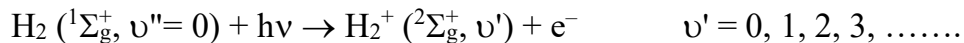
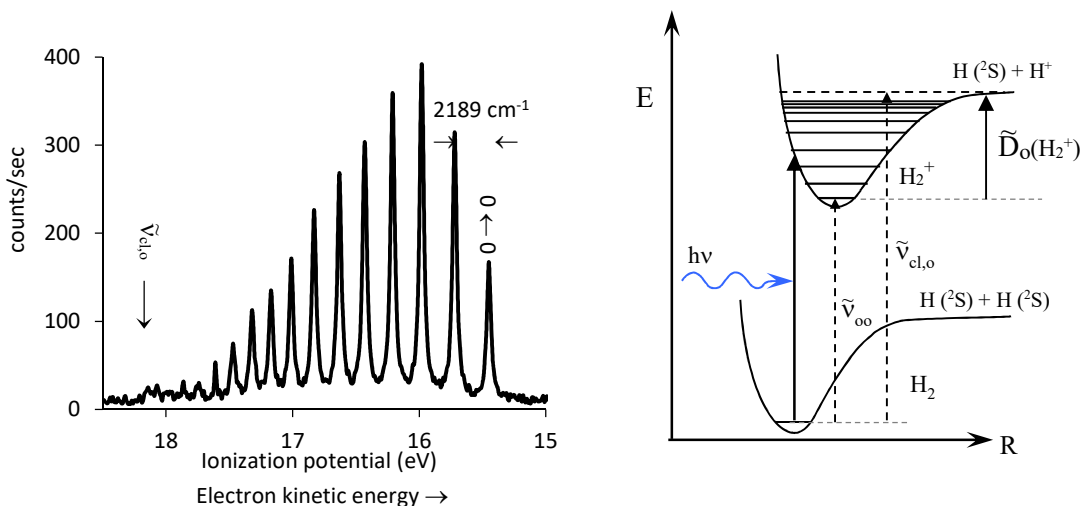


Photoelectron Spectroscopy, UPS



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



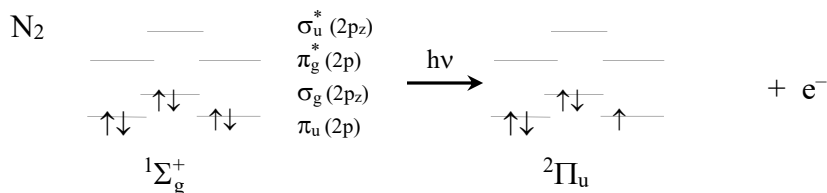
The fundamental vibration frequency of H_2 is 4158.5 cm^{-1} .

Koopmans' Theorem:

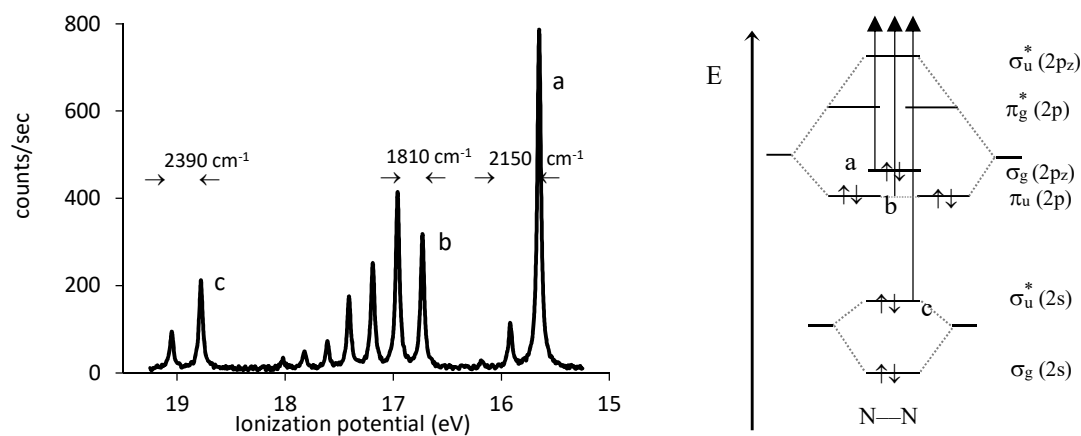
Ionization potentials at the $0 \leftarrow 0$ transitions \approx MO energies

Assumptions:

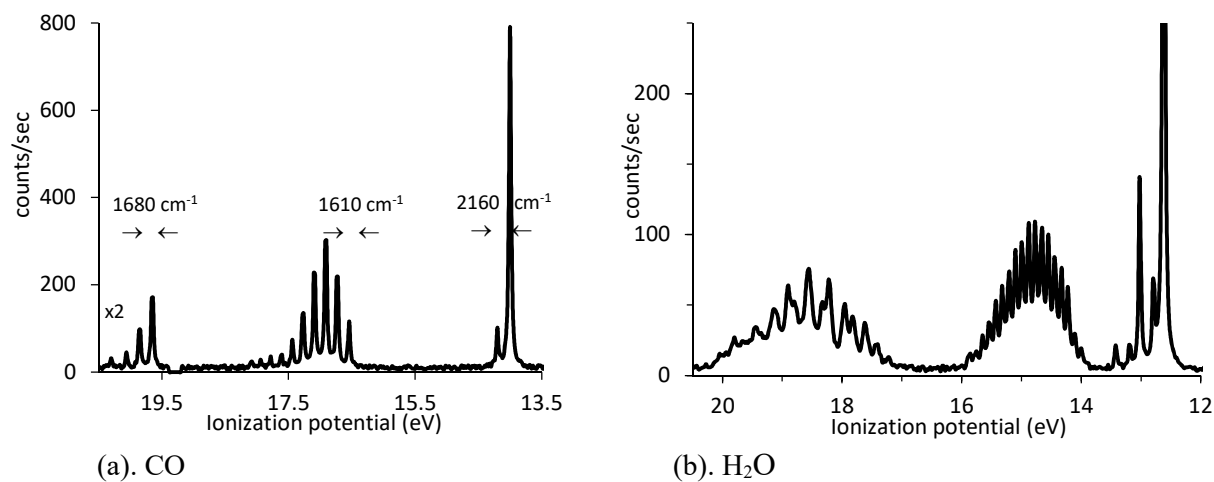
1. the orbital approximation is valid
2. the molecule does not change shape upon ionization
3. the correlation energies of the ground state and molecular ion are similar: frozen orbital approximation (valid to $\sim 1\text{-}3 \text{ eV}$).



Under Koopmans' Theorem, UPS ionization potentials are comparable to Hartree-Fock molecular orbital calculations, which do not account for correlation energies.



N_2 : The fundamental stretch of neutral N_2 is at 2345 cm^{-1}



CO : The fundamental vibration frequency for neutral CO is 2170 cm^{-1} .

H_2O : The asymmetric stretch in the molecular ion at 3220 cm^{-1} and bending at 1370 cm^{-1}
The corresponding frequencies in neutral H_2O are 3756 cm^{-1} and bending at 1595 cm^{-1}