

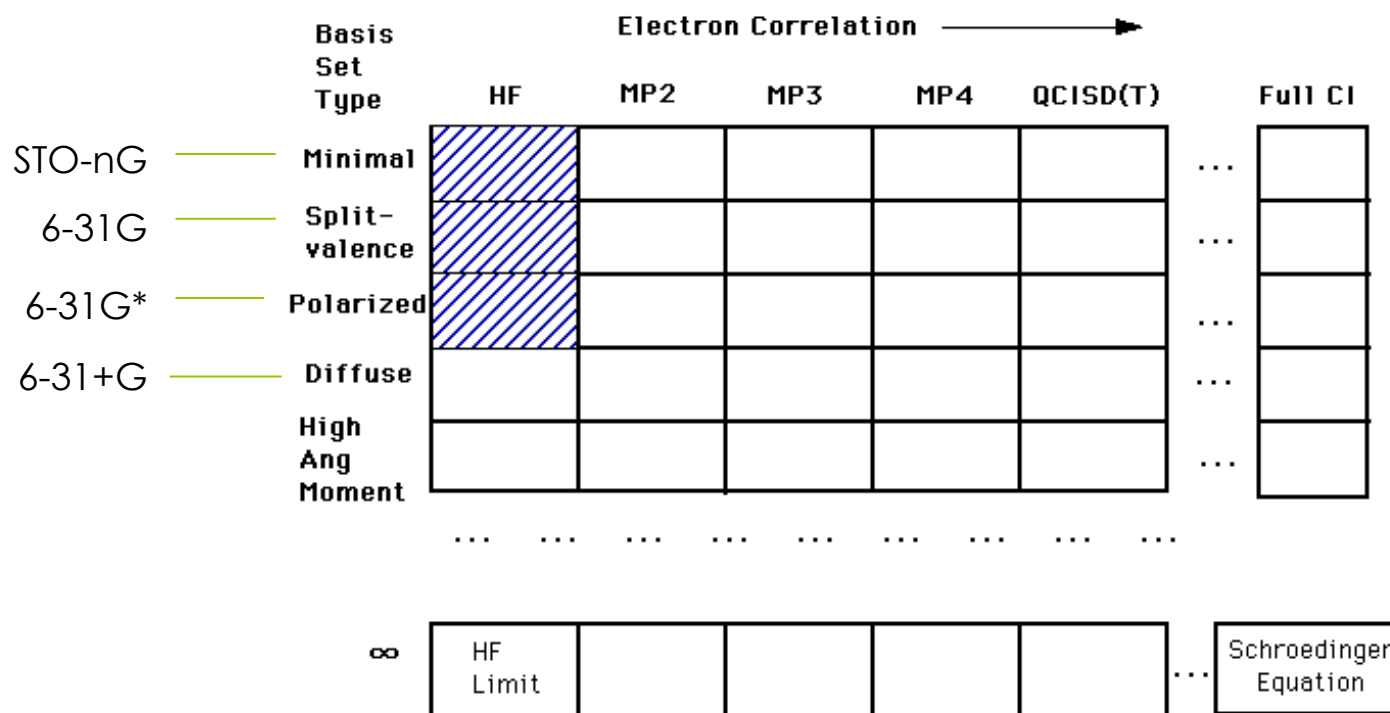
# The Effect of Basis Sets on the Absorption Spectra

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# Basis Sets

- A set of functions combined in linear combinations to create molecular orbitals
- Typically atomic orbitals centered on atoms

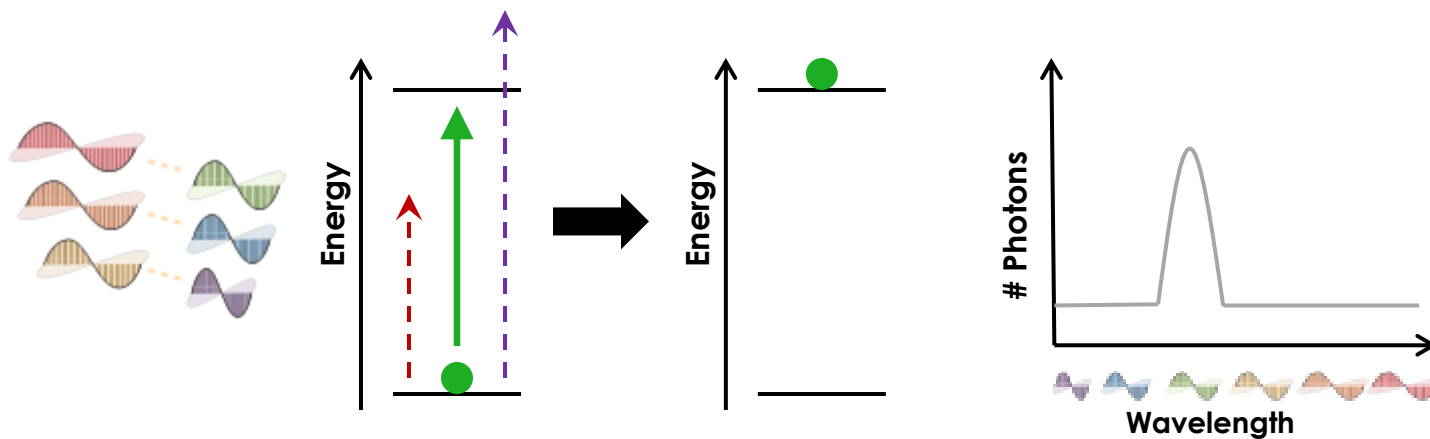


# Absorbance Spectra

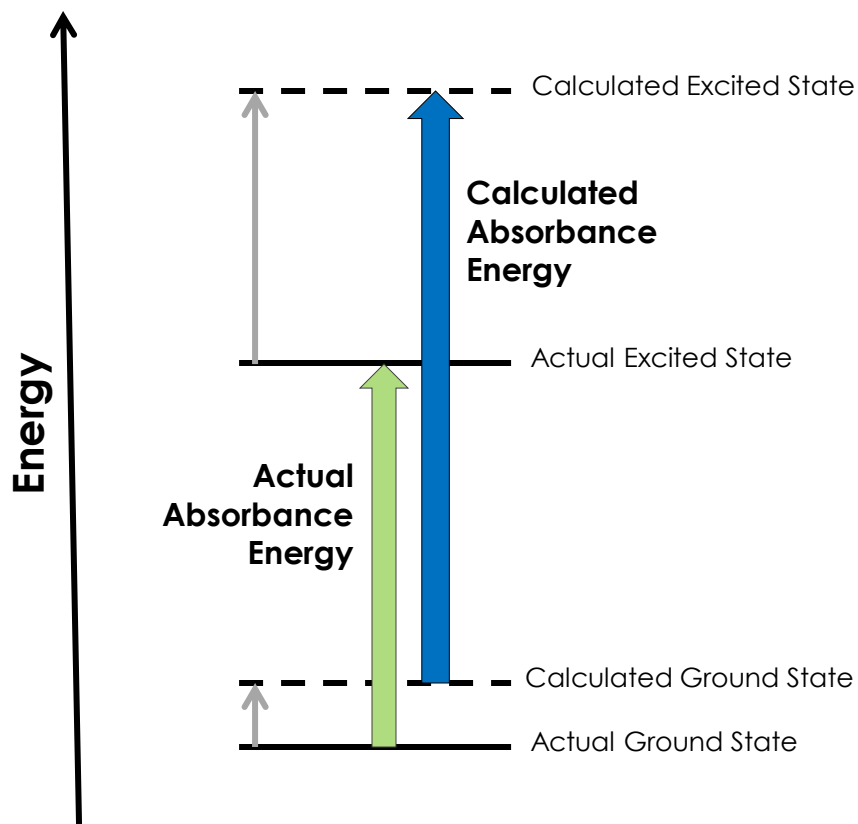
- A spectroscopic technique that measures the absorption of radiation as a function of wavelength (or energy) of light.

$$A = \epsilon bc$$

$$E = h\nu$$

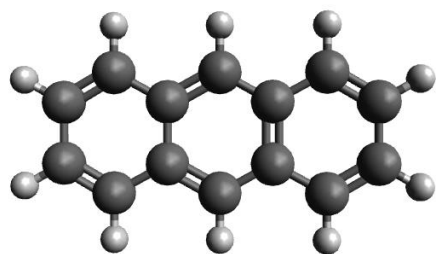


# Our Hypothesis

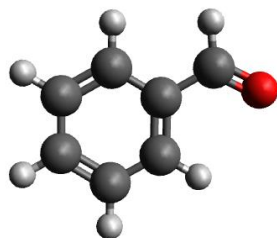


- Calculated state energies are bound (always higher)
- Excited state energies converge faster than ground state energies
- Absorbance energies are the **differences** in energies.

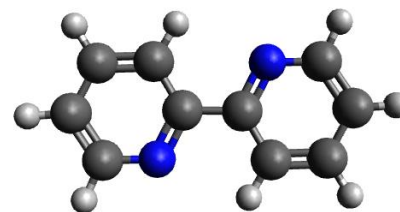
# Current Progress



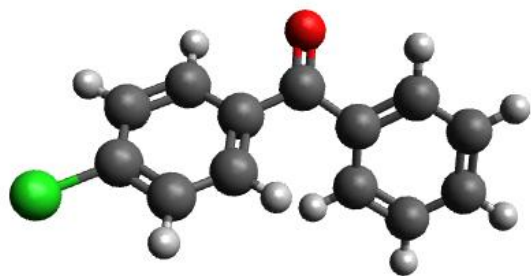
Anthracene



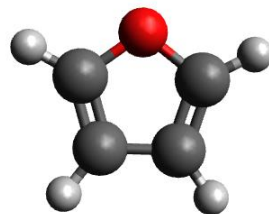
Benzaldehyde



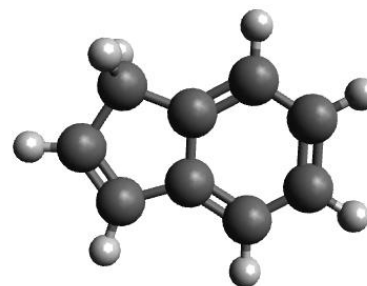
Bipyridyl



Chlorobenzophenone



Furan



Indene

# References

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- Shao, M.; Keum, J.; Chen, J., et. al.; *Nat. Comm.* **2014**. 10, 1-11.



Questions?