A Computational Study of Substituted Polycyclic Aromatic Hydrocarbons (PAHs)

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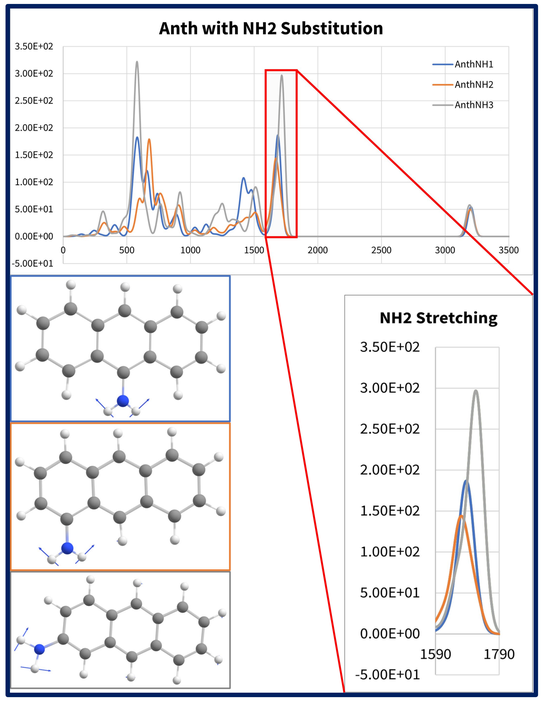
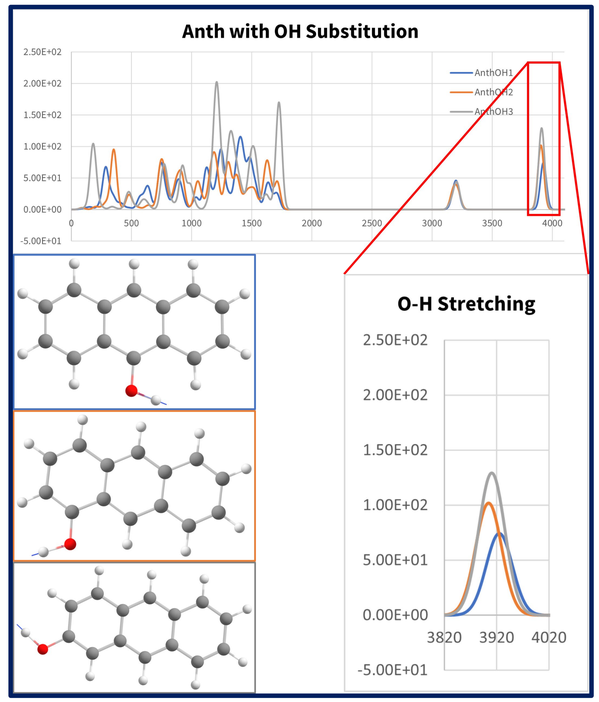
Summary

- PAHs are a molecule of interest for several fields including astrochemistry and environmental chemistry
- Classifying PAHs is often done with using robust techniques like GCMS, but these are not always available or convenient for analysis, especially with astrochemistry
- The goal of this project is to use Gaussian 09, a computational chemistry software, to access the vibrational spectra of a group of molecules (PAHs) to find trends in the IR spectra in order to better identify them

Methods

- The molecules were optimized using a M062X/6-311+G** basis set
- Analysis was done by first plotting IR frequencies and visibly evaluating the modes using Chemcraft
- Once a specific mode was determined, statistical analysis was done to see if the difference was large enough to justify a clear difference





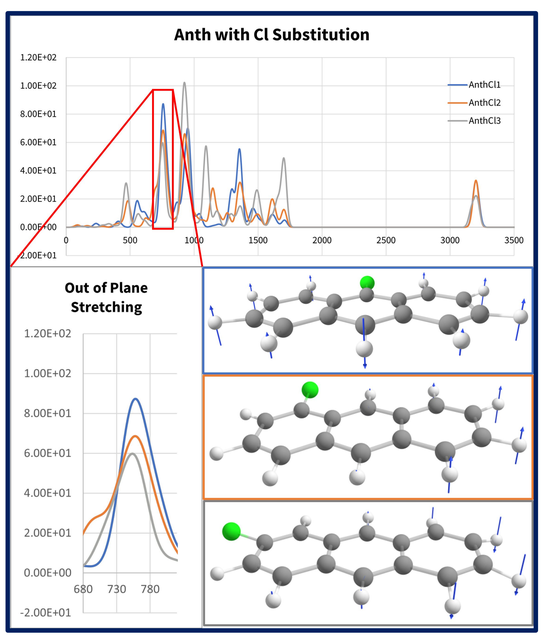


Figure 1. The first graph in each box features the full generated IR spectra for each of the molecules in the substitutions.

The substitutions for each of the molecules are featured from substitution 1 to 3 for each of the molecules. The color surrounding the molecule corresponds to the substitution number.

Lastly, a signature band that shows promise to be distinct is featured within the spectra is shown in the smaller enlarged graph

Results

- The IR spectra were all unique but finding distinct bands between the graphs was trickier
- The featured bands in Figure 1 show that there are similar modes with different frequencies and intensities which could better be able to identify these individual molecules
- Statistical analysis between the band frequencies and intensities still needs to be completed to determine if these are the best modes for determining differences between them
- With all of the molecular backbones (Naphthalene, Anthracene, and Phenanthrene), the NH2 substitution was the most distinct

Table 1. Substitutions and the exact frequency and intensity

Molecule	Frequency (cm -1)	Intensity
Anth NH2 Sub 1	1683.83	151.8942
Anth NH2 Sub 2	1668.81	119.0333
Anth NH2 Sub 3	1670.29	42.2363
Anth OH Sub 1	3925.09	74.4221
Anth OH Sub 2	3904.67	102.0260
Anth OH Sub3	3910.68	129.3568
Anth Cl Sub1	754.69	80.4166
Anth Cl Sub 2	762.87	50.3972
Anth Cl Sub 3	756.49	55.2958

Conclusions

The initial computational results show promise for finding distinctions between the different locations of the substitutions by using IR methods.

More statistical analysis has to be done to confirm the bands as the best modes.

The next steps involve completing analysis for the other two molecular backbones (Naphthalene and Phenanthrene) to determine if number of rings or arrangement significantly affect the IR spectra

Acknowledgements

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