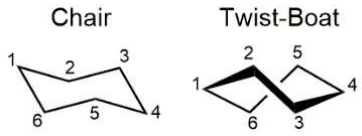
4. This question is about the molecule twistane

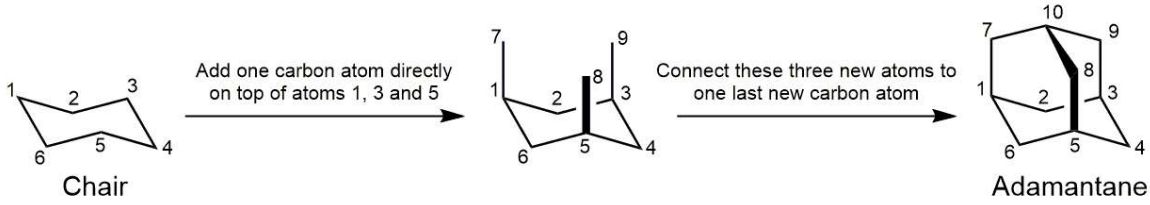
Although the skeletal structure of cyclohexane (C_6H_{12}) is often represented as a regular hexagon, it is actually a flexible molecule that exists in a variety of different shapes referred to as *conformations*. Two of these conformations, the c*hair* and the *twist-boat*, are shown below. The carbon atoms in the six-membered rings have been numbered 1-6 to show their connectivity.



The chair is the lowest energy conformation of cyclohexane with all the bond angles almost equal to the ideal angle for a tetrahedral carbon atom. The twist-boat is higher in energy.

(a) By how many degrees does the ideal C–C–C angle in the chair form of cyclohexane differ from that in a regular hexagon?

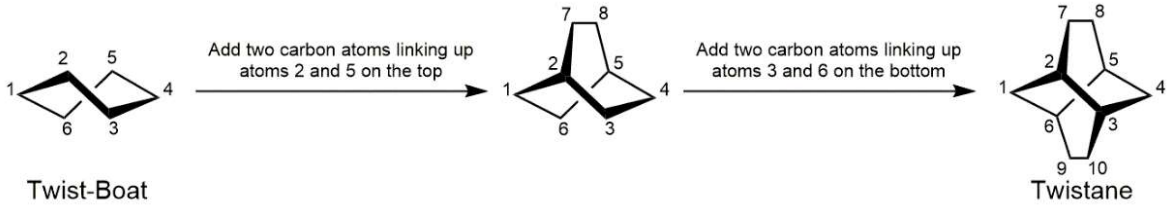
The molecule *adamantane* can be visualised by the addition of a further four carbon atoms onto the chair conformation of cyclohexane as shown below. In doing this, other six-membered rings are created. In adamantane all the six-membered rings are locked in the chair conformation.



(b) For each unique six-membered ring in adamantane, write down the numbers of the six carbon atoms in that ring in the order they are connected, beginning with the lowest number (e.g. -1-2-3-4-5-6-).

(c) How many signals are there in the ^{13}C NMR spectrum of adamantane (i.e. how many unique environments of carbon are there)?

The molecule *twistane* can be visualised by the addition of a further four carbon atoms onto the twist-boat conformation of cyclohexane as shown below. In doing this other six-membered rings are created. In twistane all the six-membered rings are locked in the twist-boat conformation, which gives the molecule its name.

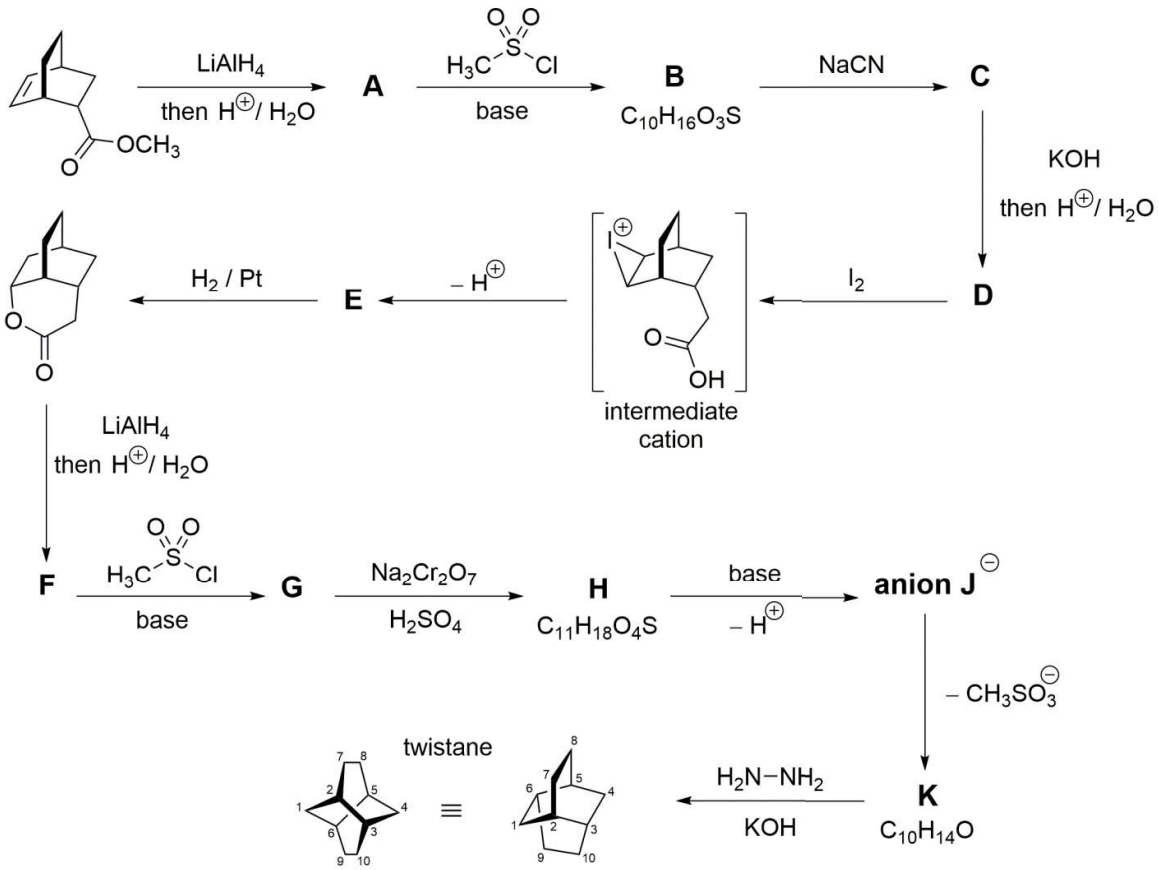


(d) For each unique six-membered ring in twistane, write down the numbers of the six carbon atoms in that ring in the order they are connected, beginning with the lowest number (e.g. -1-2-3-4-5-6-).

(e) How many signals are there in the ^{13}C NMR spectrum of twistane?

(f) Adamantane and twistane are isomers of each other. What is their molecular formula?

As all its rings are in the lowest energy chair conformation, adamantane is a very stable molecule. It was discovered as a component of crude oil in 1933. By contrast, twistane is a very strained molecule as all its rings are in the higher energy twist-boat conformation. It must be specially synthesised, which was first done in 1962. The synthesis is shown below.



No C–C single bonds are broken in the synthesis and so those present in the starting material remain throughout. They have already been drawn in your answer booklet and you must use them for your answers for part **(g)**.

(g) Draw the structure of compounds **A-H**, anion $\mathbf{J^-}$ and compound **K**.

(h) Answer the following multiple choice questions in the answer booklet.

(i) How many planes of symmetry does twistane contain?

(ii) How many rotational axes of symmetry does twistane contain?

(iii) Is twistane superimposable on its mirror image?