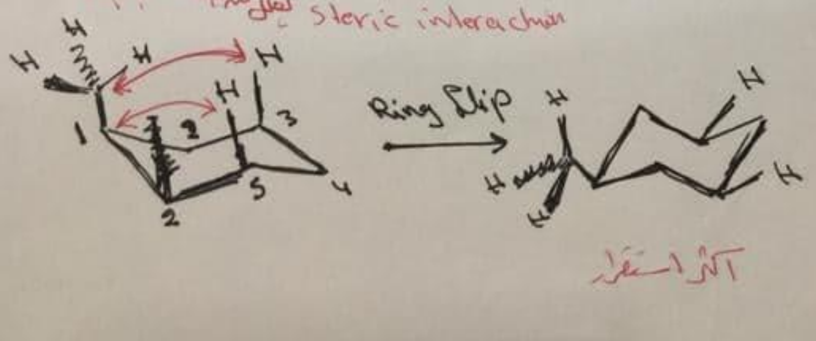
المعوض عندما يكون في حالة equal تكون الجزيئة اقل طاقة

واكثر استقرار

اي معوض يكون bigger من الهيدروجين يكون في موقع لaxial يؤدي

الى حدوث تجاذب غير مرغوب مع axial hydrogen الموجودة عند ذرة C 3 مثل هذا

التجاذب يطلق عليه 1,3-diaxial interaction



organic chemistry - cycloalkane stability and conformation

وجدان المركبات 5 و 6 الحلقة هي الأكثر الاستقرار ، والأكثر تواجد

كيف لماذا ؟

العالم Adolf Von Baeyer توصل الى توضيح الاستقراريه السبب الى المركبات 1905

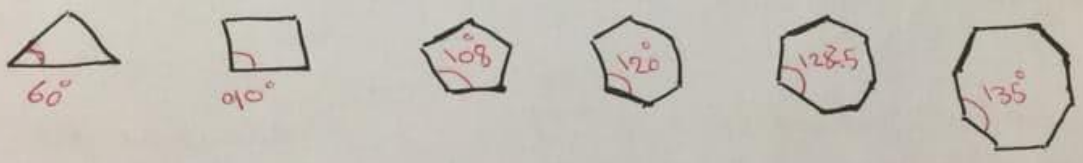
الحلقيه cyclic alkanes . وجدان المركبات او الكائنات الغير الحلقيه

(acyclic) non-cyclic لها اواصر = 109.5

وجود هذه المزاوجة تجعل الكترونات الاواصر تصيده عن بعضها as far apart as possible البعد الذي يجعلها أكثر استقرار

لهذا اذا المركبات الحلقيه لها اواصر غير 109.5 فان الاوربيتالات اواصر C - C لا تستطيع ان توصل الى تشابه اعلى overlap optimum ولهذا فيه هناك بعض (angle strain)

لاحظ conformation of cycloalkanes



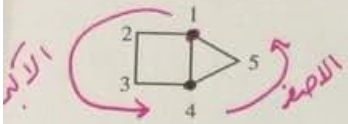
cycloalkane ليس دائما ذو تركيب مستوي (planar) وتكون الزاوية ذات صيود عن القيمة المثالية ideal value والتي تساوي 109.5

لاحظ cyclopropane

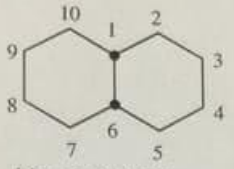
Special Topics of IUPAC Nomenclature, continued

Type 3. Two rings with two common atom – fused ring system

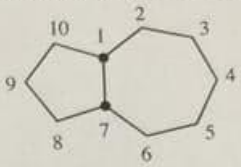
Two rings that share two common atoms are called fused rings. This ring system and the next type called bridged rings share the same designation of ring system. Each of the two common atoms is called a bridgehead atom, and there are three paths between the two bridgehead atoms. In contrast with naming the spiro rings, the *longer* path is counted first, then the shorter, then the shortest. In fused rings, the shortest path is always a zero, meaning zero atoms between the two bridgehead atoms. Numbering starts at a bridgehead, continues around the largest ring, through the other bridgehead and around the shorter ring. (In these structures, bridgeheads are marked with a dark circle for clarity.)



bicyclo[2.1.0]pentane
(path of 2 atoms and a path of 1 atom)



bicyclo[4.4.0]decane
(path of 4 atoms in each direction)

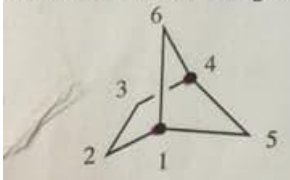


bicyclo[5.3.0]decane
(path of 5 atoms and path of 3 atoms)

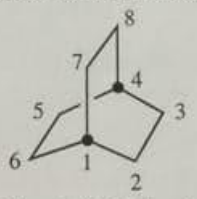
Substituents and functional groups are indicated in the usual ways. Fused rings systems are always numbered larger before smaller, and numbered in such a way as to give the highest priority functional group the lower position number.

Type 4. Two rings with more than two common atom – bridged ring system

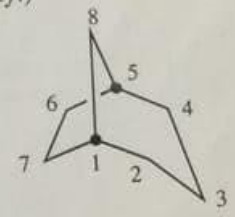
Two rings that share more than two common atoms are called bridged rings. Bridged rings share the same designation of ring system as Type 3 in which there are three paths between the two bridgehead atoms. The longer path is counted first, then the medium, then the shortest. Numbering starts at a bridgehead, continues around the largest ring, through the other bridgehead and around the medium path, ending with the shortest path numbered from the original bridgehead atom. (In these structures, bridgeheads are marked with a dark circle for clarity.)



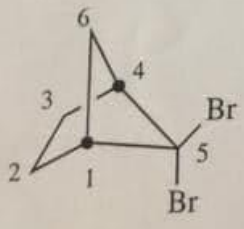
bicyclo[2.1.1]hexane
(paths of 2 atoms, 1 atom, and 1 atom)



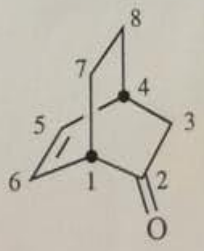
bicyclo[2.2.2]octane
(three paths of 2 atoms)



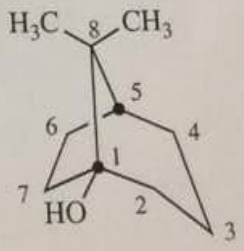
bicyclo[3.2.1]octane
(paths of 3 atoms, 2 atoms, and 1 atom)



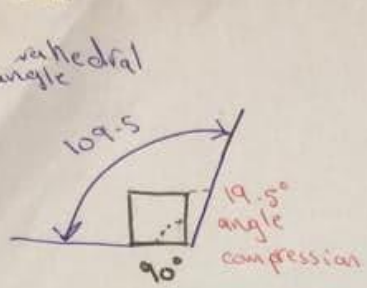
5,5-dibromo-bicyclo[2.1.1]hexane



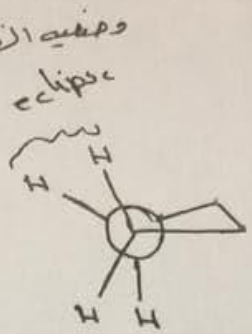
bicyclo[2.2.2]oct-5-en-2-one



8,8-dimethyl-bicyclo[3.2.1]octan-1-ol



Ring strain: 26 kcal/mol



Newmanprojection تكون الاواصر eclipsed وتؤدي الى زيادة الطاقة الالتوائية torsional strain .

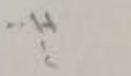
Angle strain + torsional strain = Ring strain

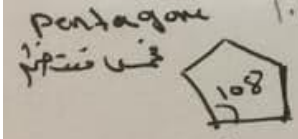
cyclopentane pentagone

التركيبة المستوية planar في سايكلوبنتان له زوايا اصرة = 108

والتي هي قريبة من القيمة المثالية الى ذرات tetrahedral

وهذا الشكل يقود الى حدوث torsional strain ينتج من عزم H---H eclipsing interaction.





مستوي

planar

all C-atoms in one plane

كل الذرات في مستوي واحد

شكل الظرف

Envelope

four C-atoms in one plane

اربع ذرات في مستوي واحد والخامسة خارج المستوى

Half-chair

Three C-atoms in one plane