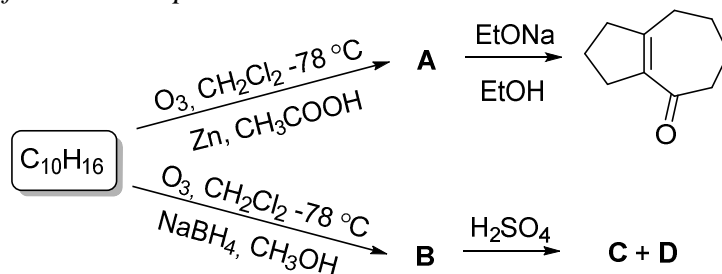


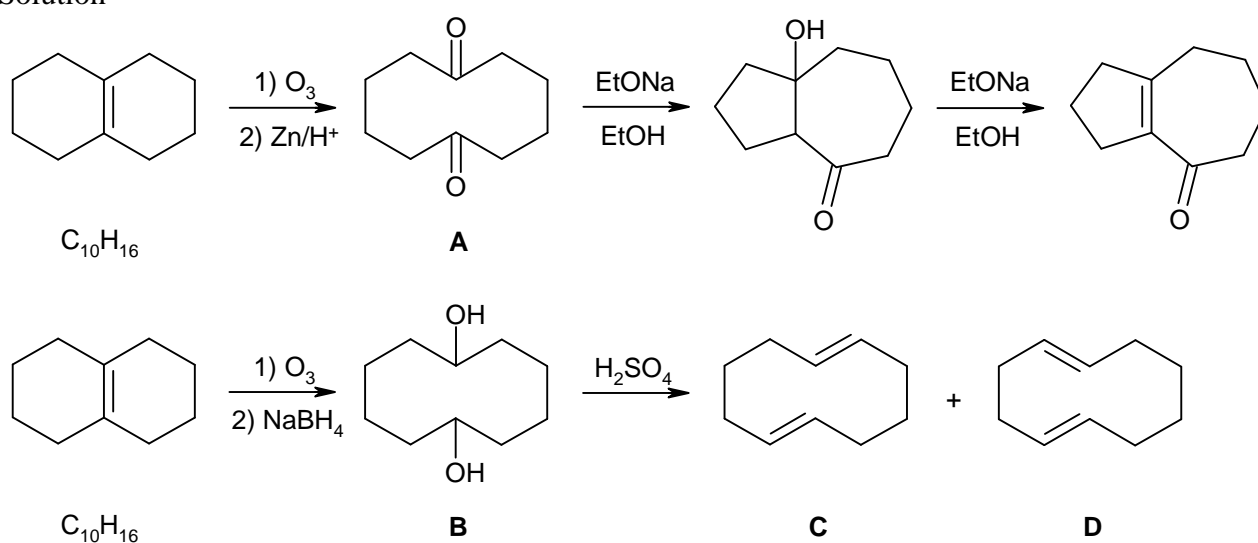
Problema 3 Essential ozone

Some hydrocarbon $C_{10}H_{16}$ participates in the transformations given in Scheme 1.

1. Determine the structural formulae of the hydrocarbon $C_{10}H_{16}$ and the molecules A–D accounting for the fact that compounds C and D are isomers of the initial hydrocarbon; the ozonolysis of C followed by the treatment of the reaction mixture with alkaline H_2O_2 produces a single product while the same transformations of D afford two compounds.



Solution

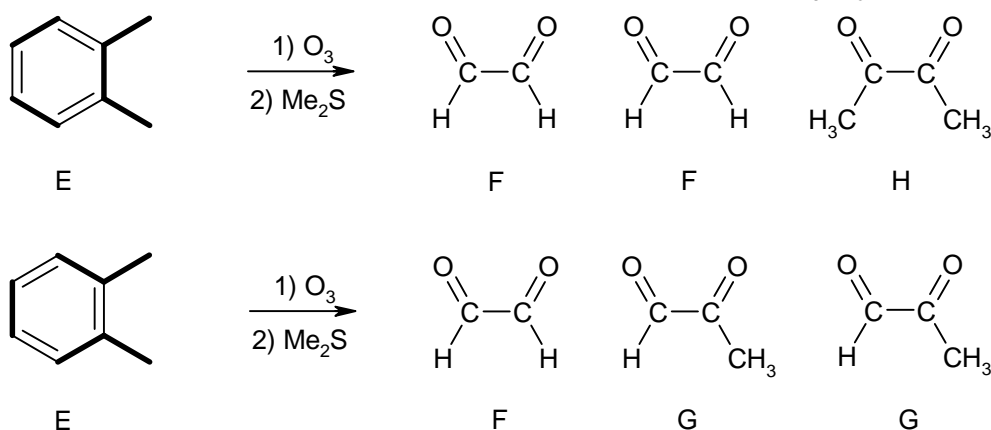


Some other hydrocarbon **E** ($\omega_C = 90.6\%$) under ozonolysis (1. O_3 , CH_2Cl_2 , $-78\text{ }^\circ\text{C}$; 2. Me_2S) forms three carbonyl compounds – **F** ($C_2H_2O_2$), **G** ($C_3H_4O_2$), and **H** ($C_4H_6O_2$) in a ratio of 3:2:1. Initial hydrocarbon **E** doesn't decolorize bromine water.

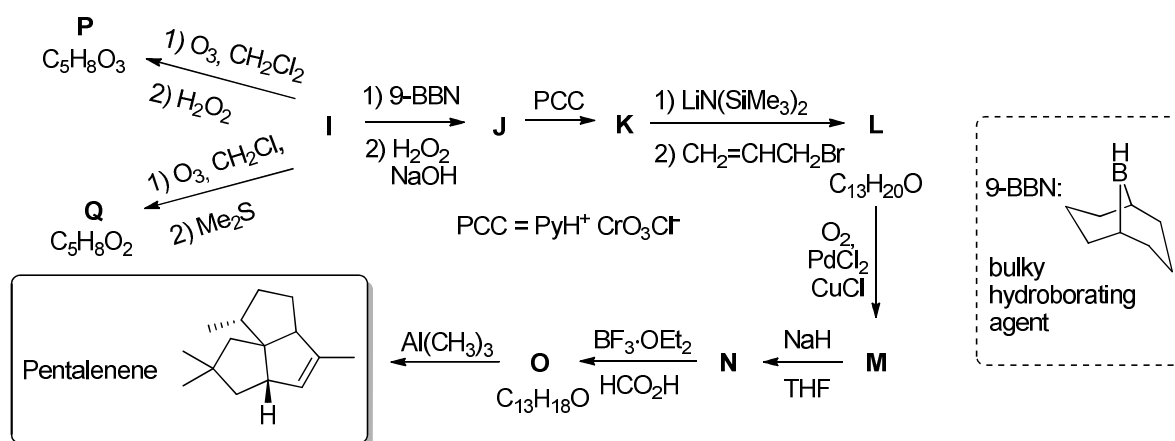
2. Write down the structural formulae of hydrocarbon **E** and products of its ozonolysis **F–H**.

Solution

Hydrocarbon **E** has 90,6% of C, 9,4% of H. Then its empirical formula is C_4H_5 . Hydrocarbon **E** is aromatic because it doesn't decolorize bromine water, so it is C_8H_{10} ortho-xylene.



Hydrocarbon **I** having center of symmetry was used as an initial material in the total synthesis of **pentalenene** (Scheme 2):

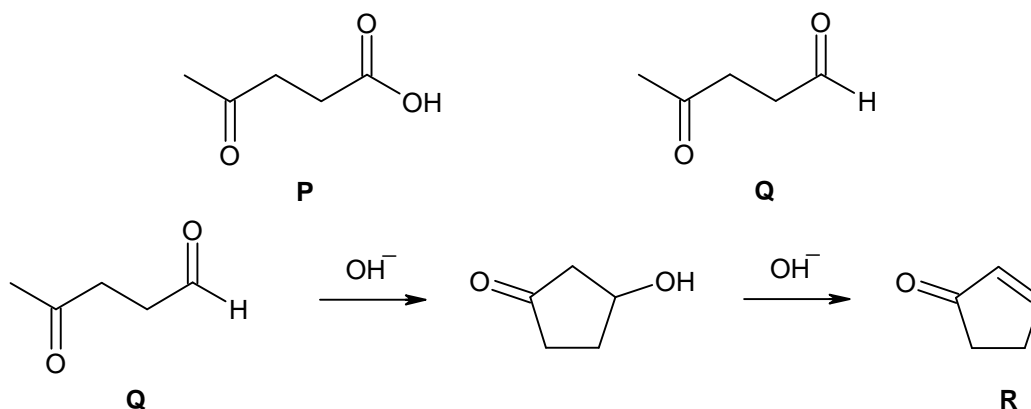


The ozonolysis of hydrocarbon **I** furnishes a single compound **P** or **Q** depending on the treatment of the ozonolysis product. Under treatment with I_2 and NaOH , compound **Q** forms a yellow precipitate containing 96.7% of iodine. Under basic conditions compound **Q** is transformed into compound **R** containing 4 types of hydrogen atoms (4 signals in ^1H NMR spectrum with integral intensity of signals 1:1:2:2). Molecular formula of **R** is $\text{C}_5\text{H}_6\text{O}$. Molecule of compound **N** has bicyclic framework containing **R** as a fragment. Molecule of **O** consists of three rings.

3. Describe the scheme of the synthesis of **pentalenene**.

Solution

P and **Q** differ for a single oxygen atom then **Q** is ketone and aldehyde and **P** is ketone and acid. **Q** is a methylketone because it gives the iodoform reaction. **Q** and **P** are then:

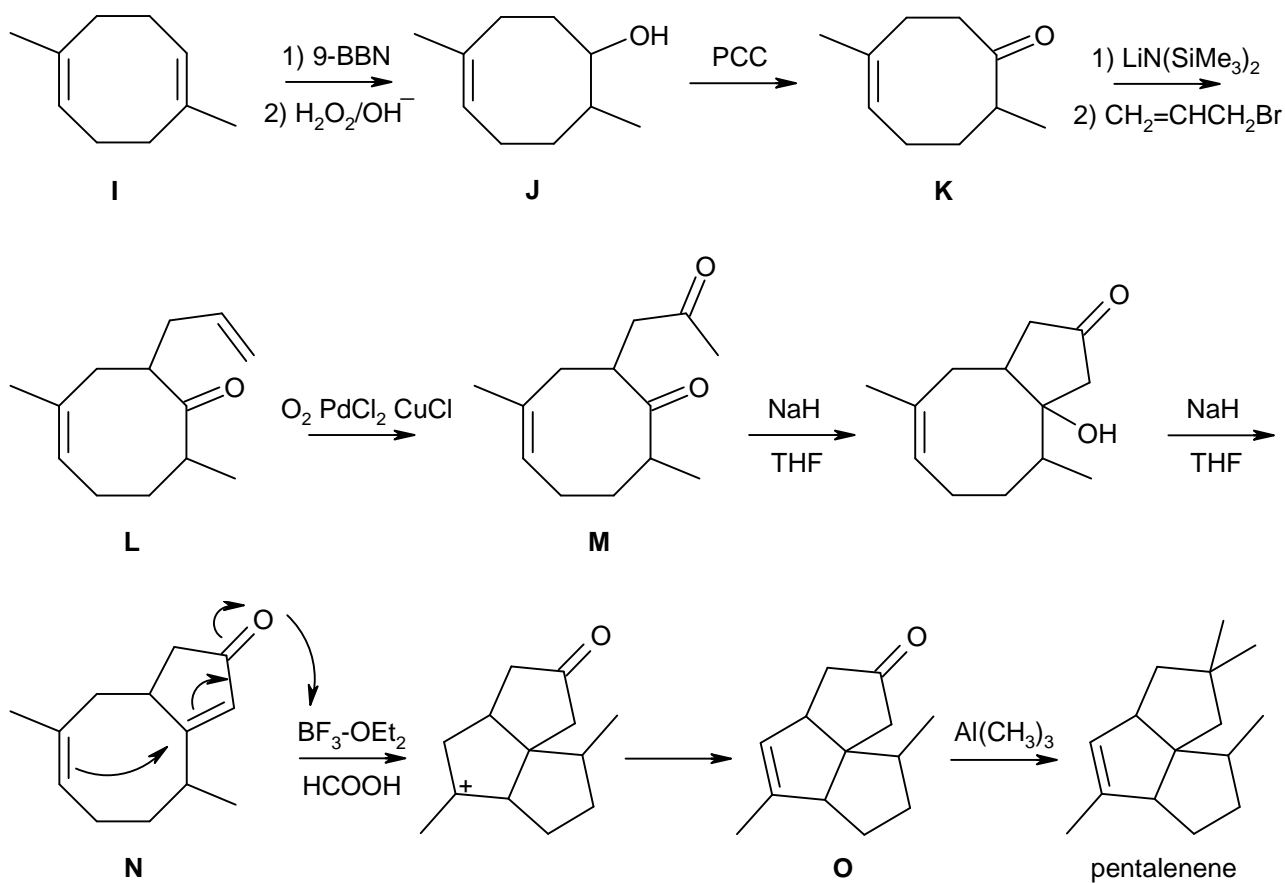


Assembling **P** and **Q** we obtain **I**. There are two possibilities:



But only the first one is correct because it has a center of symmetry.

Then the synthesis of **pentalenene** is as follows:



Soluzione proposta da
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