Problem of the Day 13
Section 4.1 4.2
Question 4.04 (c) and (d)

In Question 4.04, parts (c) and (d) are a two-step reaction sequence. The products from part (c) are the intermediates in the reaction that starts with the bromo-alcohol and ends with the 4-membered ring. Construct an energy diagram for that two-step reaction that starts with the bromo-alcohol and ends with the 4-membered ring. What are the different relative energy issues that need to be decided for drawing this diagram?

(c)

(d)

This question does not ask you to construct the Energy Diagram, but rather to reflect on what are the different relative energies needed to construct one. In fact, figuring out what these energies are would be a bit challenging here, and there would likely be debate - even among fairly experienced people (which is why we do experiments and make measurements).

| energy of A | energy of B | energy of C |
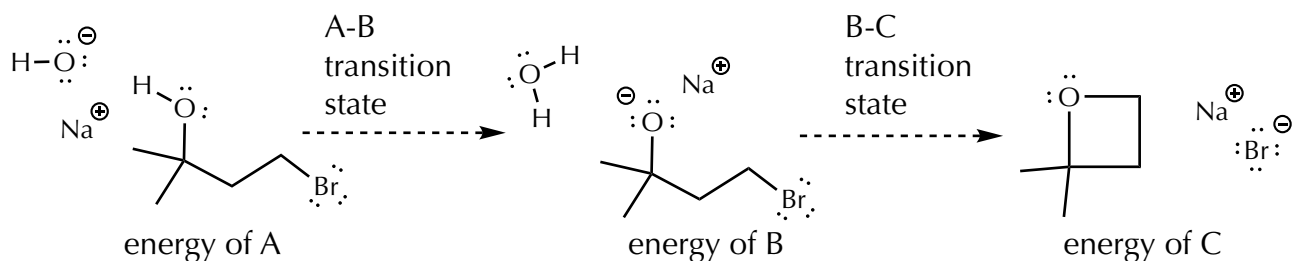
# of steps = 2 : A-to-B, B-to-C
# of intermediates = 1 (B)
# of transitions states = 2
# of energy minima = 3 : A, B, C

what is needed: relative energies of A, B, and C to place them on the diagram
what is needed: relative energies of the two transition states to place them in between

what is comparably easy to assess: A-to-B is a proton transfer (Brønsted acid base) where the pK$_a$ values of the acid (ROH) and conjugate acid (HOH) are nearly equal, to the A to B energy difference is predicted to be low (if only the organic molecule is included, then the energy of B, the anion, is higher than A, the neutral alcohol); the activation energy for proton transfer is also low; the activation energy for the second step is likely much higher, as a small ring needs to form