**Cobalt Complex Spectral Analysis**

**UV-VIS Spectra**

The three files can be opened in Excel. The first two columns are wavelength and absorbance. The third column is standard deviation, which is meaningless for a spectrum.

Plot the spectrum for wavelengths 350 – 700 nm. You should first delete the rows for Abs below 350 nm and above 700 nm. For each compounds, find the wavelength of maximum absorbance (λmax) that comes between 400 – 600 nm. Calculate the energy of λmax. and the d-orbital splitting for each compound.

Recall:

λ∙υ= c = 3.00 x 108 m/s

Ephoton = hυ

d-orbital splitting = N x Ephoton, where N = Avogadro’s number.

The greater the energy of λmax, the larger the orbital splitting, and therefore the stronger the metal-ligand interactions. Rank the three ligands (-Cl, -ONO, and –NO2) in terms of their interaction strength when bonded to Co3+ ion.

**IR Spectra**

Examine the IR spectra for the three compounds. Notice that all three compounds share four absorptions at equal energy for around 3145 cm-1, 1575-1600 cm-1, 1307 cm-1, 835 cm-1. Also notice that the NO2 compound has one additional absorption; the ONO compound has two additional absorptions. Tabulate the energies of those absorptions.

Use WebMO to construct AlCl3NO2 and AlCl3ONO and examine their IR spectra, looking for NO-based vibrations. These will most likely be the vibrations at the highest energies.

For a vibration to be “IR active” it must change the polarity of the molecule, which means the atomic motions will be asymmetric. If a vibration is symmetric it will not lead to absorption of IR radiation and no absorption will be observed.

The energies of the WebMO spectra will differ greatly from those of the experimental spectra (why?) but the trends will be the same. Given that, characterize the NO-based absorptions observed for each compound in the experimental spectra. Name them as: symmetric or asymmetric, stretch or bend, and also identify if the stretch occurs to an N-O single bond or an N=O double bond. Do the relative energies make sense?