

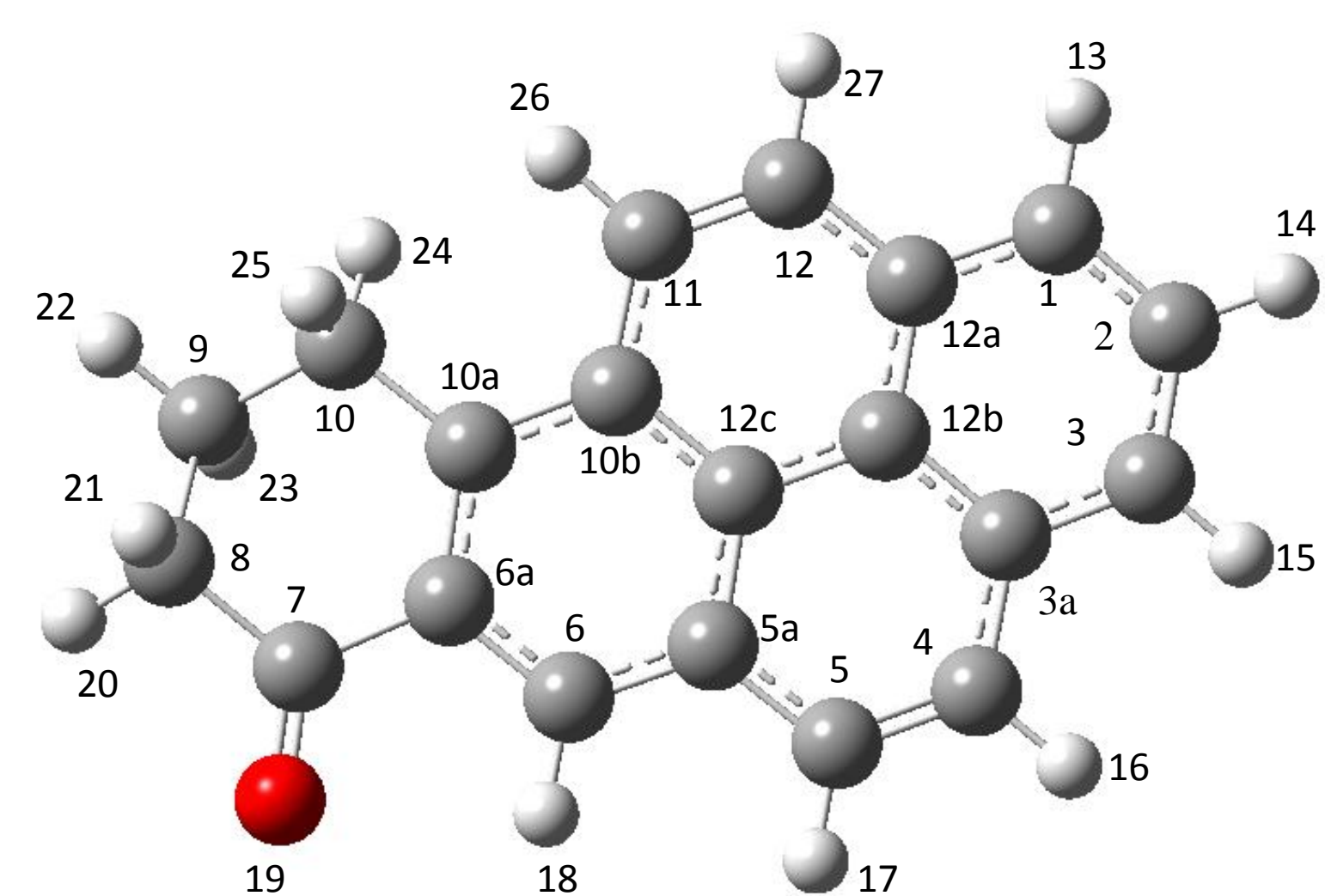
Spectroscopic Studies of 9, 10-dihydrobenzo(a)pyrene-7(8H)-one and 7, 8, 9, 10- tetrahydrobenzo(a)pyrene

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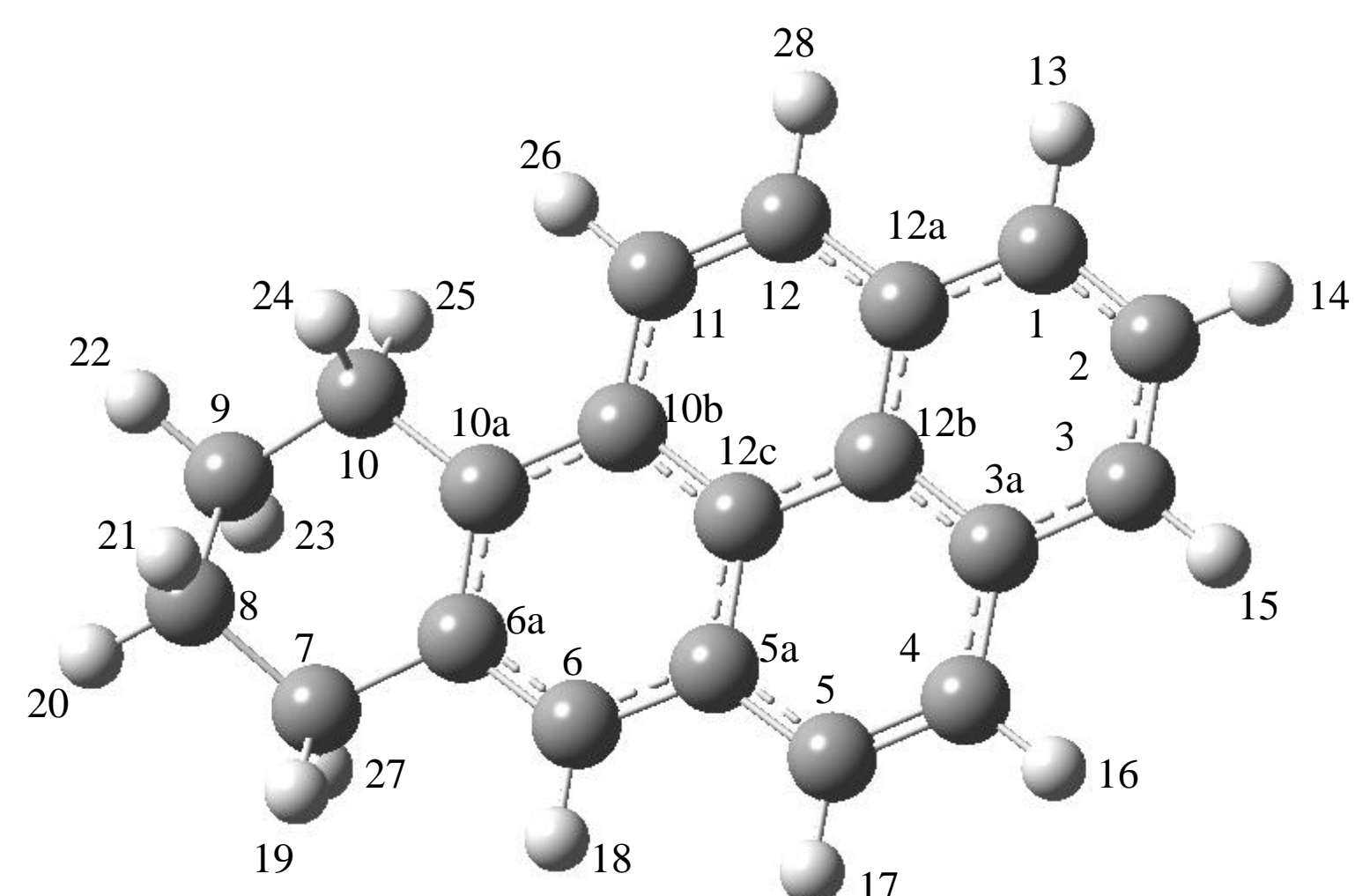
Abstract

Polycyclic aromatic hydrocarbons (PAHs) are organic molecules found in the environment. The PAHs are formed from incomplete combustion, are found in diesel exhaust particles, grilled foods, gas burners, emission from wood, and cigarette smoke. These compounds are known to be carcinogenic and mutagenic^{1,2}. Spectroscopic studies were performed on two PAHs, 9,10-dihydrobenzo(a) pyrene-7(8H)-one and 7,8,9,10-tetrahydrobenzo(a)pyrene, which helped to characterize them. Also, a theoretical infrared study was done on 9,10-H₂BaP, a scaling factor was found for a simulated infrared spectrum.

Two Compounds Studied



9,10-dihydrobenzo(a) pyrene-7(8H)-one (9,10-H₂BaP)



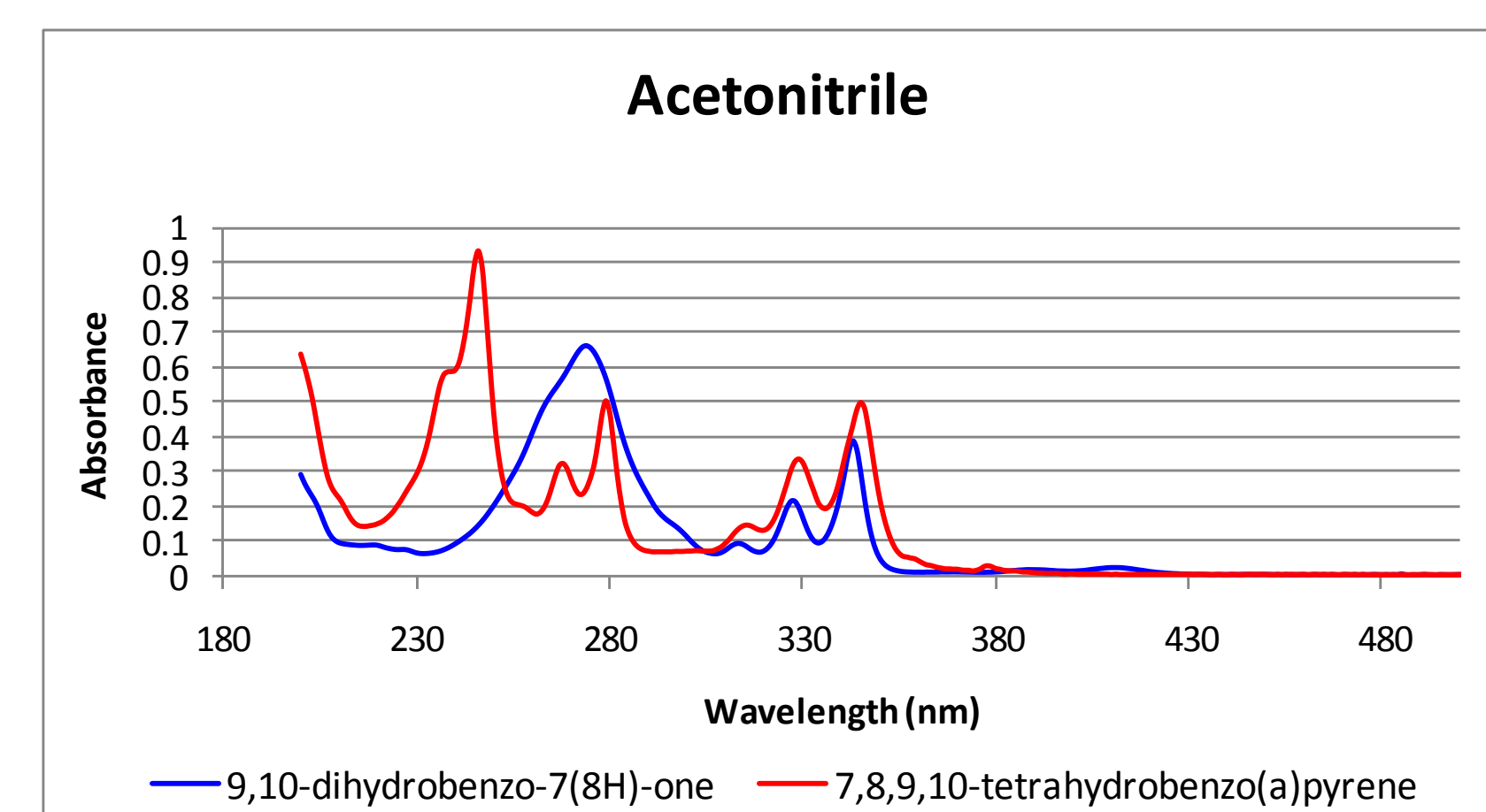
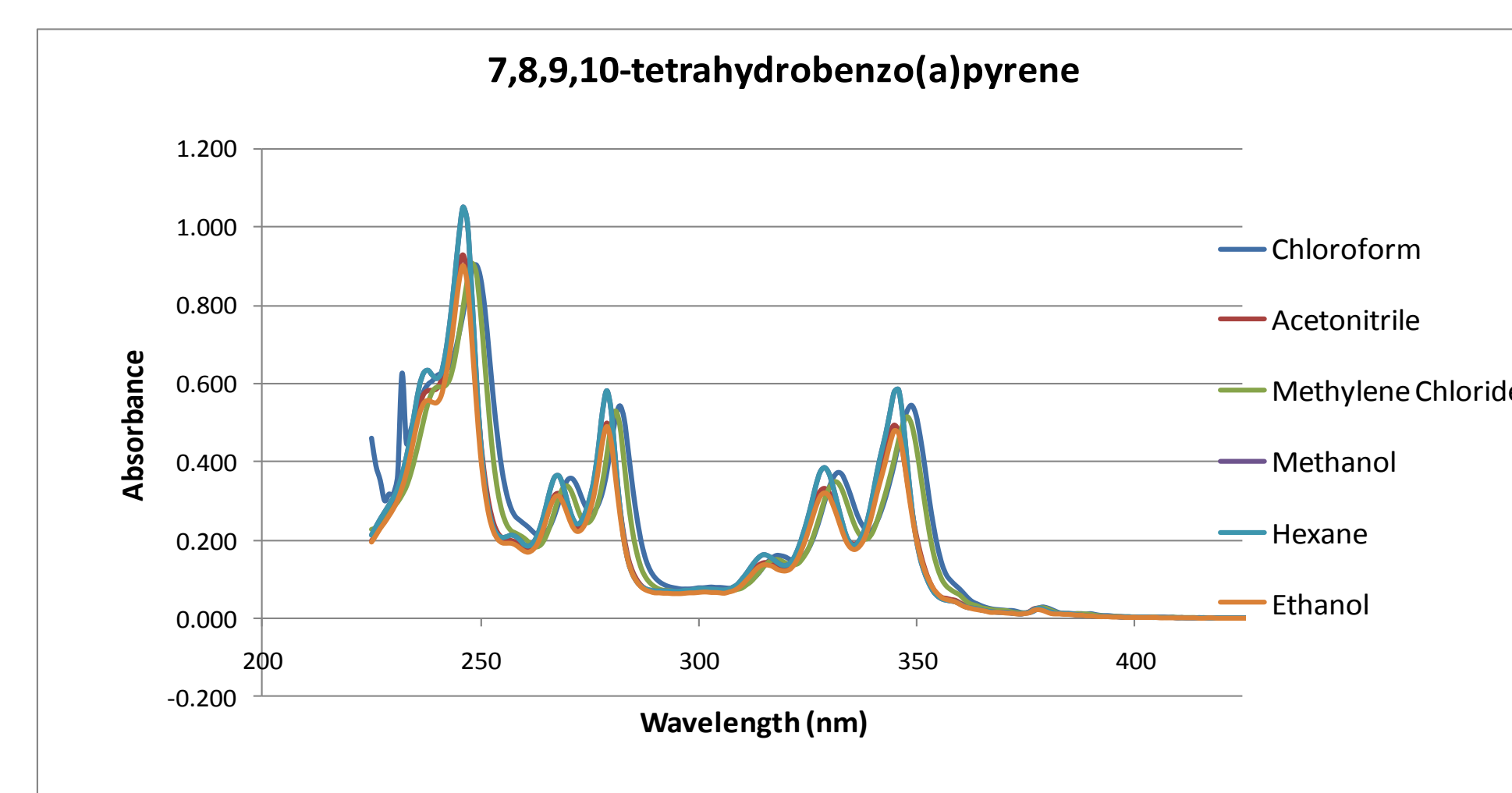
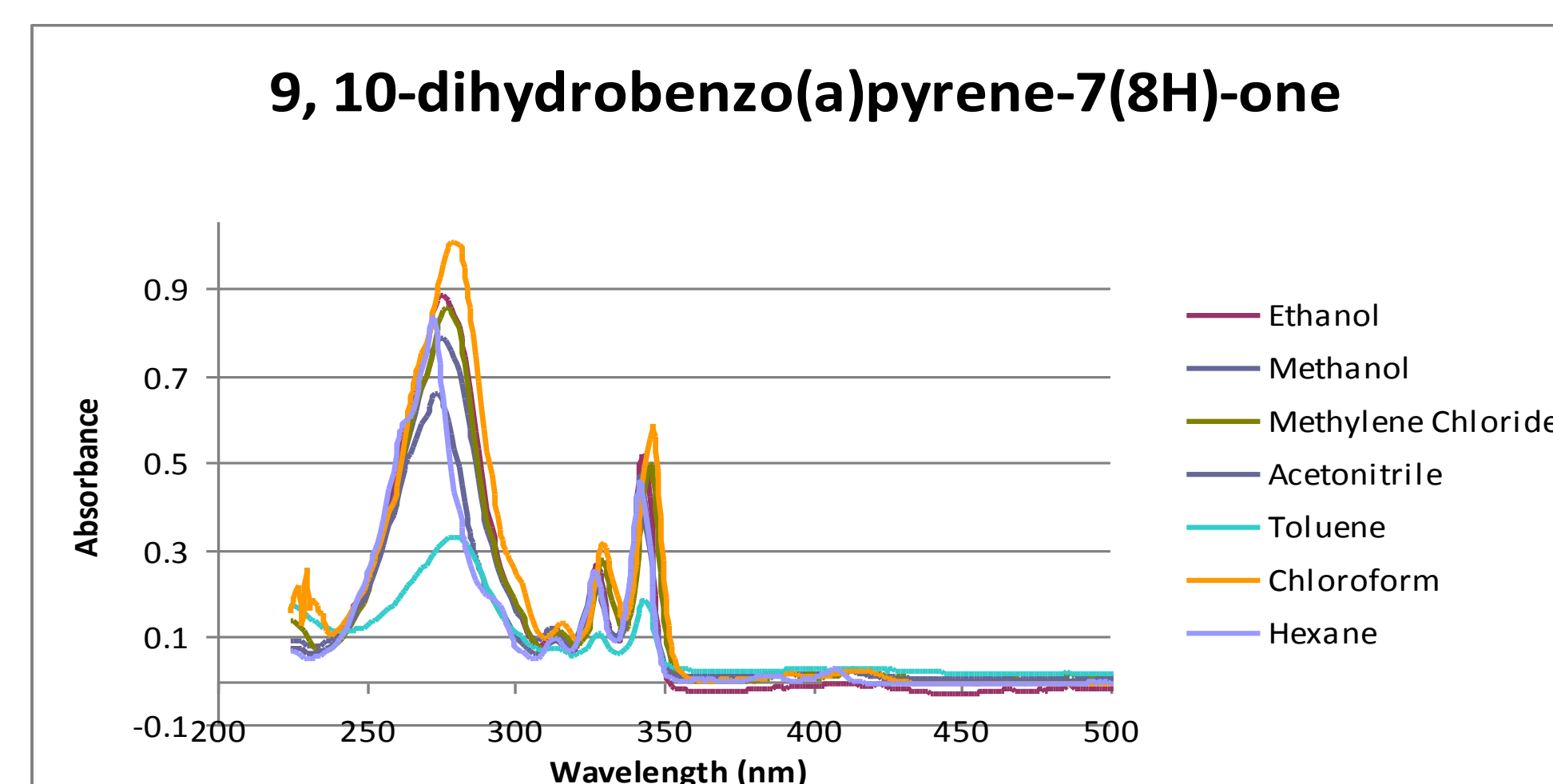
7,8,9,10-tetrahydrobenzo(a)pyrene (7,8,9,10-H₄BaP)

References

1. Herreno-Saenz, D; Evans, F; Beland, F; Fu, P, *Chem. Res. Toxicol.*, **1995**, *8*(2), 269-277
2. Shapiro, R.; Ellis, S.; Hingerty, B. E.; Broyde, S., *Chem. Res. Toxicol.*, **1998**, *11*(4), 335-341
3. Peterson, D. G.; Reichenberg, F.; Dahloff, I.; *Environ. Sci. Technol.*, **2008**, *42*(4), 1371-1376
4. Xue, J.; Liu, G.; Niu, Z.; Chou, C.; Qi, C.; Zheng, L.; & Zhang, H. *Energy and Fuels* **2007**, *21*, p. 881-890

UV-vis

These are the compiled UV-vis spectra of the two compounds dissolved in different solvents. For both compounds, the solvent, chloroform shifted the spectrum more to the red(to the right). The bottom right spectrum shows the compiled spectrum of the two compounds dissolved in the same solvent.

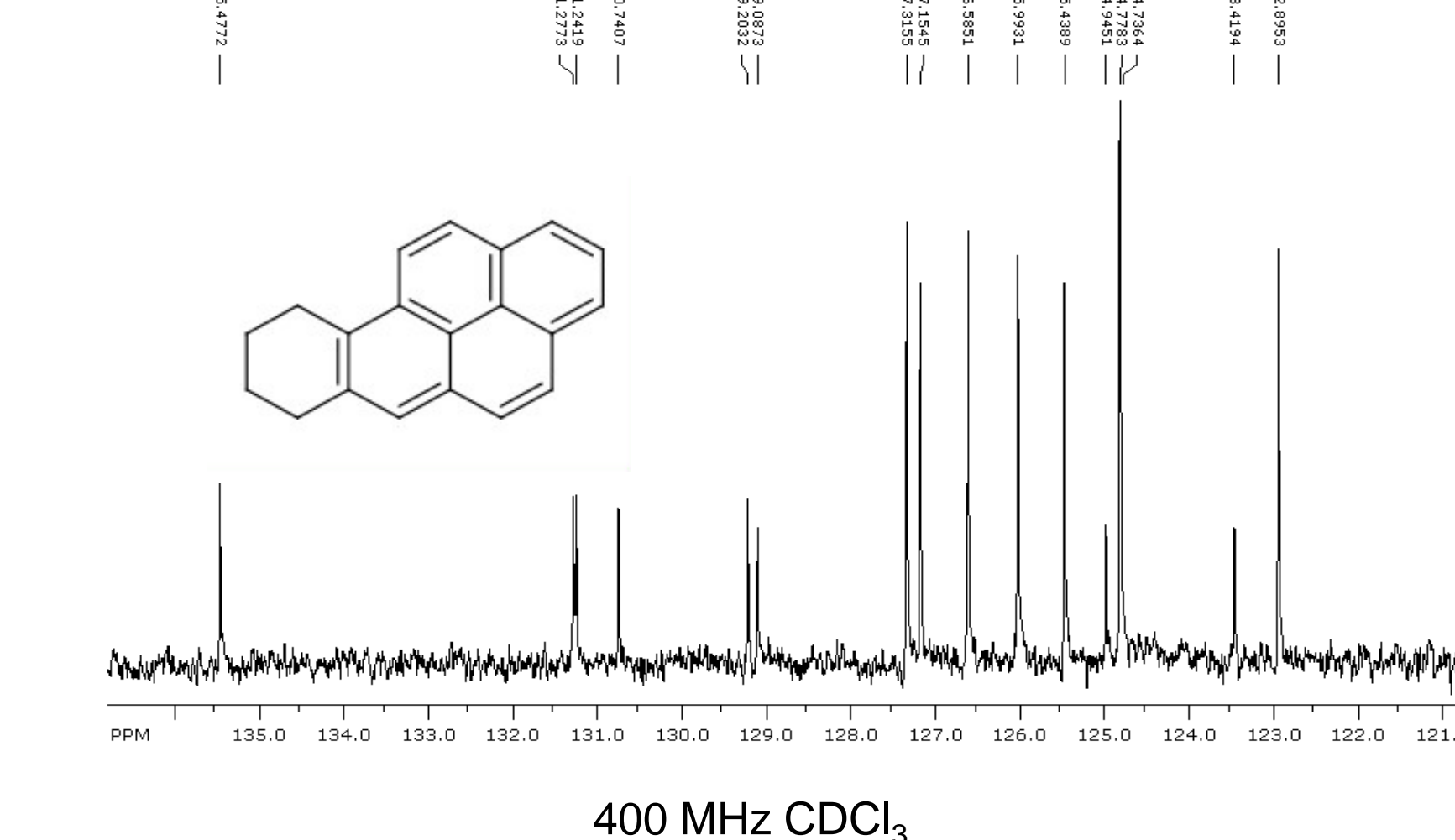
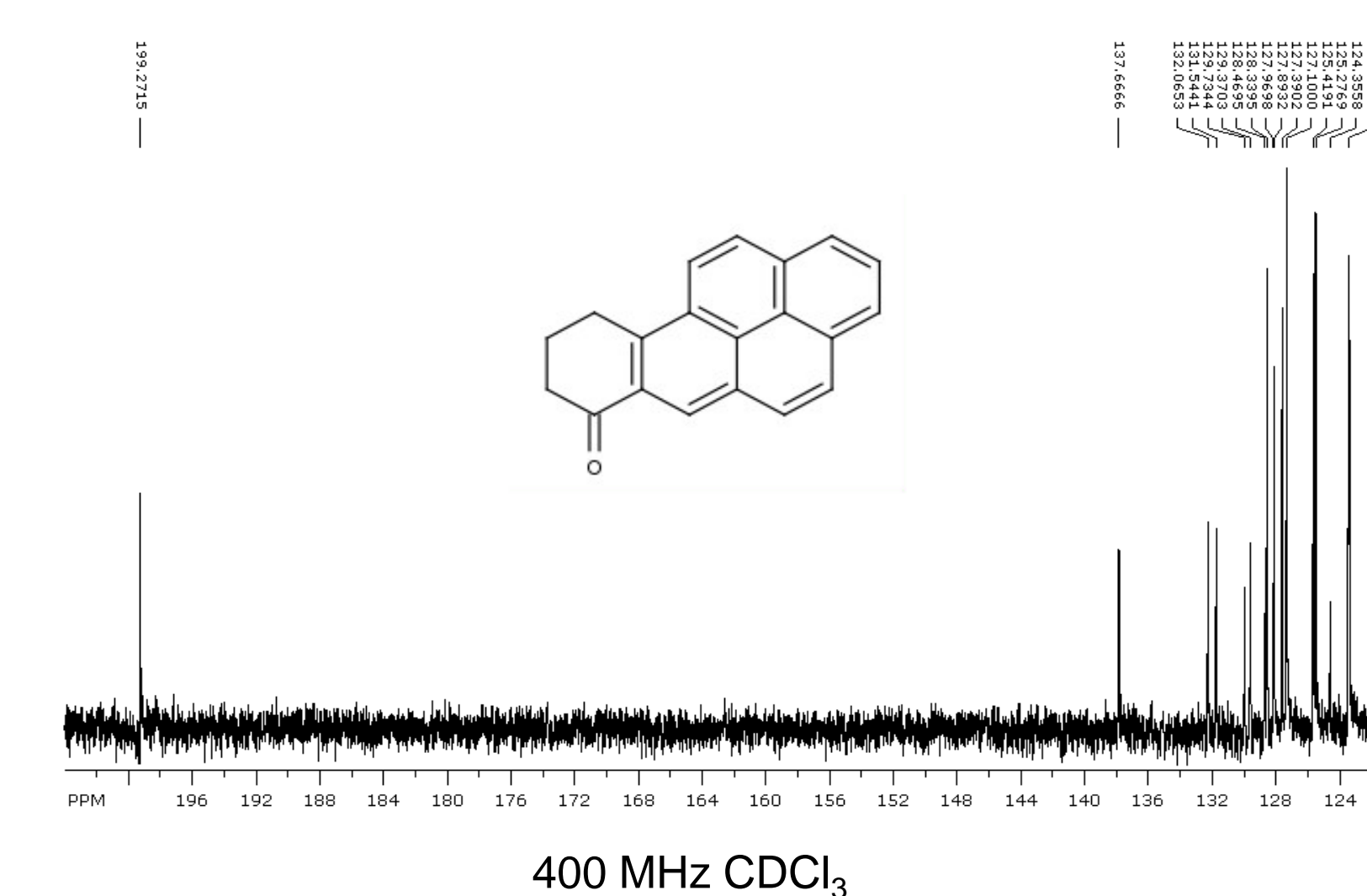


Comparison of Peak Shifts

Solvents	Chloroform	Acetonitrile	Hexane
	λ_{max} (nm)	λ_{max} (nm)	λ_{max} (nm)
9,10-dihydrobenzo(a)pyrene-7(8H)-one	317	316	309
	330	327	325
	346	343	342
7,8,9,10-tetrahydrobenzo(a)pyrene	317	315	315
	333	328	329
	349	345	346

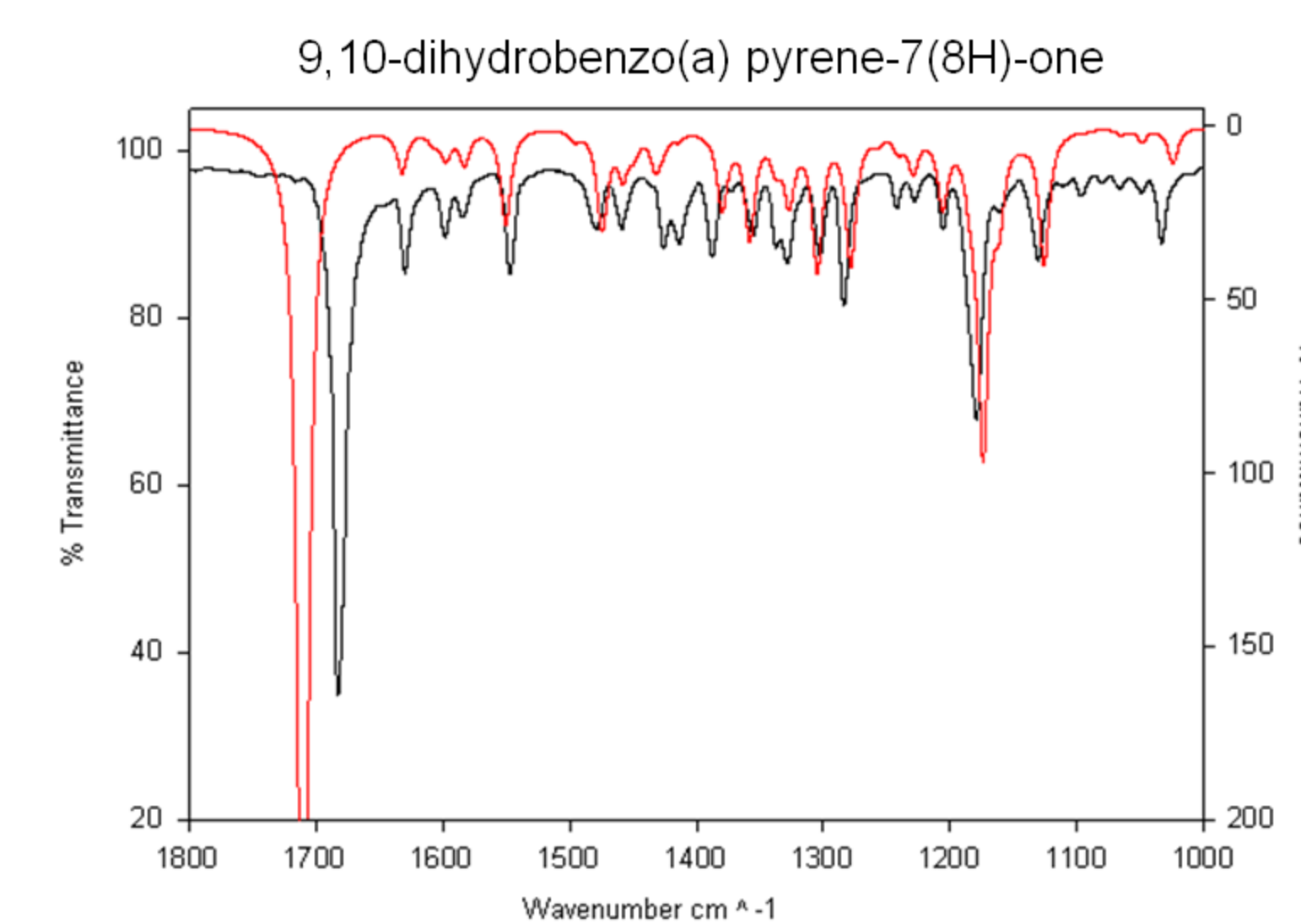
NMR

Nuclear Magnetic Resonance (NMR) spectroscopy helps in determining the structure of a compound through many different 1-D/2-D techniques. Shown below is the ¹³C spectrum for both compounds which show the number of carbons present in the molecule.



Infrared Spectrum

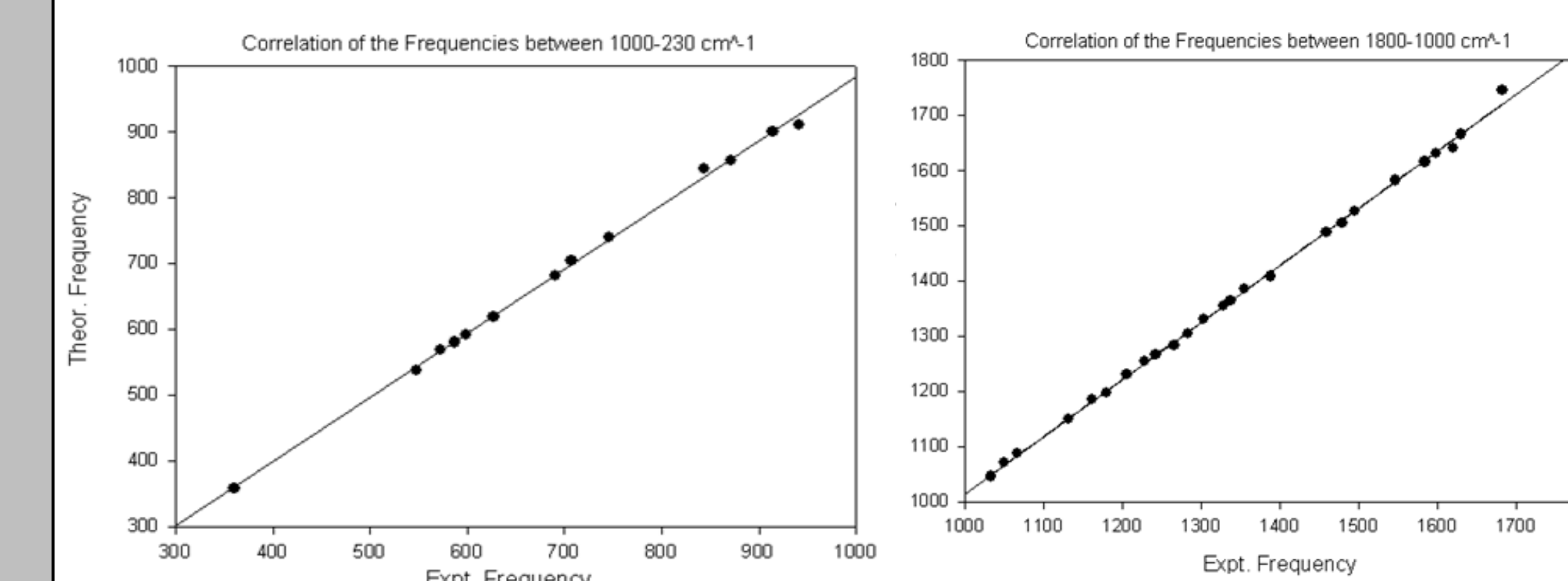
Using the density functional theory, a simulated spectrum was created. A scaling factor was found so that the experimental and the simulated spectra overlaid more closely. The scaling factor of 0.98 was used.



Infrared Spectrum

Comparison of Frequencies

Theoretical (cm ⁻¹)	Experimental (cm ⁻¹)	Theoretical *0.98 (cm ⁻¹)
1744.51	1682.36	1709.62
1629.77	1597.82	1597.17
1614.86	1583.94	1582.56
1487.56	1458.74	1457.80
1364.68	1337.39	1337.39
1230.57	1205.59	1205.96
1185.15	1161.59	1161.45



Conclusions

These experiments helped characterize these compounds with various spectroscopic techniques, so that we can understand them more and how they interact in the environment. The scaling factor was found to be 0.98 for the simulated Infrared spectrum.

Future Work

- Chromatographic Studies of PAHs on the GC/MS and the HPLC.
- Study of signaling pathways in cells on challenge to PAHs

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