

## Answer on the question #68062, Chemistry / Physical Chemistry

### Question:

a) Describe different types of electronic transitions in a molecule. Which type of transition is responsible for a band at  $\lambda_{\text{max}} = 279 \text{ nm}$  in absorption spectrum of acetone.

### Answer:

Depending on the chemistry of the molecule, chemists divide the electronic transitions into the ones that occur in organic molecules and the ones that take place in inorganics.

Electronic transitions in organics involve  $\pi$ ,  $\sigma$ , and  $n$  electrons:

- 1)  $\sigma \rightarrow \sigma^*$  (<150nm) and  $n \rightarrow \sigma^*$  (<250nm) in saturated compounds
- 2)  $\pi \rightarrow \pi^*$  and  $n \rightarrow \pi^*$  transitions: (200-700nm) in unsaturated systems with double/triple bonds.

Concerning inorganic compounds, transitions between  $d$  orbitals split by presence of ligand field are the most important. Usually they are in visible spectral region. Other type is charge-transfer transition, when the electron moves between the orbitals associated with the donor and acceptor parts (for example, ligand and metal).

The band at 279nm of acetone is the result of excitation of one of the unshared electrons of oxygen ( $n$ -level) to a higher energy level,  $\pi^*$  antibonding orbital of the carbon-oxygen double bond. The other possible transition,  $\pi \rightarrow \pi^*$  is the one of higher energy, shorter wavelength.

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