8.4: Exercise Questions

1. Using your knowledge of elimination chemistry, please indicate which solvent, water or DMSO, would you expect to better favor the E2 elimination from this exercise and why? For full credit be sure to explain your answer.
2. Using information from your calculations or your starting materials and products please complete the following tables. Please note that the solvated value of Gibbs Free Energy is the sum of G in the gas phase, ΔG_{ENP}, ΔG_{CDS}, and $\Delta G^{\circ}{}_{\text{Conc}}$.

Starting Materials

Solvent	G (Eh) Gas Phase	ΔG_{ENP} (Eh)	ΔG_{CDS} (Eh)	$\Delta G^{\circ}{}_{\text{Conc}}$ (Eh)	Solvated G (Eh)
DMSO	-693.3164	-0.083226	-0.001211	0.003012	-693.3978
Water	-693.3416			0.003012	

Transition States

Solvent	G (Eh) Gas Phase	ΔG_{ENP} (Eh)	ΔG_{CDS} (Eh)	$\Delta G^{\circ}{}_{\text{Conc}}$ (Eh)	Solvated G (Eh)
DMSO	-693.3157			0.003012	
Water	-693.3291			0.003012	

Products

Solvent	G (Eh) Gas Phase	ΔG_{ENP} (Eh)	ΔG_{CDS} (Eh)	$\Delta G^{\circ}{}_{\text{Conc}}$ (Eh)	Solvated G (Eh)
DMSO	-693.3805			0.00301	
Water	-693.3804			0.00301	

3. To make our reaction coordinate diagram easier to interpret we will be normalizing all of our energy values to the energy of the starting materials in water. To do this, all you need to do is add the value of the Solvated Gibbs free energy (G) you are interested into the Solvated Gibbs free energy (G) of the starting materials in water. Using the values that you have documented in question 2 please complete the following tables. Please note that he conversion between energy in Hartree (Eh) and kcal/mol is 1 Eh = 627.5 kcal/mol. **Hint**: you will have completed this calculation correctly if the Normalized Solvated G for the starting materials in water is 0 Eh.

Water Solvent

Water Solvent	Solvated G (Eh) (See Question 2)	Normalized Solvated G (Eh)	Normalized Solvated G (kcal/mol)
Starting Materials			
Transition State			
Products			

DMSO Solvent

DMSO Solvent	Solvated G (Eh) (See Question 2)	Normalized Solvated G (Eh)	Normalized Solvated G (kcal/mol)
Starting Materials	-693.39786		
Transition State			
Products			

4. Using the thermodynamic data (in kcal/mol) please create a reaction coordinate diagram that includes a pathway for both the reaction in DMSO and in Water.

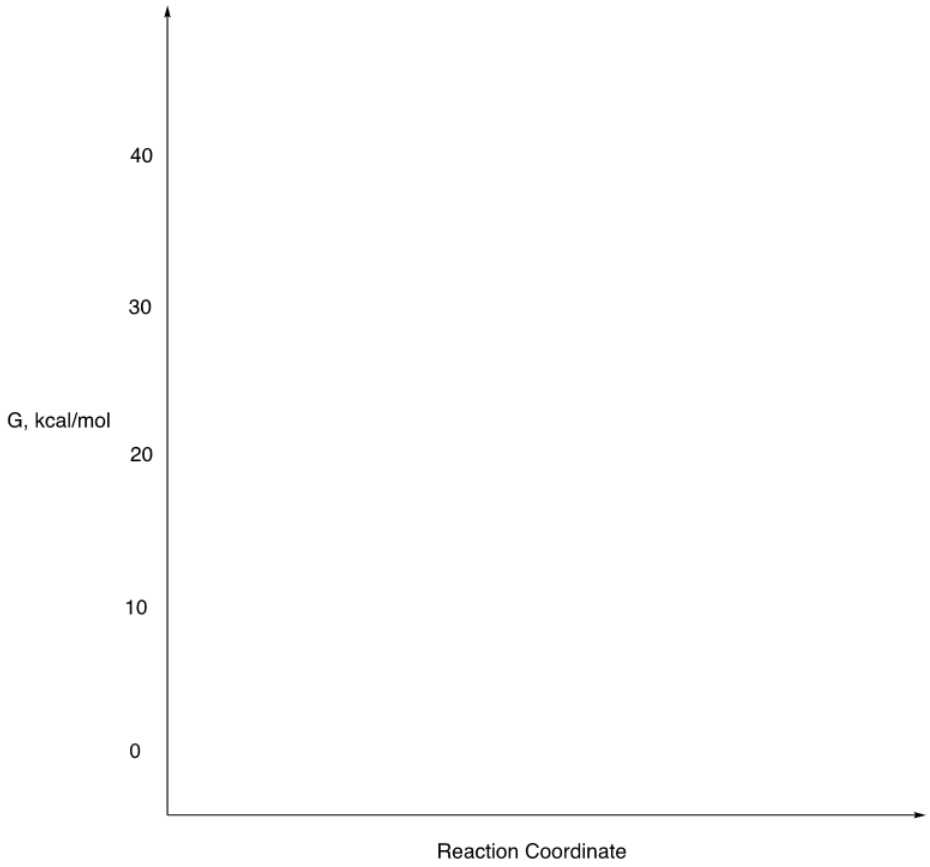

Figure 8.4.1: Copy and Paste Caption here. (Copyright; author via source)

5. Using your data and the reaction coordinate diagram in question 4 for support, please indicate which reaction you would expect to proceed more quickly and explain why you believe this is the case.
