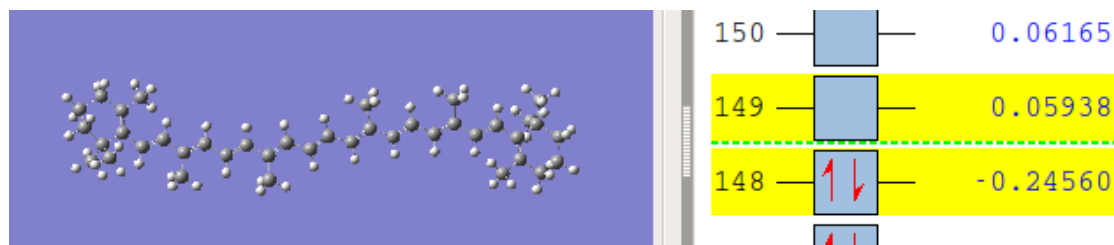


# Assignments to ComputChem

## Q1

1. Estimate its HOMO-LUMO energy gap using the particle-in-a-box model.



Command: b3lyp/6-31g(d) pop=(nbo,savenbos) geom=connectivity

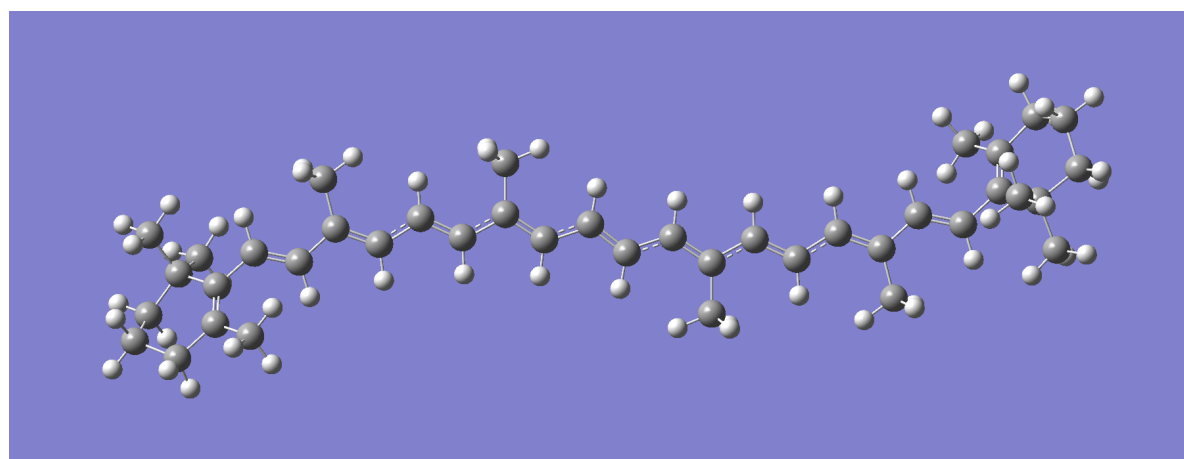
After the implementation of particle in a box model, I get the molecule orbit as follows.

NBO index	Molecular units	Energy(Hartree)	Class
148	CR (1) C 40	-0.024560	HOMO
149	RY*(1) C 1	0.05938	LUMO

Consequently, the HOMO-LUMO energy gap is 0.08394 Hartree

2. Obtain its stable structure using a proper quantum mechanical method and briefly

describe the structure.



Command: opt=calcfc b3lyp/6-31g(d)

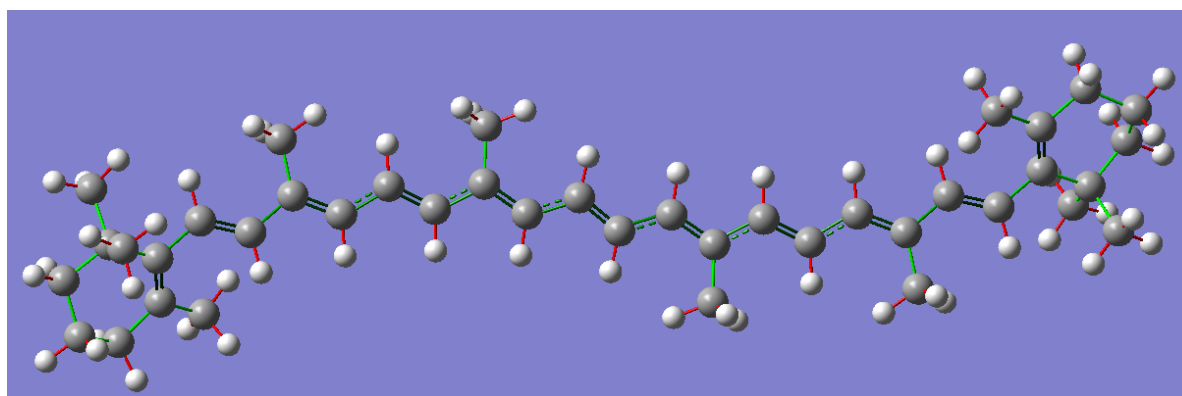
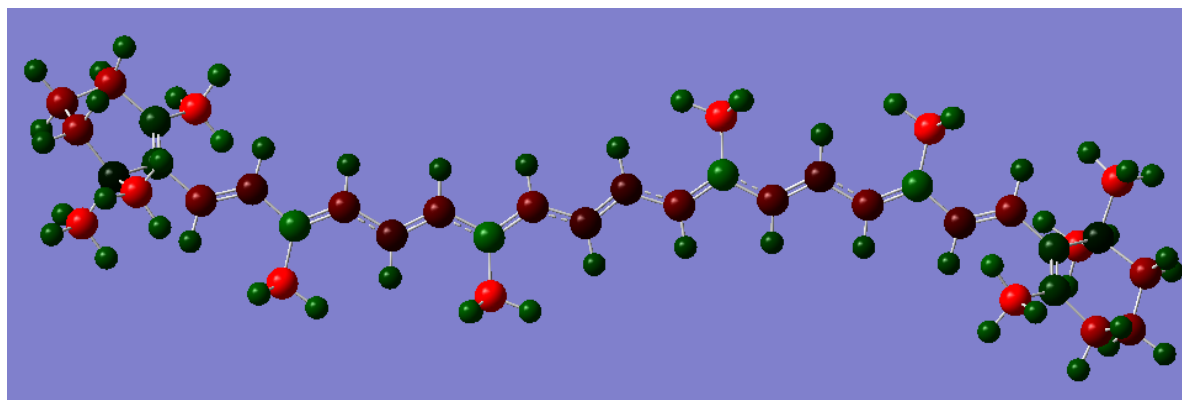
In this case, I choose B3LYP and 6-31G(d) as the calculation parameters. And after 13 steps, the total energy converge at around -1557.9 Hartree. Indicating the normal termination of optimization process. The description of the optimized molecule

Beta-carotene, with the molecular formula  $C_{40}H_{56}$ , owns a long chain of conjugated double bonds together with two retinyl groups. The huge conjugated structure equip this molecule of highly-delocalized electron groups.

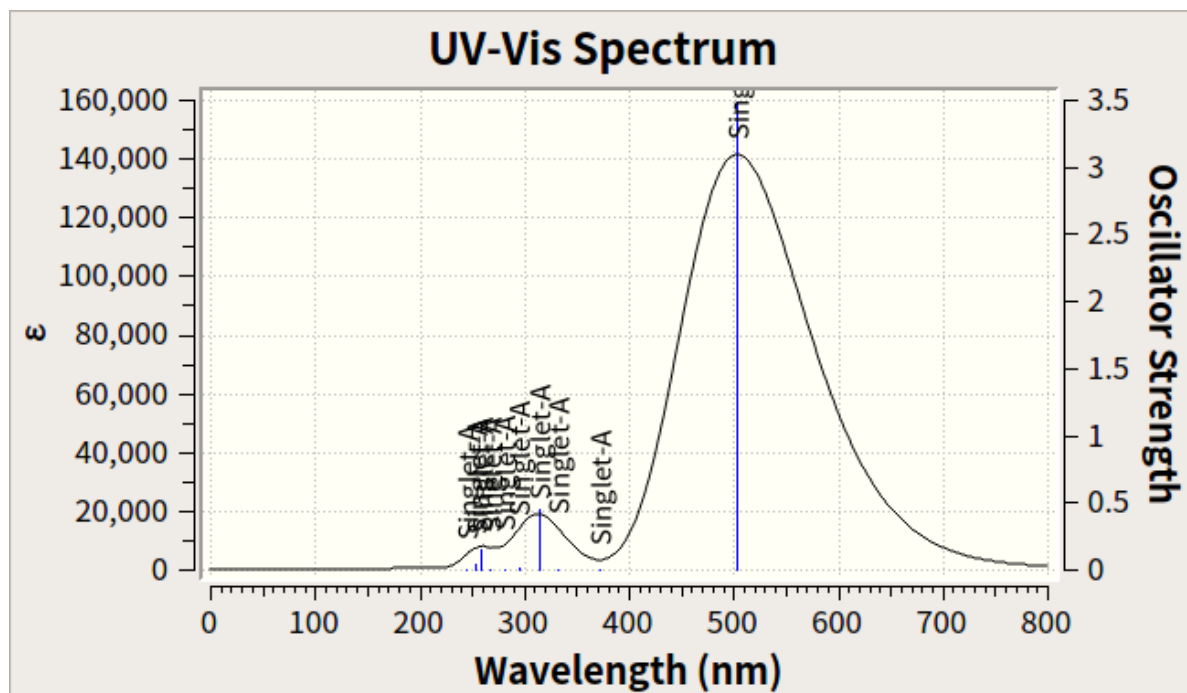
As the picture describes, there are up to 40 electron pairs located in a same energy level, illustrating the delocalization of the electrons.

The distribution of charge and bonds' length also prove the delocalization of electrons. As is shown in the figure, the charge of the central chain goes through a sort of equalization, which also happens in the bond length.

Class	Typical Bond Length(pm)	Typical Bond Order
<i>Ethylene</i>	(C=C) 133.9	2
<i>Ethene</i>	(C-C) 152.8	1
$\beta$ - Carotene	(C=C)137.4 (C-C) 144.3	(C=C)2 (C-C)1.5

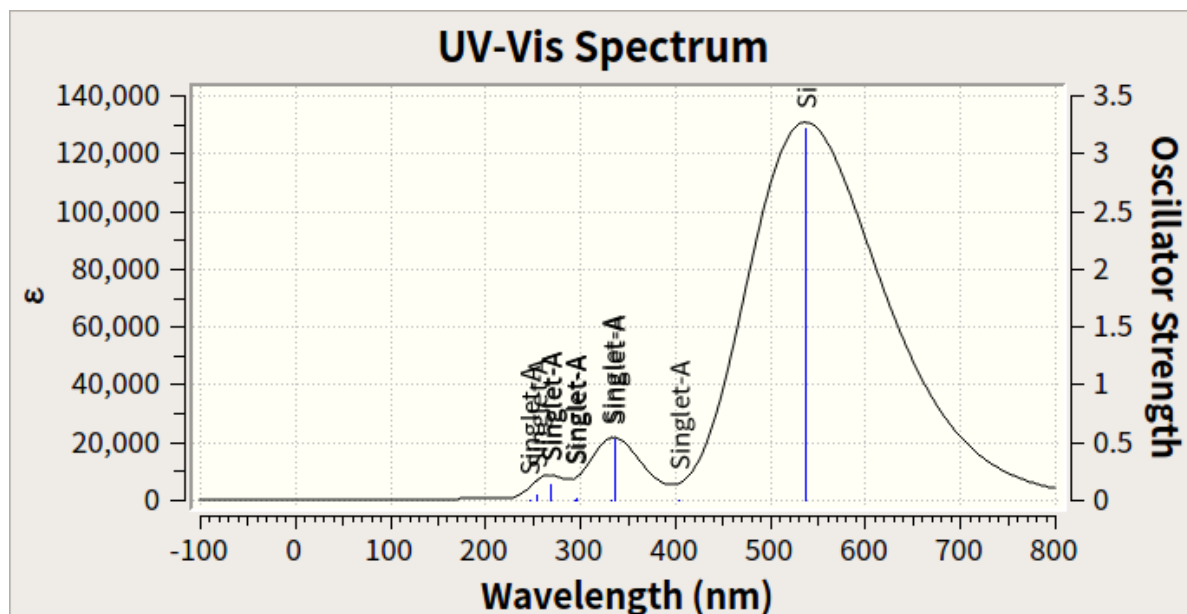


**3. Based on the structure obtained in step 2, compute its UV-Vis spectra in the gas phase, using the ZINDO method (nstates=10).**



Command: zindo=(astates=10)

**4. Re-compute its UV-Vis spectra in ethanol using the same method with the IEFPCM solvation model**

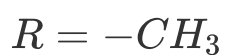
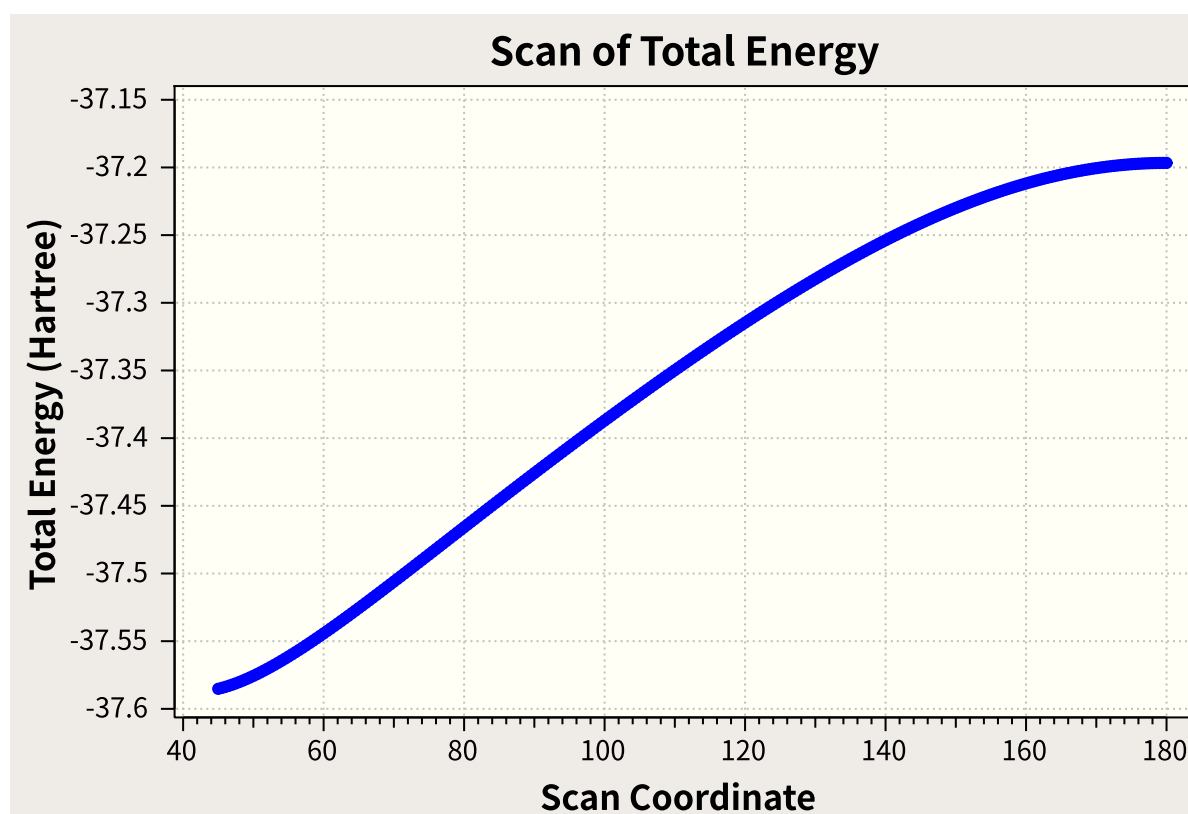
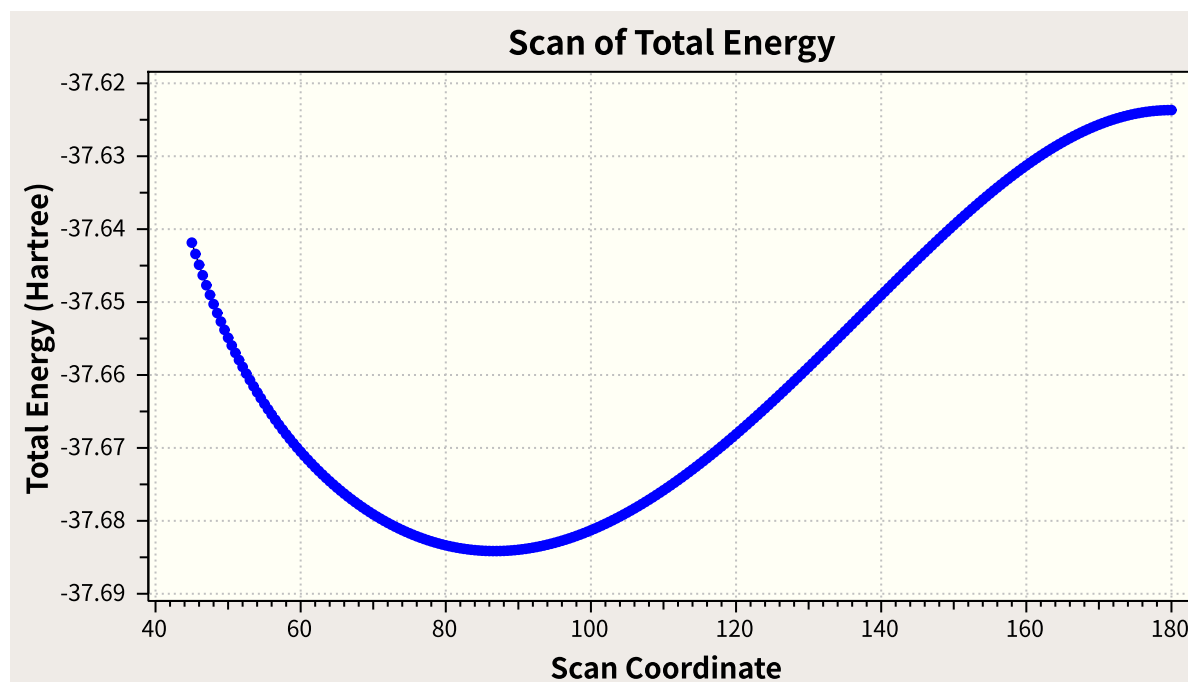
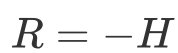


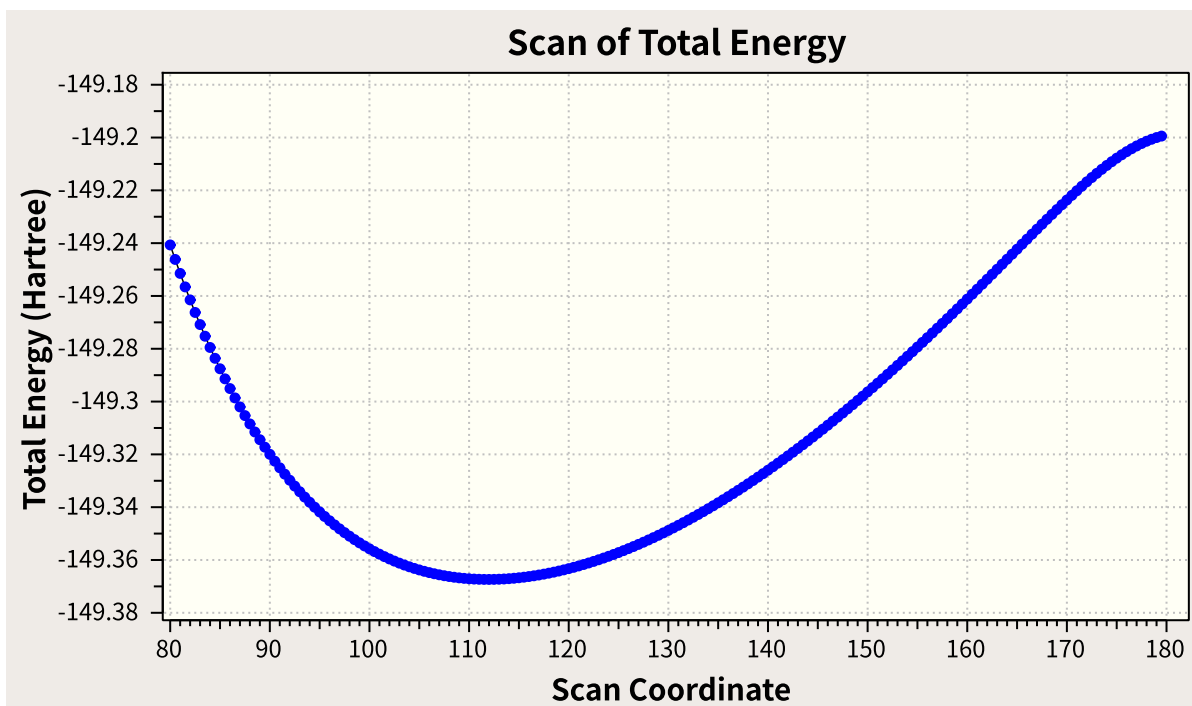
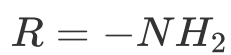
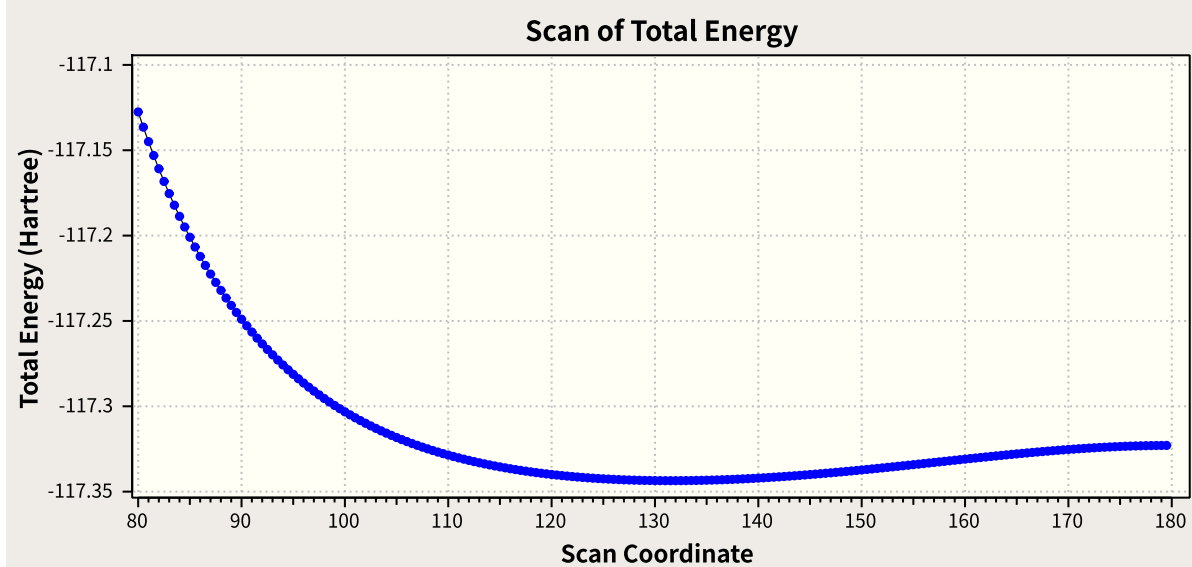
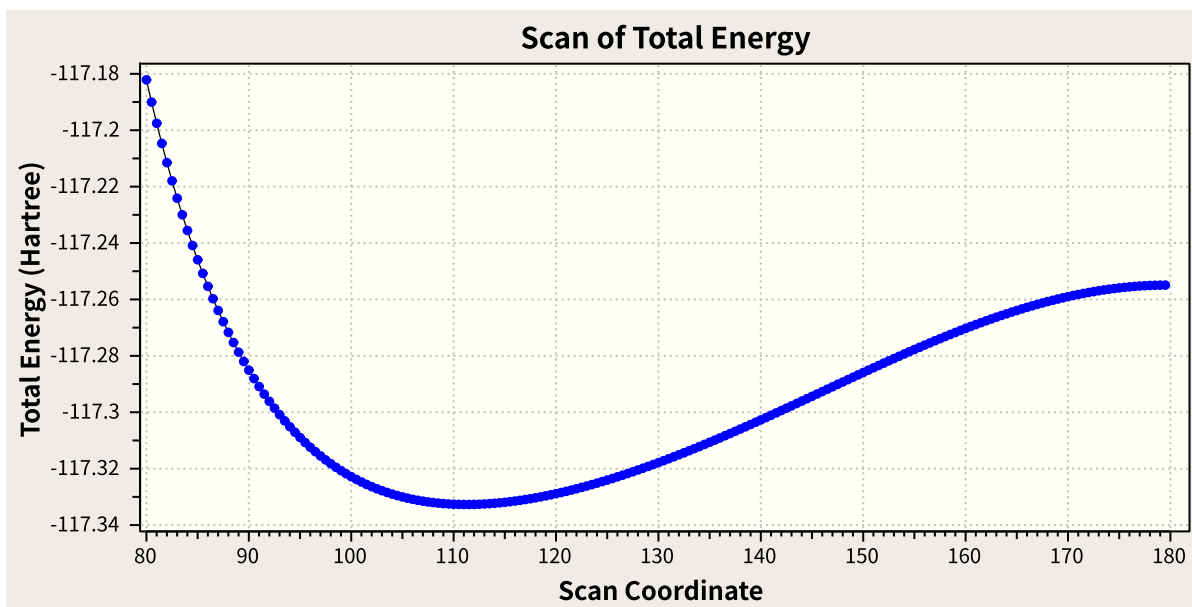
Command: zindo=(nstates=10) scrf=(iefpcm,solvent=ethanol)

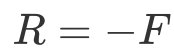
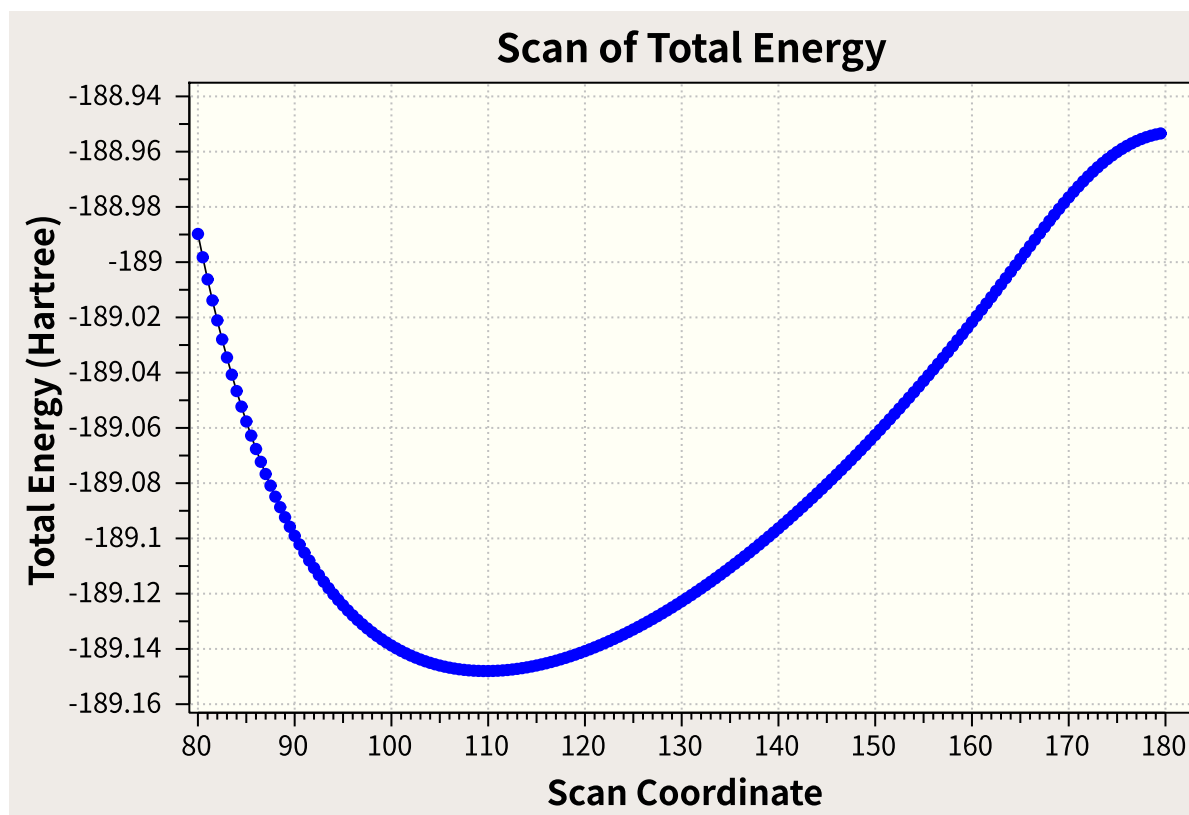
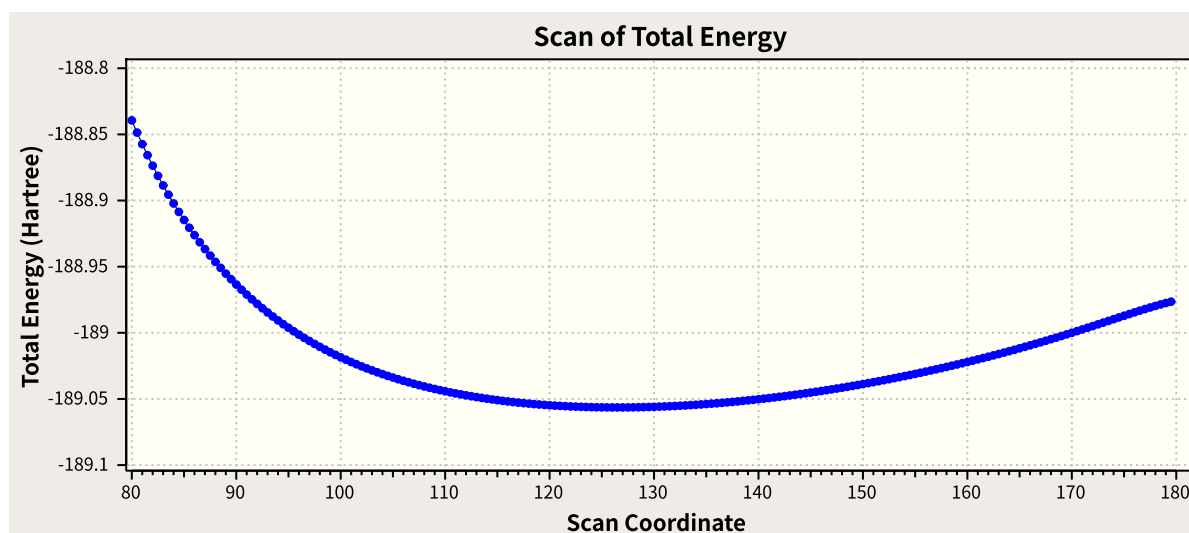
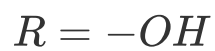
**5. The experimentally measured maximum UV-vis absorption peak in ethanol is 450 nm. Discuss all the computed and the experimental excitation energy values and comment on**

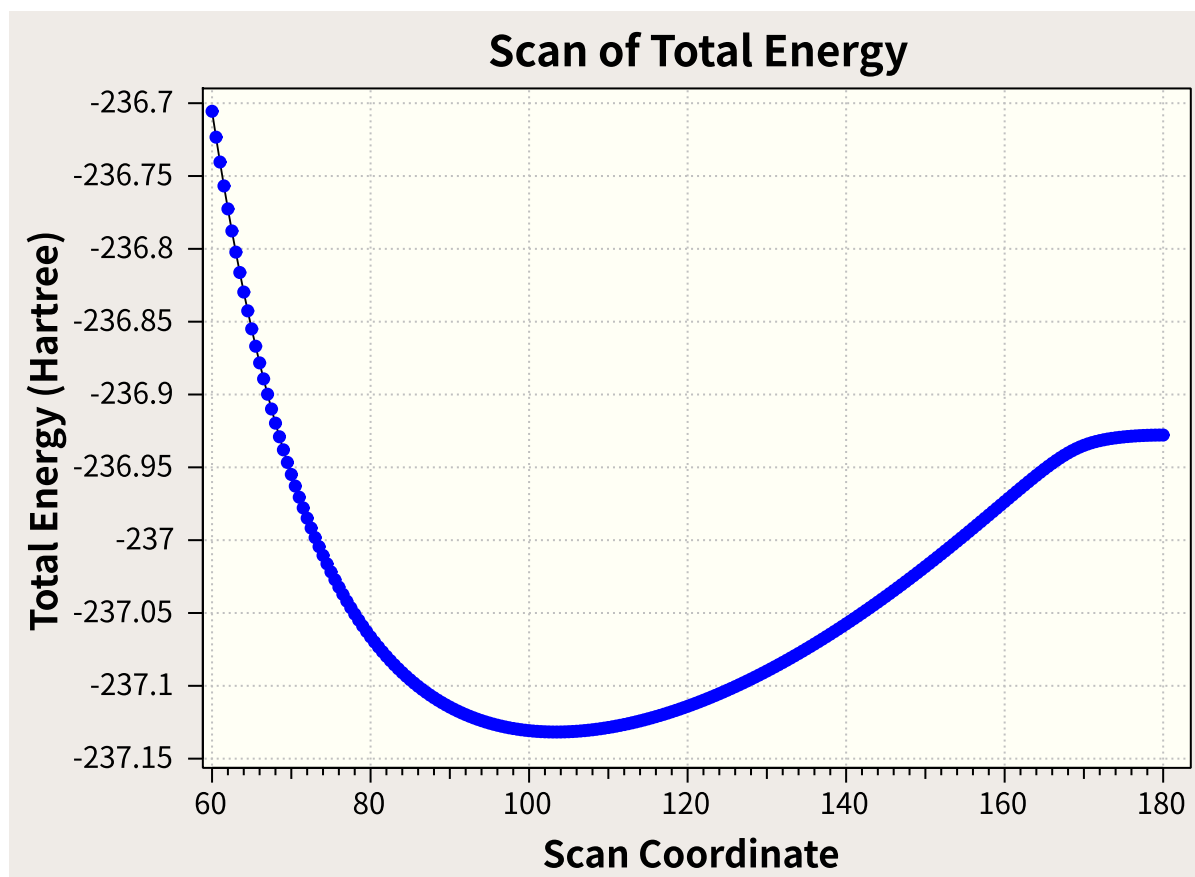
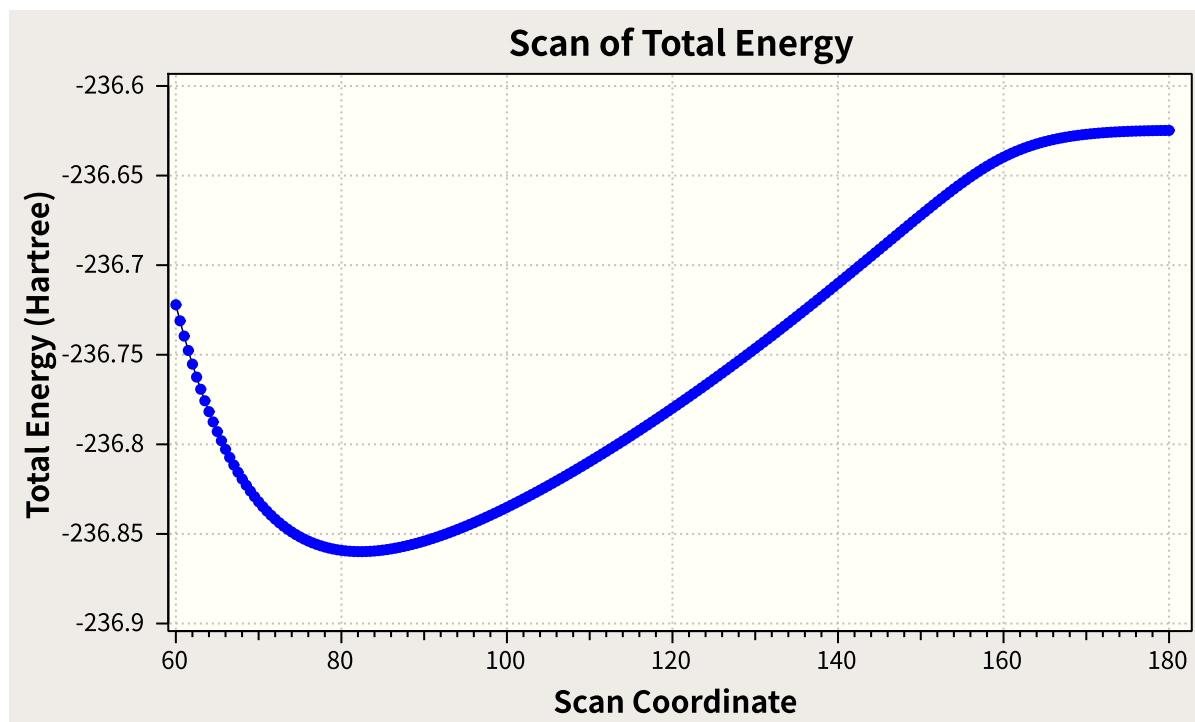
the models used.

Q2









Q3