Infrared Spectroscopy of Heptane and Mineral Oil under High Pressure

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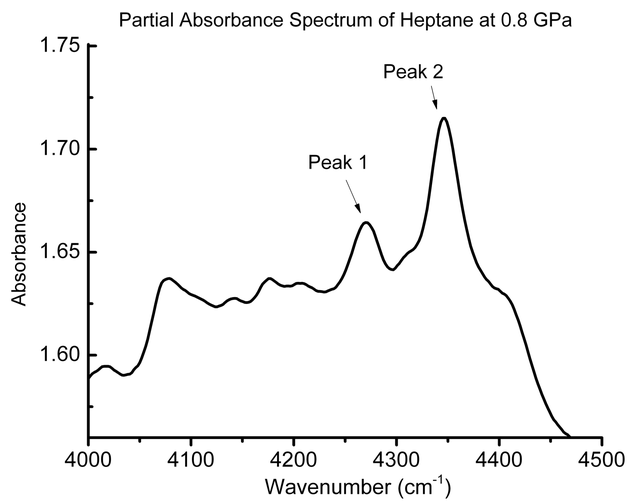
Introduction:

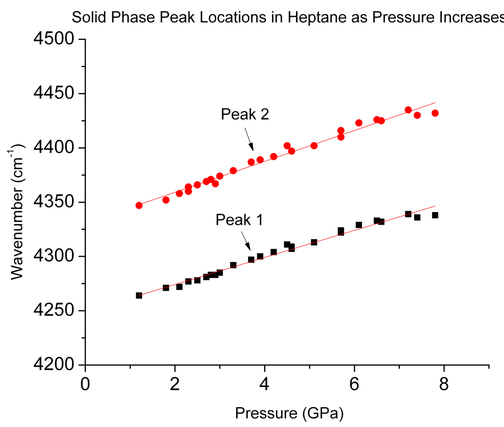
- **The liquid to solid phase transition of heptane under increasing pressure is well-documented. Other transitions, such as liquid-liquid or solid-solid transitions, could also be occurring at certain pressures.**
- **The behavior of heptane under high pressures would also useful for pressure calibrations in certain experiments where samples are immersed in heptane.**
- **Mineral oil, which is similar to heptane in chemical composition, behaves similarly under pressure and could also be used for pressure calibration.**

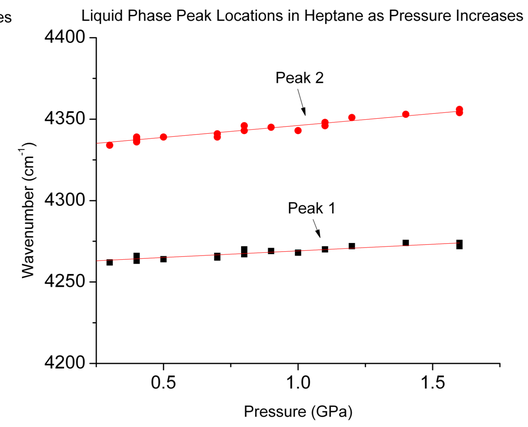
Methods:

- **A diamond anvil cell was used to compress samples of heptane and mineral oil to pressures ranging from 0.1 to 8 GPa. A stainless steel gasket was placed between the two opposing surfaces of the diamonds to hold the fluid sample in place. Ruby microspheres were included in the fluid sample in order to calibrate the pressure. A Fourier transform infrared (FTIR) spectrometer was used to obtain the IR absorption spectrum.**
- **Prominent absorption peaks that occurred in the frequency range of 4250-4450 cm^{-1} (labeled Peak 1 and Peak 2) were tracked across a range of pressures.**

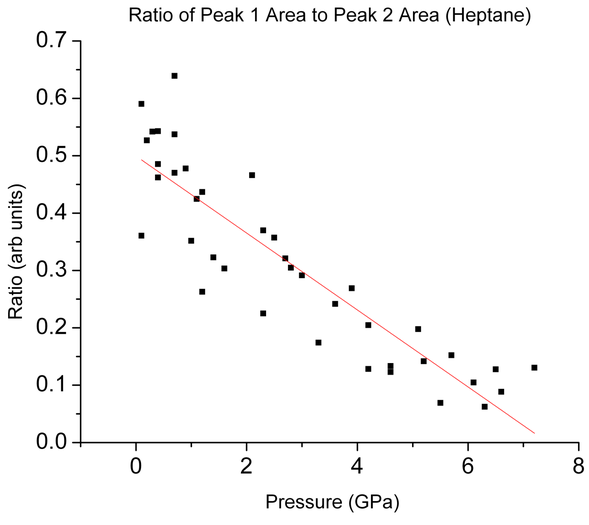
Results:







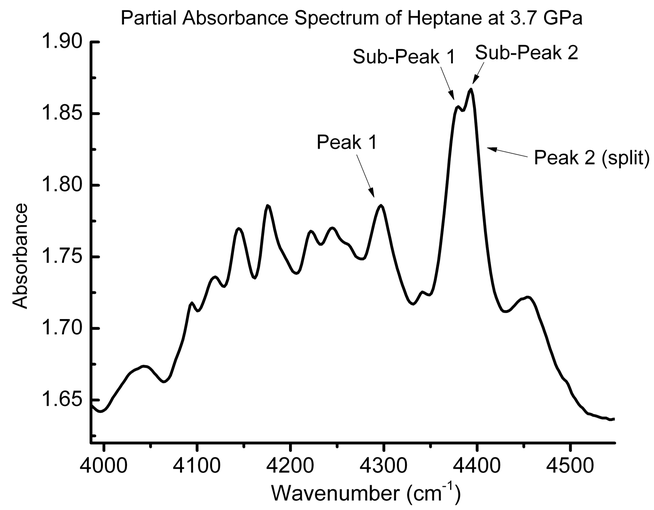
- **The peaks of interest were found to increase linearly in wave number as pressure increased.**



- **The ratio of the area of Peak 1 over the area of Peak 2 appeared to decrease linearly with pressure.**
- **These same trends also appeared in samples of mineral oil.**

Results (cont.):

- **Peak 2 was also found to split after heptane samples solidified (the peak did not split in mineral oil samples). The two sub-peaks labeled below shifted in intensity as pressure increased, with Sub-Peak 1 decreasing and Sub-Peak 2 increasing.**



Conclusions:

- **Based on the strong correlation between pressure and peak location, it appears that either mineral oil or heptane would work well for pressure calibrations in future experiments, although more research should be done to better quantify this relationship.**
- **Further research should also seek explanations for the observed correlation between the ratio of the areas of Peak 1 and Peak 2 and explore what happens as this ratio approaches zero. More data could also try to explain the splitting of Peak 2. These features may be caused by additional phase transitions.**

References:

Yamaguchi, M., S. Serafin, T. H. Morton, and E. L. Chronister. “Infrared Absorption Studies of n-Heptane under High Pressure”. American Chemical Society, 2003.

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