Chapter-12

INNOVATIVE METHODS FOR THE IUPAC NOMENCLATURE OF BICYCLO AND SPIRO COMPOUNDS

Arijit Das

In this last chapter 12, IUPAC nomenclature of bicyclo and spiro compounds have been discussed, which is vitally important to students of organic chemistry from undergraduate to post-graduate level. These innovative mnemonics has to be introduced for informal determination of IUPAC nomenclature of bicyclo and spiro compounds in a very simple, metabolic and time economic way.

Conventional methods which are generally used for determination of IUPAC nomenclature of bicyclo and spiro compounds are time consuming[1,2,3]. To keep the matter in mind, two innovative methods have been introduced for the IUPAC nomenclature of bicyclo and spiro compounds in a very simple way[4].

METHODOLOGY

A. Innovative Method for IUPAC Nomenclature of Bicyclo Compounds

In *bicyclo* compounds, two rings are fused with each other and the common points of two fused rings are at least 02 (two). It may be three, four etc. but not less than two. The common points (cp) may also be treated as carbons, which are common in two fused rings.

The format of IUPAC nomenclature for bicyclo compounds is *'bicyclo[a,b,c]alkane'*, where, 'a' and 'b' are the maximum and minimum number of points respectively in the fused ring system excluding common points and variable 'c' = no of common points (cp) – 2.

B. Innovative Method for IUPAC Nomenclature of Spiro Compounds

In *spiro* compounds, two rings are passing through one point (intersecting point = 1) elected as the common point. In such case, common point (cp) is always one. It is fish like structure.

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1. I.L.Finar, *Organic Chemistry* 1 (Pearson, 6th ed.: 2004), 532.
2. R.T. Morrison et.al., *Organic Chemistry* (Pearson, 7th ed.: 2011), 208.
3. T.W.Graham Solomons and C.B.Fryhle, *Organic Chemistry* (Wiley India, 10th ed.: 2012), 150.
4. A. Das, "Review of Innovative Mnemonics for Inorganic and Organic Chemical Education", *Chemistry Journal* 4(July 2018): 11-31, http://www.publicscienceframework.org/journal/paperInfo/cj?paperId=3979.

The format of IUPAC nomenclature for *spiro* compounds is *'spiro[a,b]alkane'*, where, 'a' and 'b' are the minimum and the maximum number of points respectively in the fused ring system excluding common point (cp).

RESULTS AND DISCUSSION

A. Innovative Method for IUPAC Nomenclature of Bicyclo Compounds

The format of IUPAC nomenclature for non-substituted *bicyclo* compounds format is *'bicyclo[a,b,c]alkane'* and for substituted *bicyclo* compounds formats are *'x-substituent bicyclo[a,b,c]alkane'* (in presence of only one substituent); *'x-substituent bicyclo[a,b,c]alkene/alk-y-ene'* (in presence of one double bond and one substituent); *'x, x-disubstituent bicyclo[a,b,c]alkene/alk-y-ene'* (in presence of one double bond and two same substituents) and *'x,x-disubstituent bicyclo[a,b,c]alka-y,z-diene'* (in presence of two double bonds and two same substituents).

Here 'a' and 'b' are the maximum and minimum number of points respectively in the fused ring system excluding common points and variable 'c' = no of common points (cp) – 2; x = position number of the substituents present in the ring system; y and z = position numbers of the double bonds and the suffix 'alkane' corresponding to the total number of points (or carbons) in the fused ring system including common points (bridging points).

Since, *'bicyclo'* starts with letter 'b' and 'b' stands for 'big' (maximum), so, during IUPAC nomenclature of *bicyclo* compounds, first, write in the third parenthesis '[ ]', maximum no of points followed by minimum no of points and then variable number 'c' always accomplish by the deduction of 02 (two) from the total number of common points [i.e. variable c = no of common points (cp) – 2]. Sometimes, where, a = b, then write, 'a' after 'b' or vice versa.

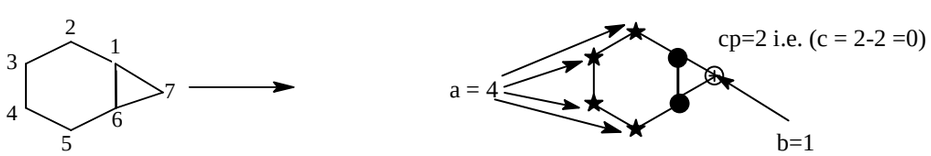
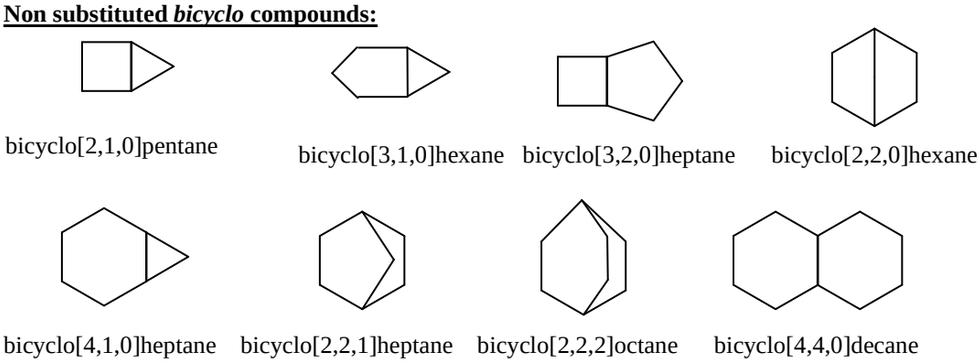


Fig. 12.30. Bicyclo[4,1,0]heptane.

In bicyclo[4,1,0]heptanes, (**Fig. 12.30**), the maximum no of points, 'a' = 4, have denoted by asterisk mark, minimum no of the point, 'b'=1, has denoted by positive sign and common points, cp = 2, are denoted by shadow circle.

Adequate examples for the nomenclature of non substituted *bicyclo* compounds are given in (**Fig. 12.31).**

Non substituted *bicyclo* compounds:



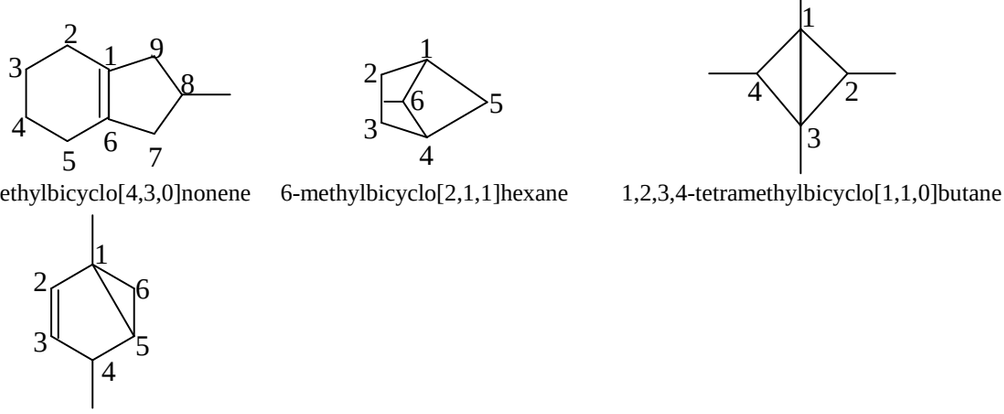
bicyclo[2,1,0]pentane bicyclo[3,1,0]hexane bicyclo[3,2,0]heptane bicyclo[2,2,0]hexane

bicyclo[4,1,0]heptane bicyclo[2,2,1]heptane bicyclo[2,2,2]octane bicyclo[4,4,0]decane

Fig. 12.31. IUPAC Nomenclature of non-substituted bicyclo compounds.

In case of substituted *bicyclo* compounds (**Fig. 12.32)** numbering is to be started from the common point vertex and is continued to the next longest fused ring and thus the shortest fused ring is numbered later on.

Substituted *bicyclo* Compounds:-



8-methylbicyclo[4,3,0]nonene 6-methylbicyclo[2,1,1]hexane 1,2,3,4-tetramethylbicyclo[1,1,0]butane

1,4-dimethylbicyclo[3,1,0]hex-2-ene.

Fig. 12.32. IUPAC Nomenclature of substituted bicyclo compounds.

B. Innovative Method for IUPAC Nomenclature of Spiro Compounds

The format of IUPAC nomenclature of non substituted *spiro* compounds is *'spiro[a,b]alkane'* and for substituted *spiro* compounds formats are *'x-substituentspiro[a, b]alkane'* (in presence of only one substituent);

'x-substituentspiro[a,b]alkene/alk-y-ene' (in presence of one double bond and one substituent); *'x,x-disubstituentspiro[a, b]alkene/alk-y-ene'* (in presence of one double bond and two same substituents) and *'x, x-disubstituentspiro[a, b]alka-y, z-diene'* (in presence of two double bonds and two same substituents).

Here 'a' and 'b' are the minimum and maximum number of points respectively in the fused ring system excluding common point (cp); x = position no of the substituents present in the ring system; y and z = position numbers of the double bonds and the suffix 'alkane' corresponding to the total number of points i.e. carbon atoms in the ring system including common point.

Since in *'spiro'*, the starting letter 's' stands for 'small' (minimum), so, during IUPAC naming of *spiro* compounds first write in the third parenthesis'[ ]', minimum no of points 'a' followed by maximum no of points 'b'. Sometimes, where a = b, then write 'a' after 'b' or vice versa.

In case of numbering of substituted spiro compounds, give priority to the smaller ring system and the numbering starts from the atom next to the common point (cp) of *spiro* and proceeds to the smaller ring first and then bigger ring later on (**Fig. 12.33)**.

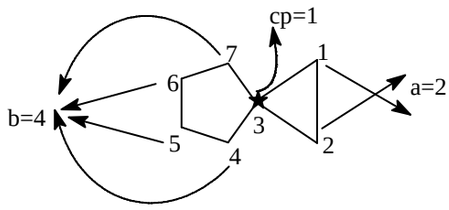
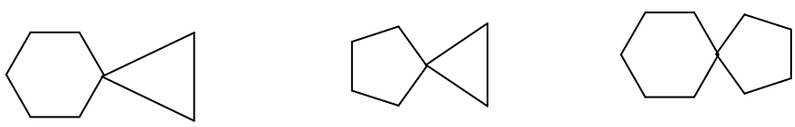


Fig. 12.33. Spiro[2, 4]heptane.

In spiro[2,4]heptane (**Fig. 12.33)**, the minimum no of points, 'a' = 2, and maximum no of points, 'b'=4, is denoted by arrow mark and the common point (cp = 1), is denoted by an asterisk mark.

Adequate examples for the nomenclature of non substituted and substituted *Spiro* compounds are given in Figure (**Fig. 12.34)** and (**Fig. 12.35)** respectively.

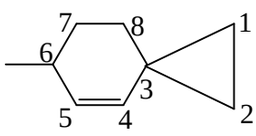
Non Substituted *Spiro* compounds:-



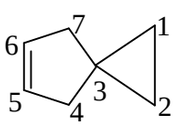
Spiro[2,5]octane Spiro[2,4]heptane Spiro[4,5]decane

Fig. 12.34. Nomenclature of non substituted spiro compounds.

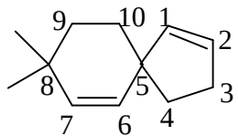
Substituted *Spiro* compounds:-



6-methylspiro[2,5]oct-4-ene



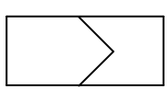
Spiro[2,4]hept-5-ene



8,8-dimethylspiro[4,5]deca-1,6-diene

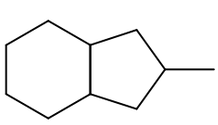
Fig. 12.35. Nomenclature of substituted spiro compounds.

PROBLEMS ON IUPAC NOMECLATURE OF BICYCLO AND SPIRO COMPOUNDS

Q.1. The compound,  **is named as:**

a.bicyclo[2,2,1] heptane b.bicyclo[2,2,0] hexane c.bicyclo[2,2,0] heptane d.bicyclo[2,1,0] heptane

Ans: a.bicyclo[2.2.1] heptane

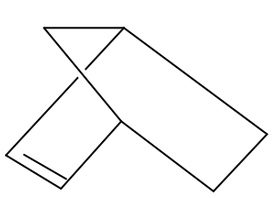
Q.2. The compound,  **is named as:**

a.1-methylbicyclo[4,3,0] nonane b.8-methylbicyclo[4,3,0] nonane c.3-methylbicyclo[4,3,0] nonane

d.4-methylbicyclo[4,3,0] nonane

Ans: b.8-methylbicyclo[4,3,0] nonane

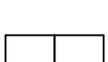
Q.3. Following is named as bicyclo[x,y,z] hept-2-ene



here, (x+y+z) is

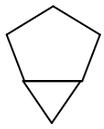
a.4 b.3 c.5 d.6

Ans: c. bicyclo[2,2,1] hept-2-ene, where, x = y = 2 & y = 1, hence, x+y+z = 5

Q.4. The compound,  **is named as:**

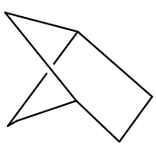
a.bicyclo[2,2,2] hexane b.bicyclo[3,2,1] hexane c.bicyclo[2,1,1] butane d.bicyclo[2,2,0] hexane

Ans: d.bicyclo[2,2,0] hexane

Q.5. The compound,  **is named as:**

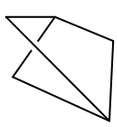
a.bicyclo[3,2,0] hexane b.bicyclo[3,1,0] hexane c.bicyclo[3,2,1] hexane d.bicyclo[2,2,0] hexane

Ans: b.bicyclo[3,1,0] hexane

Q.6. The compound,  **is named as:**

a.bicyclo[2,1,1] hexane b.bicyclo[2,2,0] hexane c.bicyclo[3,1,1] hexane d.bicyclo[3,1,0] hexane

Ans: a.bicyclo[2,1,1] hexane

Q.7. The compound,  **is named as:**

a.bicyclo[2,1,0] pentane b.bicyclo[1,1,1] pentane c.bicyclo[1,1,1] pentane d.bicyclo[2,1,1] hexane

Ans: b.bicyclo[1,1,1] pentane

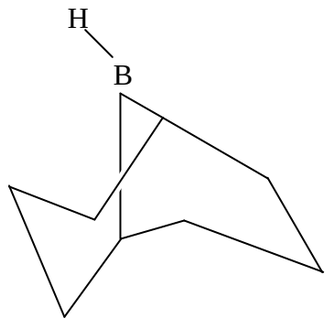
Q.8.The order of priority of the functional groups in IUPAC system of nomenclature is (STGT 2017)

(a) — CHO > >C=O > —OH > >C=C< (b) >C=O > —CHO > —OH > >C=C<

(c) —CHO > —OH > >C=O > >C=C< (d) >C=C< > —CHO > >C=O > —OH

Ans: a) — CHO > >C=O > —OH > >C=C< **(see appendix H)**

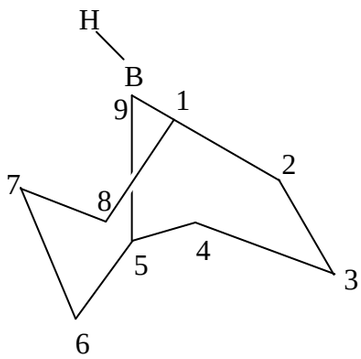
Q.9. The IUPAC name of the following compound is **(NET 2017)**



a)9-borabicyclo[3.3.1]nonane b)1-borabicyclo[3.3.1]nonane c)9-borabicyclo[3.3.0]octane

d)1-borabicyclo[3.3.0]octane

Ans: a) 9-borabicyclo[3.3.1]nonane (here, X = Y = CP = 3 - see below)



It may be expected that these time economic organic innovative mnemonics for the IUPAC nomenclature of bicyclo and spiro compounds, would go a long way to help the students of chemistry from Undergraduate to Post-Graduate level. Experiments, *in vitro,* on 100 students, showed that by using these formulae students can save up to 2-3 minutes' time in the examination hall. On the basis of this, I can strongly recommend using these time economic innovative methods in the field of hydrocarbons in general organic chemistry.