Section Question 2

Petroleum fuels for vehicles are usually composed of alkanes with intermediate carbon-chain lengths—high enough molecular weight so that they are non-volatile and non-explosive, but low enough so that they aren't too viscous. (Octane, C_8, has these optimal characteristics.) Gaseous hydrocarbons with lower molecular weights are more readily available, and it would be very useful to be able to convert butane (C_4) from natural petroleum gas, for example, to higher molecular weight chains.

Brookhart and coworkers recently reported a method for "metathesizing" short alkanes to a distribution of shorter and longer ones by simultaneously exposing them to two catalysts.[1] The overall reaction can be summarized in three steps, which are shown on the next page. (I've drawn the catalysts active in each step, but you can ignore them for this problem.)

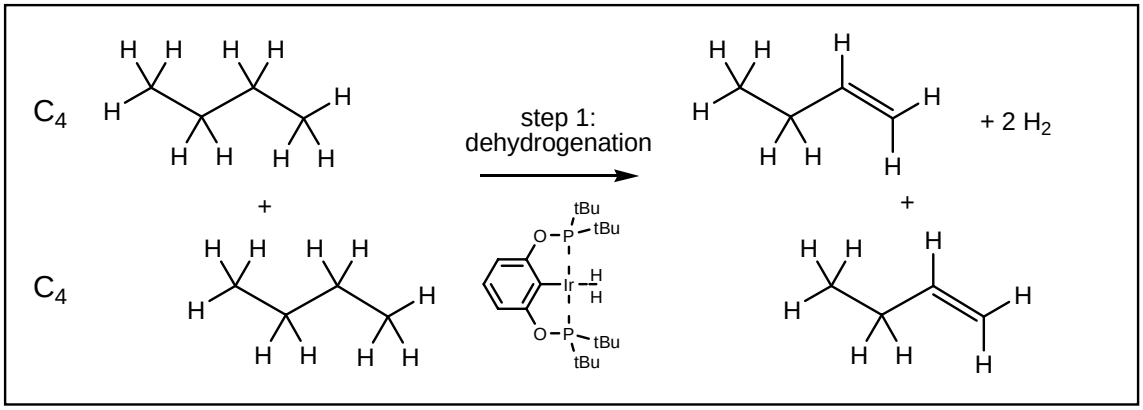
a. For each of the three steps, which bonds are made and which bonds are broken? How much energy is each of these bonds worth? Write your answers in the worksheet on page 3.

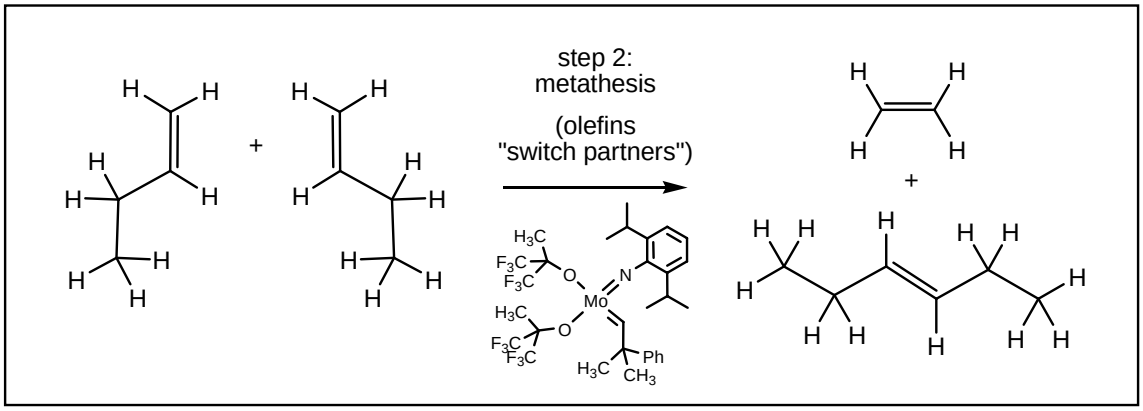
b. What is the overall $\Delta H°$, then, for each reaction step? Again, answer on the worksheet.

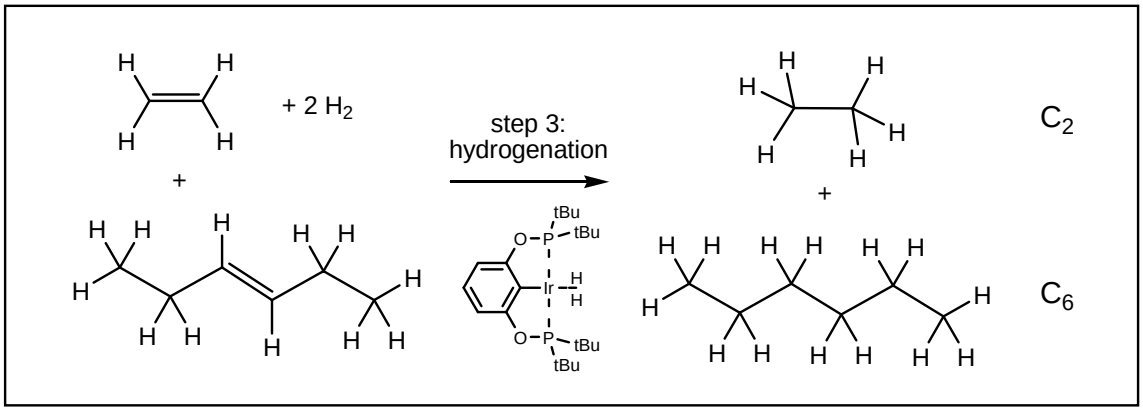
c. What would you guess ΔG to be for each step? Are there any entropy contributions to each step's ΔG?

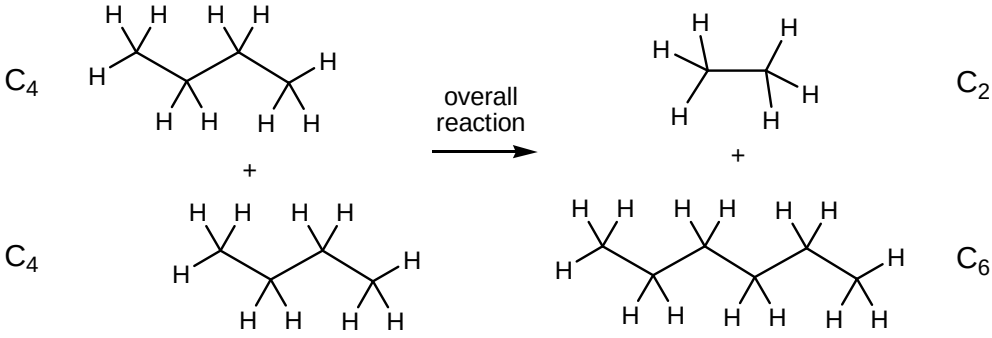
d. Draw a potential energy diagram for the overall reaction on page 4, by drawing energy levels for each intermediate state. Is the overall reaction exothermic, thermoneutral, or endothermic (all relating to ΔH)? Is it exergonic, energy neutral, or endergonic (all relating to ΔG)?

[1] Goldman, A. S.; Roy, A. H.; Huang, Z.; Ahuja, R.; Schinski, W.; Brookhart, M. *Science* **2006**, *312*, 257-261.

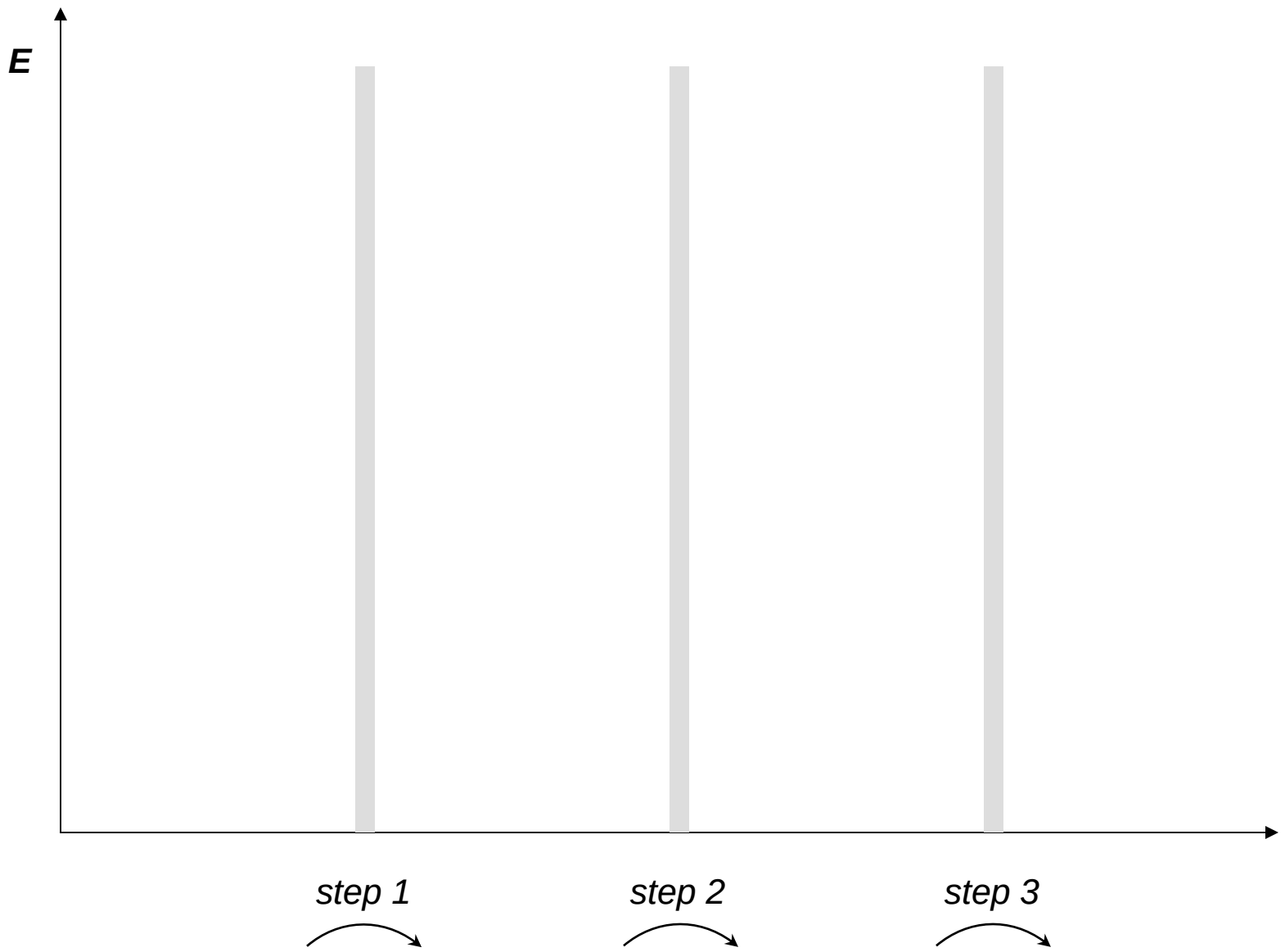

C4
step 1:
dehydrogenation
+ 2 H2
C4
tBu
tBu
O
P
Ir
H
H
O
P
tBu
tBu
tBu


step 2:
metathesis
(olefins
"switch partners")
H3C
F3C
F3C
O
N
Mo
O
H3C
F3C
F3C
H3C
Ph
CH3


+ 2 H2
step 3:
hydrogenation
C2
C6
tBu
tBu
O
P
Ir
H
H
O
P
tBu
tBu


C4
overall
reaction
C2
C4
C6

	Bonds made	Bonds broken	Bond energy gained/lost	Overall ΔH	Overall ΔG
Step 1					
Step 2					
Step 3					
Overall reaction					


E
step 1
step 2
step 3