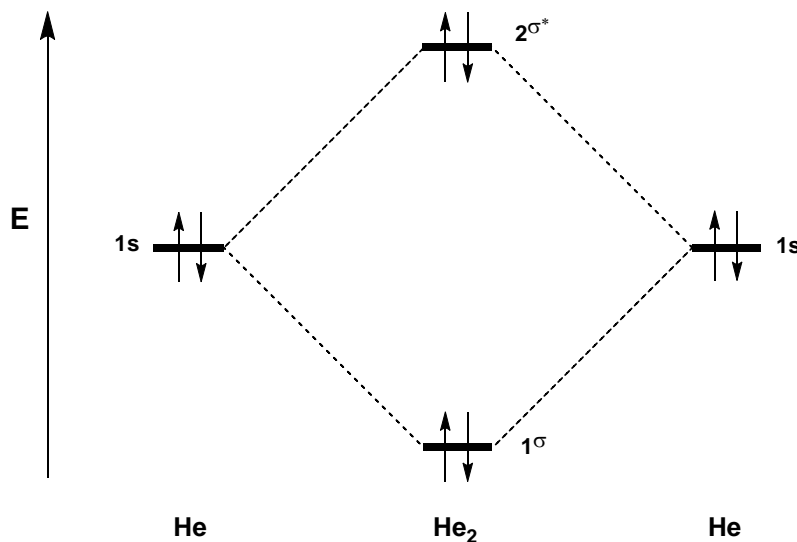


Answers to Exercise 2.3

Molecular Orbital Energy Level Diagrams: Hydrogen and Helium

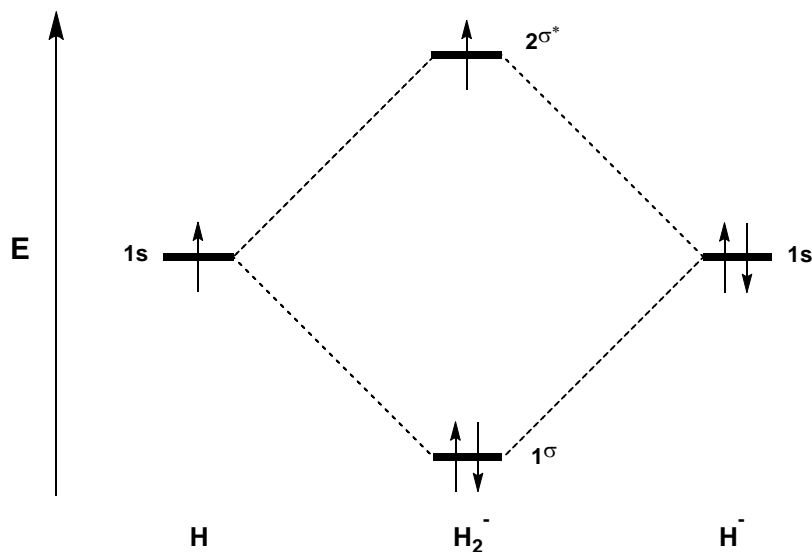
1.



The bond order in He_2 is $\frac{2-2}{2} = \frac{0}{2} = 0$.

Since the calculated bond order is 0, the He-He bond does not form and He_2 does not exist.

2.



The orbital occupancy for H_2^- is $(1\sigma)^2(2\sigma^*)^1$.

The extra electron in H_2^- is in an antibonding orbital, so it weakens the H-H bond compared to H_2 .

The bond order in H_2^- is $\frac{2-1}{2} = \frac{1}{2}$ which is lower than the bond order of 1 in H_2 .

To be totally accurate, the energies of both MOs should be raised (relative to their energies in H_2) since adding the extra electron to H_2 increases electron-electron repulsion and raises the energies of all three electrons. Similarly, the energy of the electrons in H^- should be higher than the energy of the electrons in H . The simplified diagram above, however, is sufficient to answer the question.