**Photoclectron Spectroscopy, UPS**

\[ H_2 \left( ^1\Sigma_g^+, \nu'' = 0 \right) + h\nu \rightarrow H_2^+ \left( ^2\Sigma_g^+, \nu' \right) + e^- \quad \nu' = 0, 1, 2, 3, \ldots \]

\[ D_0^{\text{ion}} = 18.07 \text{ eV} - 15.43 \text{ eV} = 2.64 \text{ eV}. \]

The fundamental vibration frequency of \(H_2\) is 4158.5 cm\(^{-1}\).

**Koopmans’ Theorem:**

Ionization potentials at the \(0 \leftrightarrow 0\) transitions \(\approx\) MO energies

**Assumptions:**

1. the orbital approximation is valid
2. the molecule does not change shape upon ionization
3. the correlation energies of the ground state and molecular ion are similar: frozen orbital approximation (valid to \(\sim\)1-3 eV).

\[ N_2 \quad \sigma^*_u \quad \pi_g \quad \pi_u \quad \sigma^*_g \quad \pi_u \quad \rightarrow \quad + e^- \]

Under Koopmans’ Theorem, UPS ionization potentials are comparable to Hartree-Fock molecular orbital calculations, which do not account for correlation energies.
**N₂**: The fundamental stretch of neutral N₂ is at 2345 cm⁻¹.

**CO**: The fundamental vibration frequency for neutral CO is 2170 cm⁻¹.

**H₂O**: The asymmetric stretch in the molecular ion at 3220 cm⁻¹ and bending at 1370 cm⁻¹. The corresponding frequencies in neutral H₂O are 3756 cm⁻¹ and bending at 1595 cm⁻¹.