What Happens to the Orbitals as a One-Dimensional Box Gets Longer?

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Part 1 Questions

1. C_2H_2 Job number: _____

(a) Bond lengths (in Å)

$C_1 - H$	1.064
$C_1 - C_2$	1.192
$C_2 - H$	1.064

(b) Energy (in E_h)

π occupied	1st π unoccupied
-0.409	0.203
-0.409	0.203

(c) # of occupied

σ orbital	π orbital
5	2

2. C_4H_2 Job number: _____

(a) Bond lengths (in Å)

$C_1 - H$	1.064
$C_1 - C_2$	1.194
$C_2 - C_3$	1.392
$C_3 - C_4$	1.194
$C_4 - H$	1.064

(b) Energy (in E_h)

π occupied	1st π unoccupied
-0.489	0.203
-0.489	0.203
-0.373	0.634
-0.373	0.634

(c) # of occupied

σ orbital	π orbital
9	4

3. C_6H_2 Job number: _____

(a) Bond lengths (in Å)

$C_1 - H$	1.064
$C_1 - C_2$	1.194
$C_2 - C_3$	1.387
$C_3 - C_4$	1.196
$C_4 - C_5$	1.387
$C_5 - C_6$	1.194
$C_6 - H$	1.064

(b) Energy (in E_h)

π occupied	1st π unoccupied
-0.520	0.085
-0.520	0.085
-0.448	0.233
-0.448	0.233
-0.354	0.407
-0.354	0.407

# of occupied

σ orbital	π orbital
13	6

4. C_8H_2 Job number: _____

(a) Bond lengths (in Å)

$C_1 - H$	1.064
$C_1 - C_2$	1.194
$C_2 - C_3$	1.386
$C_3 - C_4$	1.197
$C_4 - C_5$	1.382
$C_5 - C_6$	1.197
$C_6 - C_7$	1.386
$C_7 - C_8$	1.194
$C_8 - H$	1.064

(b) Energy (in E_h)

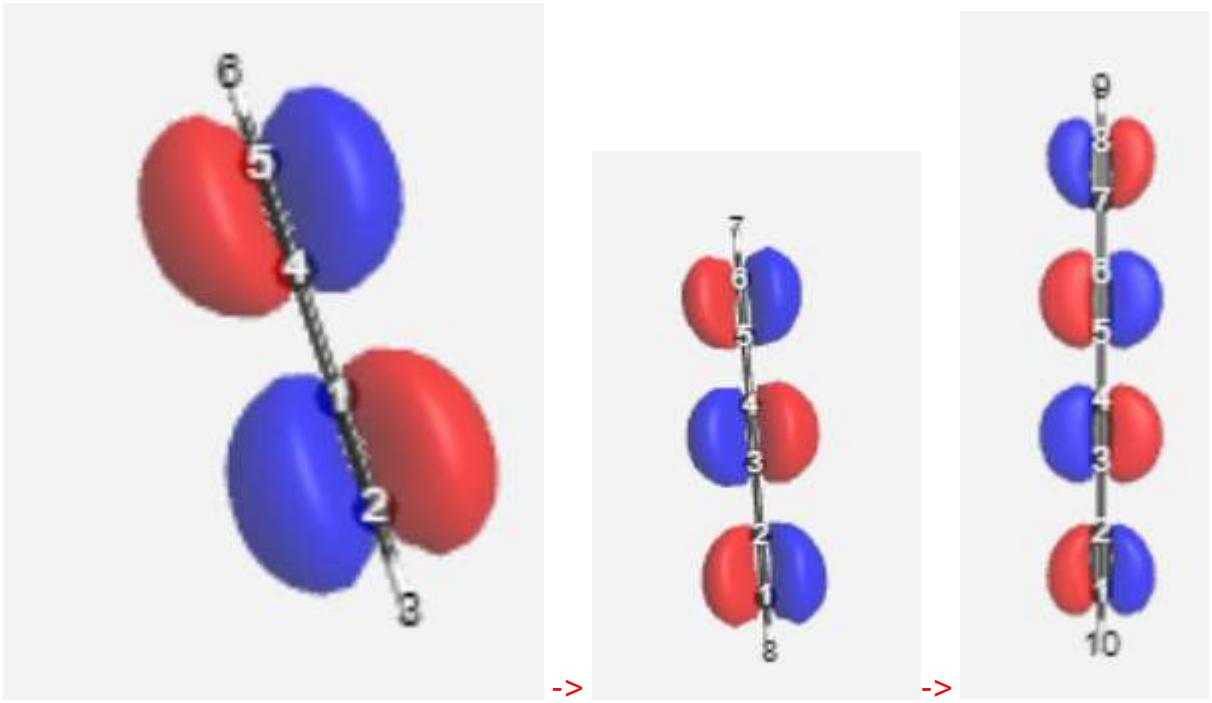
π occupied	1st π unoccupied
-0.535	0.061
-0.535	0.061
-0.488	0.174
-0.488	0.174
-0.420	0.306
-0.420	0.306
-0.344	0.449
-0.344	0.449

(c) # of occupied

σ orbital	π orbital
17	8

5. What is the visual difference in the π orbitals for each successive level for each molecule?

The more the molecule is lengthy, the bigger the number of the pi orbital rooms for the electrons; The electrons will be localized between carbon atoms



6. What happens to the energy of the π highest occupied molecular orbital (HOMO) for each successively longer for molecule?

The HOMO energy becomes less negative as we change the molecule to a longer one

7. How does this relate to the particle-in-a-box model and to the pattern of bond lengths (Hint: think nodes)? To properly view the MOs, you may need to change the opacity in the settings.

The electrons will be trapped in the pi bonding and behave like an electron trapped in a PIB, and the length of the box is related to the conjugated system's.