

Key Molecular Energy Integrals

$$\text{Overlap: } S \equiv \int AB d\tau = \left[1 + \frac{R}{a_0} + \frac{1}{3} \left(\frac{R}{a_0} \right)^2 \right] e^{-R/a_0}$$

$$\text{Coulomb: } j \equiv \frac{e^2}{4\pi\epsilon_0} \int \frac{A^2}{r_B} d\tau = \frac{e^2}{4\pi\epsilon_0 R} \left[1 - \left(1 + \frac{R}{a_0} \right) e^{-2R/a_0} \right]$$

$$\text{Exchange: } k \equiv \frac{e^2}{4\pi\epsilon_0} \int \frac{AB}{r_B} d\tau = \frac{e^2}{4\pi\epsilon_0 a_0} \left(1 + \frac{R}{a_0} \right) e^{-R/a_0}$$

(where the explicit formulas depending on the internuclear distance R apply to H_2^+)

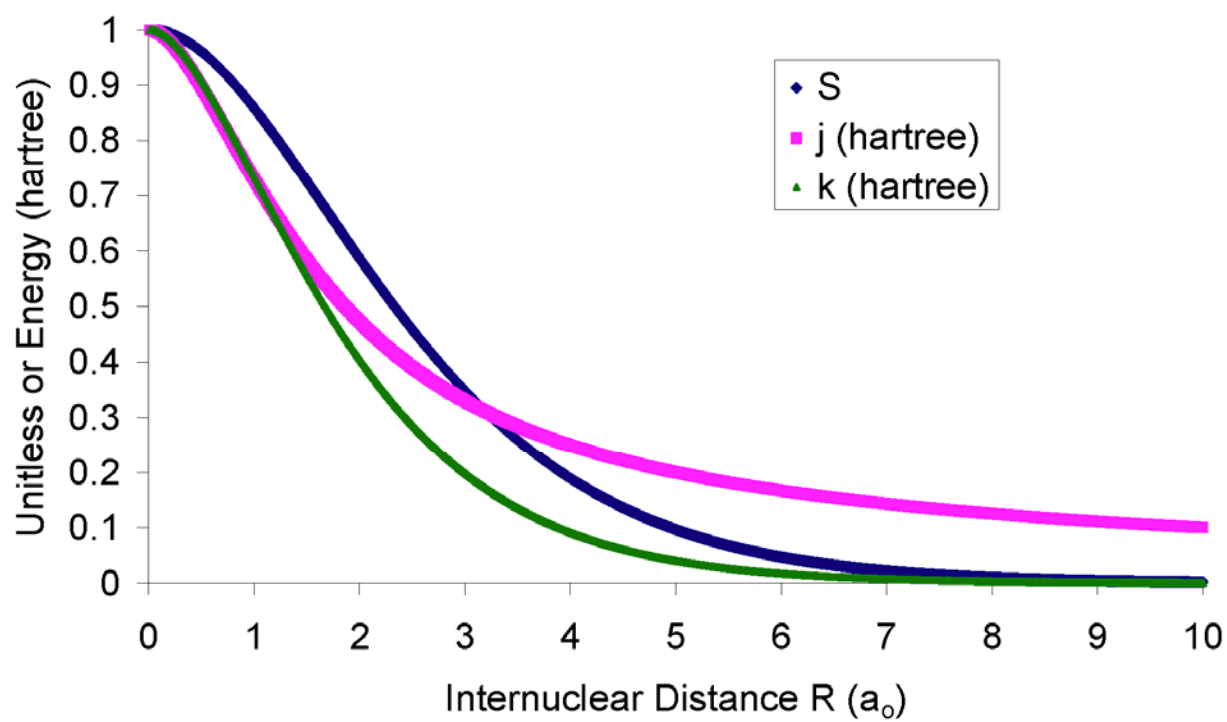
Atomic Units

$$\text{Length: } 1 \text{ bohr} = 1 a_0 = 52.9177 \text{ pm}$$

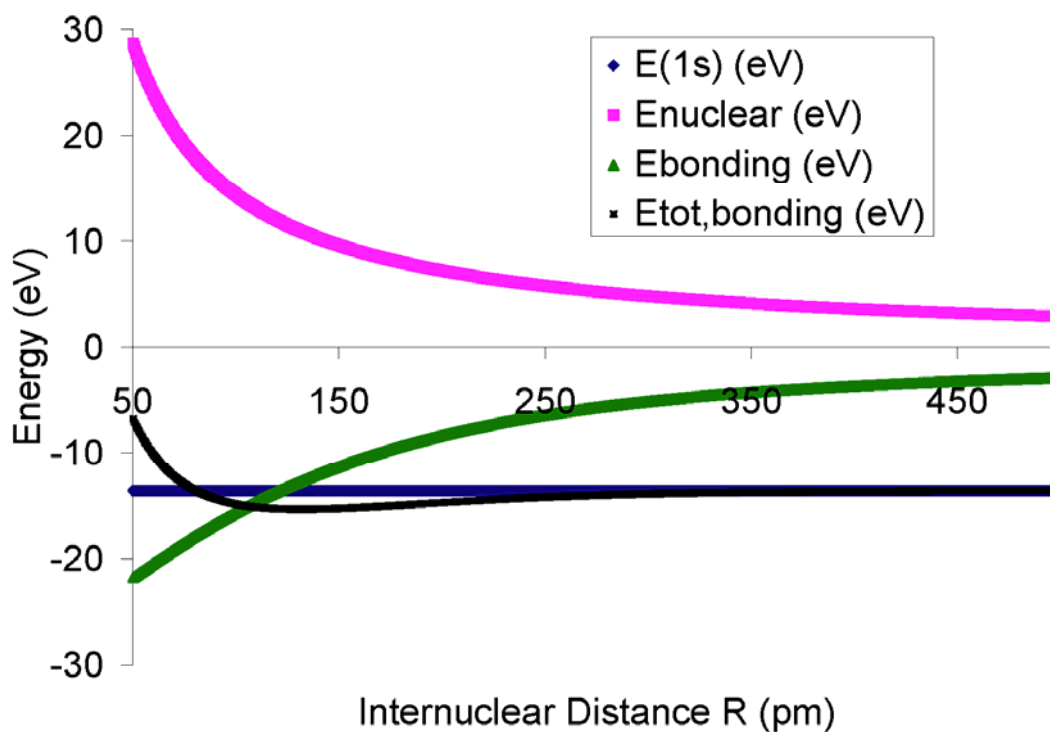
$$\text{Energy: } 1 \text{ hartree} = 1 \frac{e^2}{4\pi\epsilon_0 a_0} = 27.212 \text{ eV}$$

(so reporting j and k in units of hartree is tantamount to setting $\frac{e^2}{4\pi\epsilon_0 a_0} = 1$)

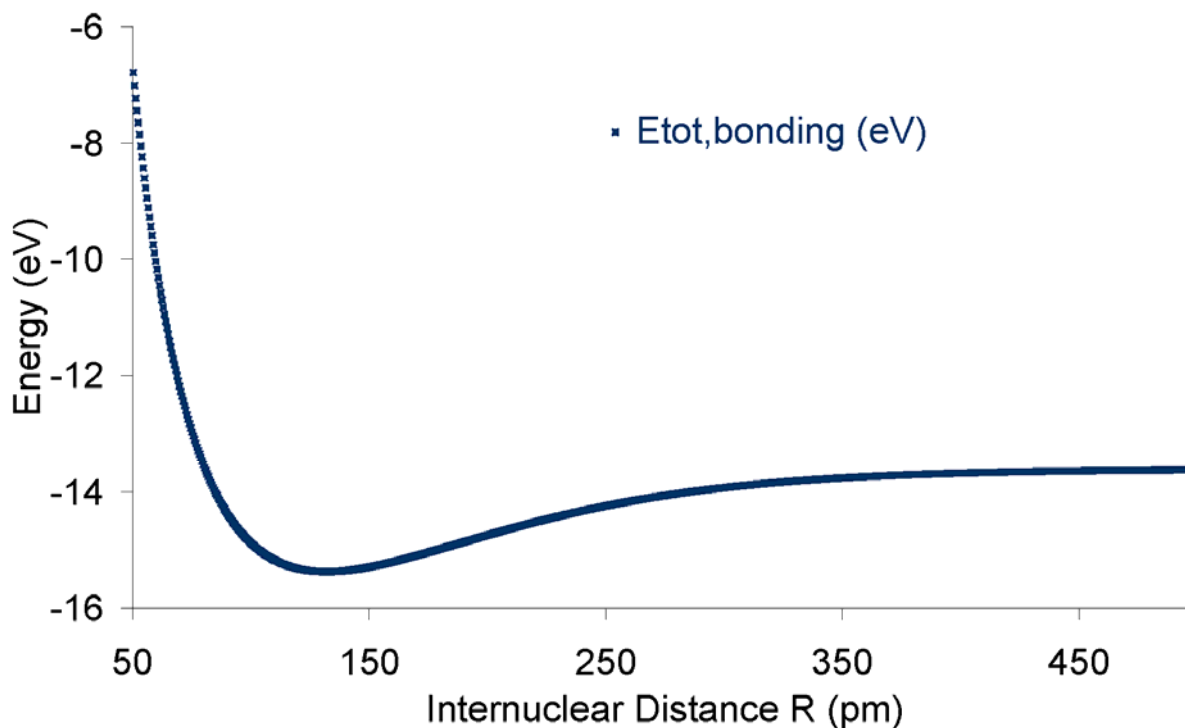
H_2^+ Energy: Key Integrals



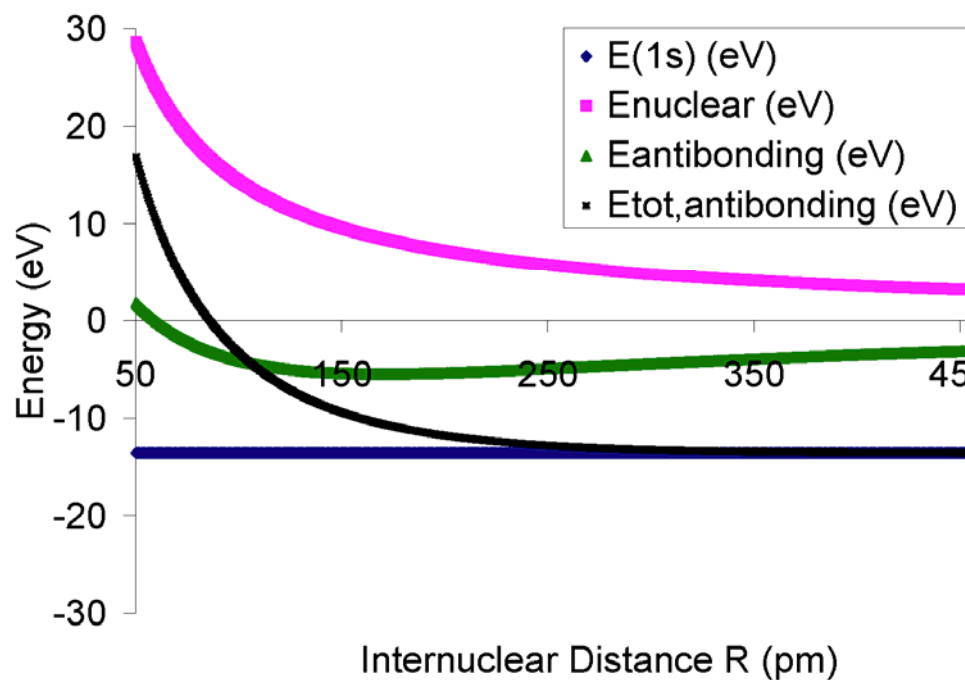
H_2^+ : Energy of the Bonding Molecular Orbital



H_2^+ : Energy of the Bonding Molecular Orbital



H_2^+ : Energy of the Antibonding MO



H_2^+ : Energies of the Atomic and Molecular Orbitals

