When does water become OH + H?

Name: Ibraheem Al-Yousef

Part 1 Questions

1. O-H bond length: 0.969 A

2. H-O bond angle: 102.718 Degrees

3. Total # of occupied orbitals: 5 Total # of unoccupied orbitals: 19

4. What atomic orbitals (1s, 2s, $2p_x$, $2p_y$, $2p_z$) from each of the three atoms (H, H, & O) make up each of the MOs (remember that the H orbitals here come in H+H and H-H combinations) for:

MO #1: 1s

MO #2: 2s

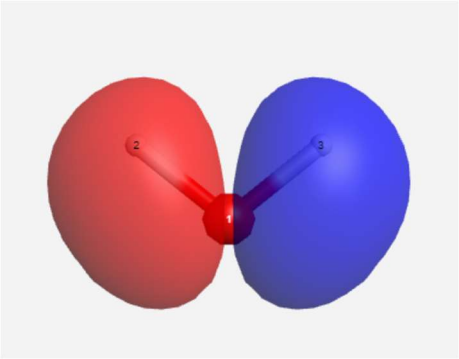
MO #3: 2px

MO #4: 2pz

MO #5: 2py

MO #6:

5. Draw MO #3.



6. Write the MO energies for each MO:

MO #1: -20.553 au MO #2: -1.332 au MO #3: -0.690 au

MO #4: -0.568 au MO #5: -0.493 au MO #5: 0.183 au

7. For each specified O-H bond stretched distance:

a) Write each corresponding MO energy:

O-H Bond	MO #1	MO #2	MO #3	MO #4	MO #5	MO #6
1.5 Å	-20.593	-1.278	-0.625	-0.493	-0.490	0.079
2.0 Å	-20.618	-1.282	-0.630	-0.507	-0.416	-0.022
2.5 Å	-20.630	-1.289	-0.538	-0.517	-0.368	-0.084
3.0 Å						

b) Look at the MOs and indicate which MO number(s) corresponds to MO #3 in the standard water molecule. (Hint: The MO orderings may change as some orbitals destabilize.)

1.5 Å: MO#3

2.0 Å: MO#3

2.5 Å: MO#3

3.0 Å:

c) Thought question: At what bond length do you expect the H atom finally to dissociate and "destroy" the water molecule? (Hint: this is a roughly linear function) Explain your answer.

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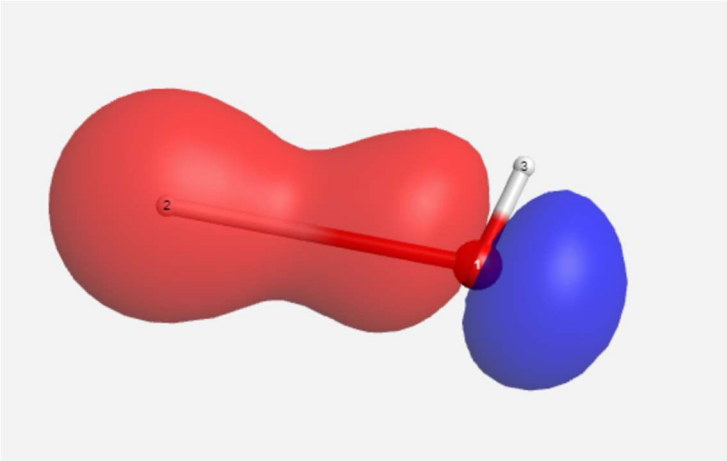

Between 2.75~2.79 Å, after that the psi4 engine will fail to calculate the Mos, and from the look of the MO at 2.75 Å, it looks like it is very close to disassociate

d) Discuss why and how the orbital energies are changing.

Each time we increase the bond length, the orbital energies are decreasing because the molecule will become less stable.