計算生物（二）第三周作業
0317033 謝明修

For hydrogen molecule:

1. Construct the PES of $H_2$ dissociation at the level of UHF/6-31G. Plot the curve and calcuate the bond dissociation energy (BDE). (Figure1.)
2. Calculate BDE for 2H →$H_2$ at the level of CCSD(T)/aug-cc-pVTZ. (Table1.)

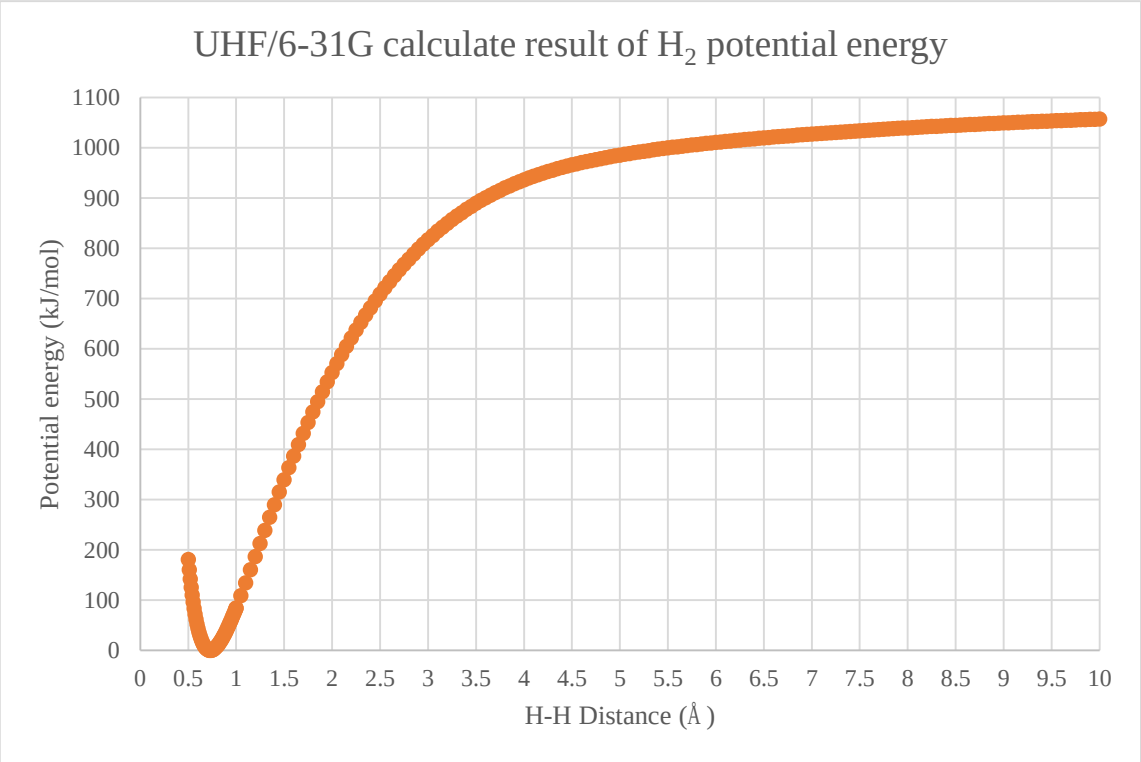


**Figure1.** The potential energy curve with different H—H distance. Calculated at the level of UHF/6-31G. Note that the energy is much larger than experimental value.

**Table1.** The bond dissociate energy computed at the level of UHF/6-31G and CCSD(T)/aug-cc-pVTZ.

| | UHF/6-31G | CCSD(T)/aug-cc-pVTZ | Experimental value |
|---|---|---|---|
| H (neutral doublet) | | | |
| Energy (hartree) | -0.4982329 | -0.4998212 | |
| $H_2$ (neutral singlet) | | | |
| Energy (hartree) | -1.1268277 | -1.1726356 | |
| H—H optimized bond length (angstrom) | 0.730 | 0.743 | 0.7414 |
| BDE(kJ/mol) | 342.3 | 454.2 | 432 |
| Error(%) | -20.77 | 5.14 | |

For water molecule:

1. Optimize the structure of $H_2O$ at the level of HF/6-31G. (Table2)
2. Construct the rigid PES of water in symmetry, at the geometry of O–H bondlength of 1.0Å and ∠H–O–H changing from 30° to 175°. Plot the potential energy surface. (Figure2)
3. Construct the rigid PES of water with two or more changing geometric parameters. Choose the variables by yourself. (Figure3)

**Table2.** Optimized geometry of $H_2O$ at the level of UHF/6-31G

| | UHF/6-31G | Experimental value |
|---|---|---|
| $H_2O$ (neutral singlet) | | |
| Energy (hartree) | -76.0107465 | |
| O—H Bond length (angstrom) | 0.947 | 0.958 |
| ∠H–O–H (degree) | 105.50 | 104.5 |

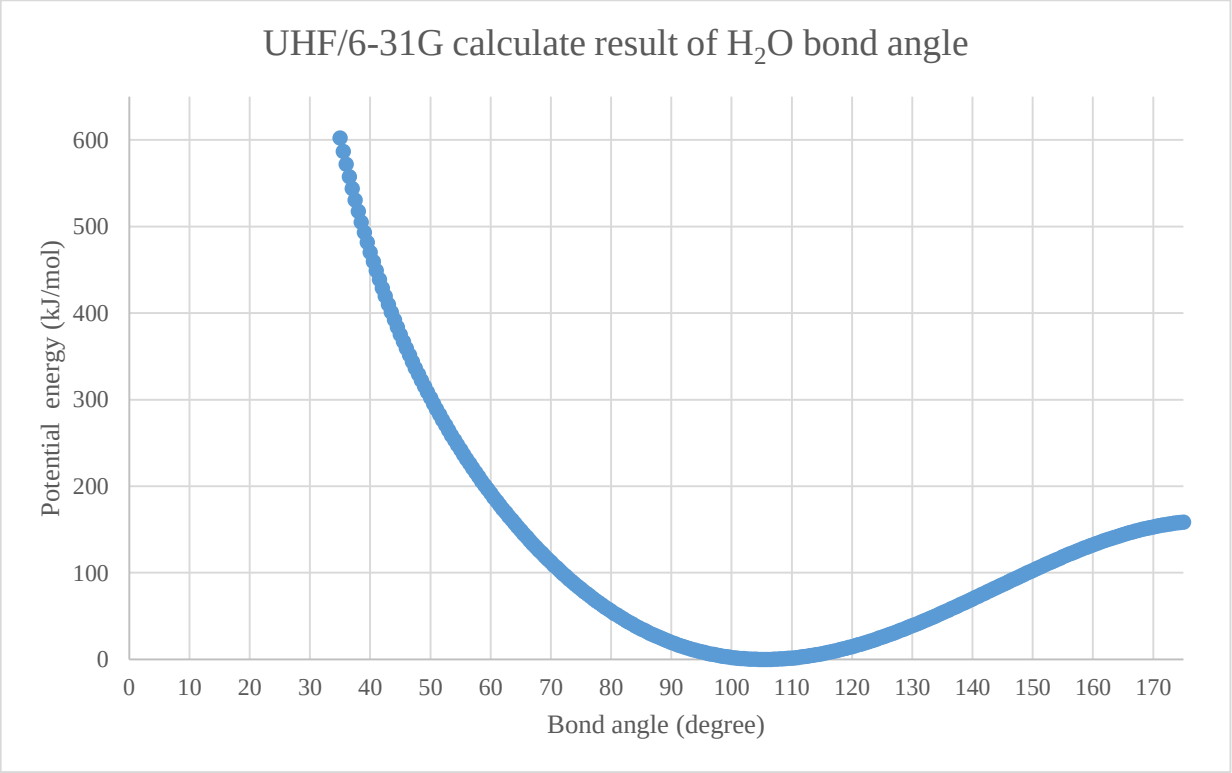


**Figure2.** Calculated results of potential energy with different bond angle at the geometry of O—H bond length of 1 Å. Computed at the UHF/6-31G level.

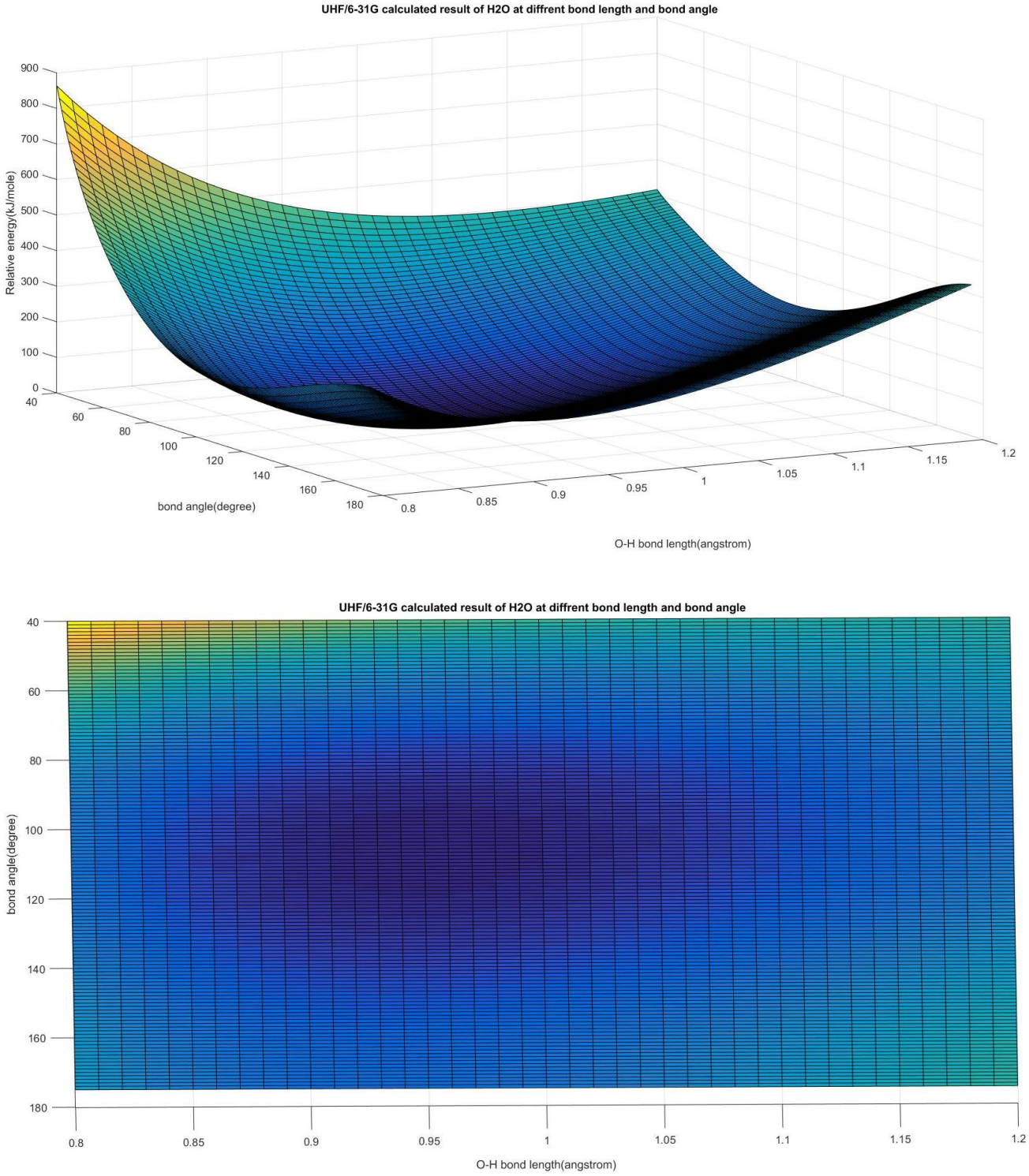


**Figure3.** The potential energy surface with different O—H bond length and ∠H–O–H bond angle at the level of UHF/6-31G.