"Classical" and Quantum Mechanical (exchange) Conrtibutions to the Bonding Energy in H_2^+

from: D.A. McQuarrie and J.D. Simon,
Physical Chemistry A Molecular Approach,
University Science Books, Sausalito, p. 332.

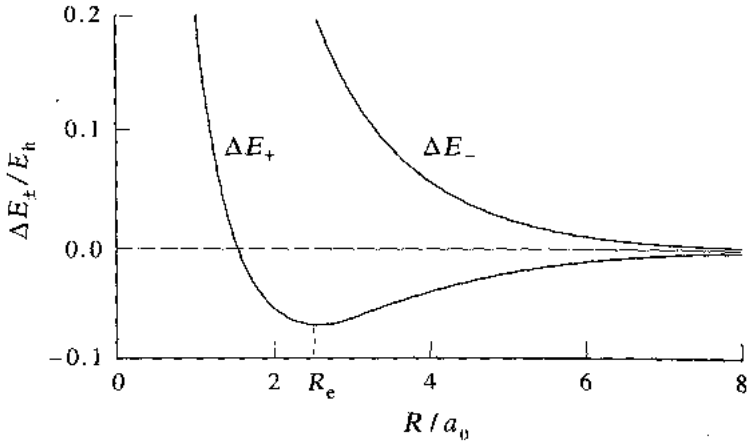

FIGURE 9.6
The energies $\Delta E_+ = E_+ - E_{1s}$ and $\Delta E_- = E_- - E_{1s}$ corresponding to the ψ_+ and ψ_- molecular orbital wave functions given in Equation 9.6 (with $c_1 = c_2$) plotted as a function of intermolecular separation R for H_2^+. The plot shows that ψ_+ leads to a bonding molecular orbital whereas ψ_- leads to an antibonding molecular orbital.

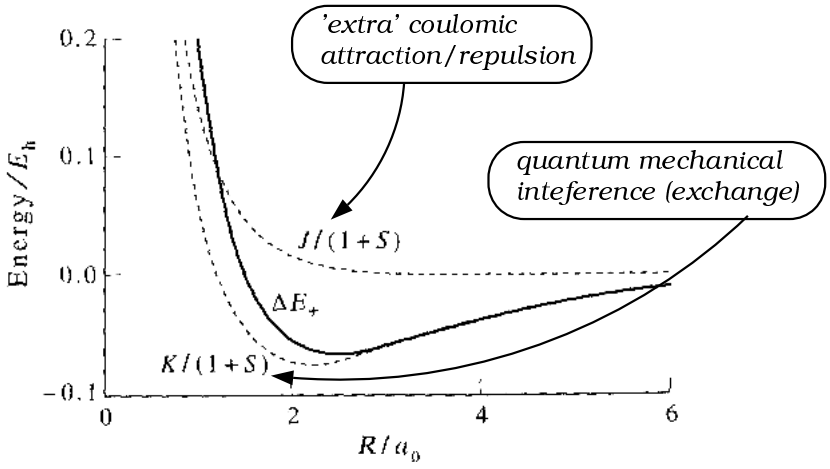

FIGURE 9.7
The separate contributions of the Coulomb integral, J, and the exchange integral, K, to the stability of H_2^+.