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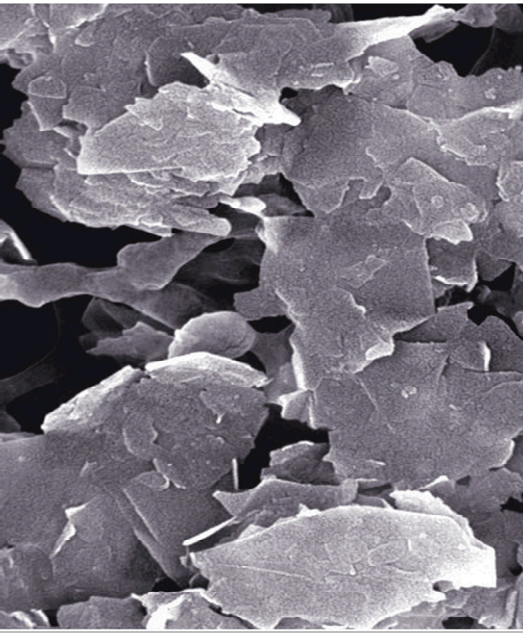

Effects of Doping Graphene onto CTAB-d_3 in H_2O

Using NMR to investigate the magnetic alignment of liquid crystal/graphene composites

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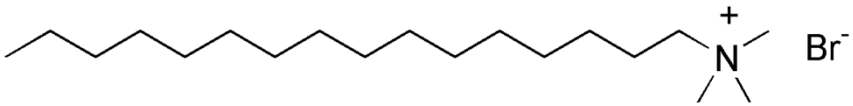
http://www.azonano.com/article.aspx?ArticleID=3206

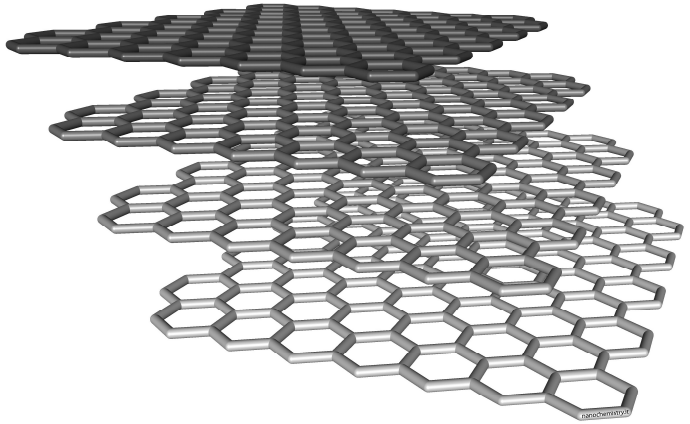
Background

- Hexadecyltrimethylammonium bromide (CTAB) forms liquid crystal (LC) in H_2O
- LC is combination of physical phases:
  - Liquid, solid
  - Has electric/magnetic alignment
- Graphene (GP) is 2-D carbon sheets
- GP has many applications:
  - Reduce electro-optical switching response times through mitigation of free ions in LC.
  - GP nanoplatelets can be used as an ultrafiltration unit
  - Essentially act as a barrier between two substances (batteries)

CTAB Structure



Graphene sheets

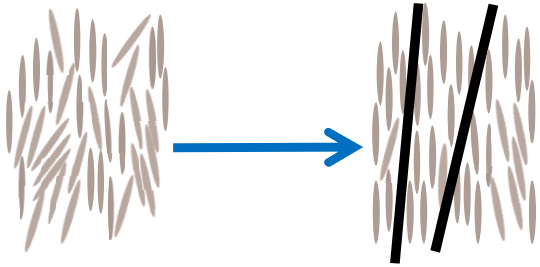


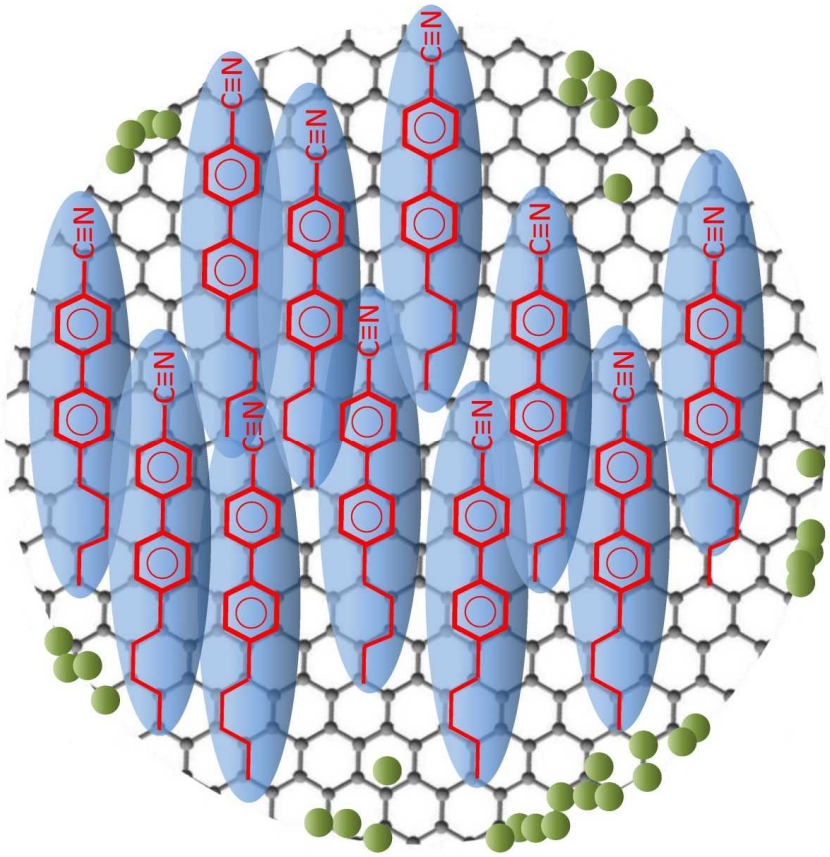
Can Graphene be used to modify CTAB liquid crystal?
Can we increase the order in LC?

http://www.nanochemistry.it/download/download.html
http://chemistry.about.com/od/factsstructures/ig/Chemical-Structures---C/Cetrimonium-Bromide.htm

Previous Work

- Electro-Optical: Graphene nanocomposites increase orientational order on 5CB LC in nematic phase [1]
- $\pi - \pi$ stacking of the hexagonal carbon structure
- Work done in Todd Alam's lab using NMR has also shown this result on 5CB [2]





5CB= 4-Cyano-4'-pentylbiphenyl

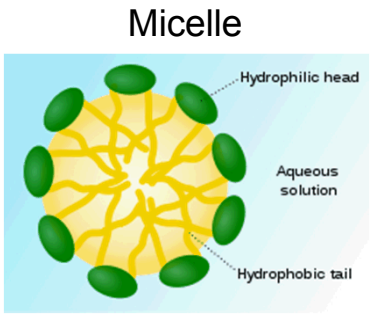
Can Graphene be used to modify CTAB liquid crystal?
Can we increase the order in LC?

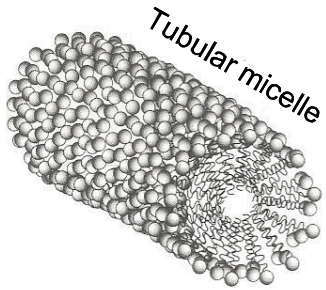
[1] Rajratan Basu, Daniel Kinnamon, and Alfred Garvey, Appl. Phys. Lett. **106**, 201909 (2015)
[2] Todd Alam and Charles Pierce, Chemical Physics Letters, Volume 592, 30 January 2014, Pages 7–13

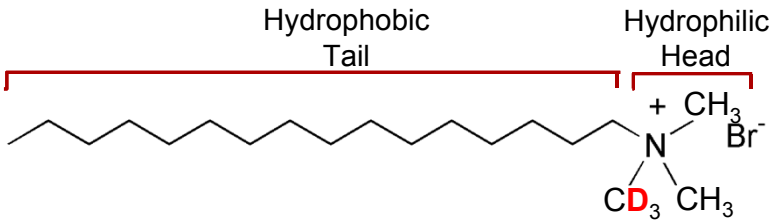
Why use CTAB-d_3?

D=^{2}H

- Surfactant: Decreases surface tension in H_2O
  - Part hydrophilic head that attracts water
  - Chain is hydrophobic tail
- Naturally forms micelles in solution
  - Tubular micelles have magnetic susceptibility: torque produced at large temperature can overcome viscosity in solution
- CTAB can be used during the production process of graphene nanoplatelets
- ^{2}H NMR detects only the deuterium atoms in samples







https://en.wikipedia.org/wiki/Micelle
http://www.metafysica.nl/ontology/general_ontology_29m1b.html

Goals for Summer Project: ^{2}H NMR

Determine the impact of graphene on the liquid crystal order of CTAB

- Use ^{2}H NMR spectroscopy
- Magnetic alignment?

What's the impact of the process of sample preparation?

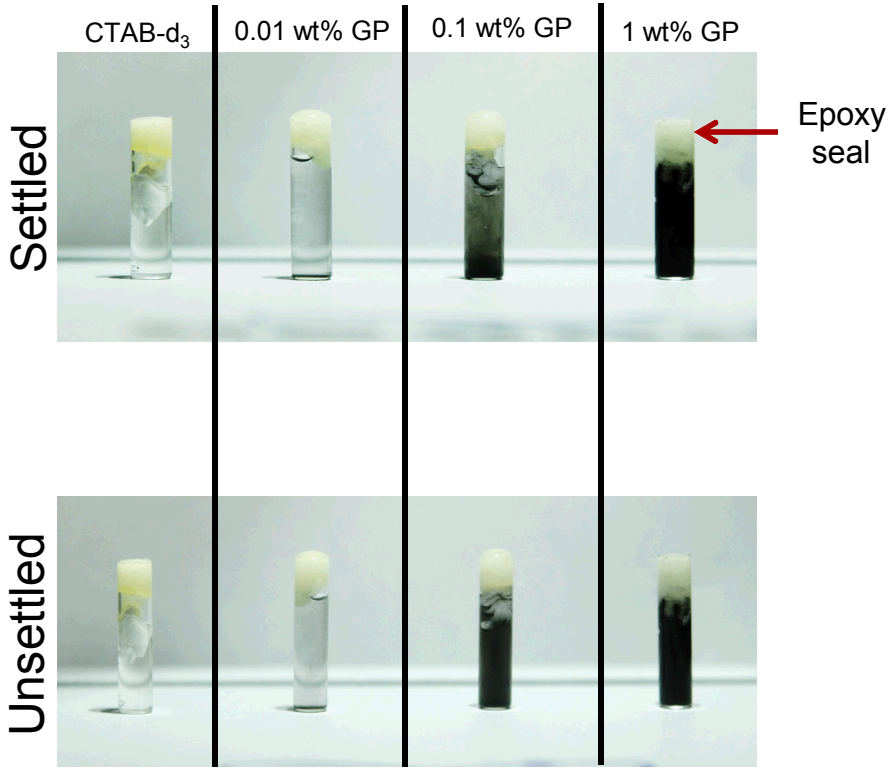
- Try a few different methods for sample prep and see what works best
- Vortex?
- Sonication?

Sample Preparation

- 25 wt.% CTAB-d_3 in H_2O
  - 0.01 wt.% Graphene
  - 0.1 wt.% Graphene
  - 1 wt.% Graphene

Bruker NMR 400

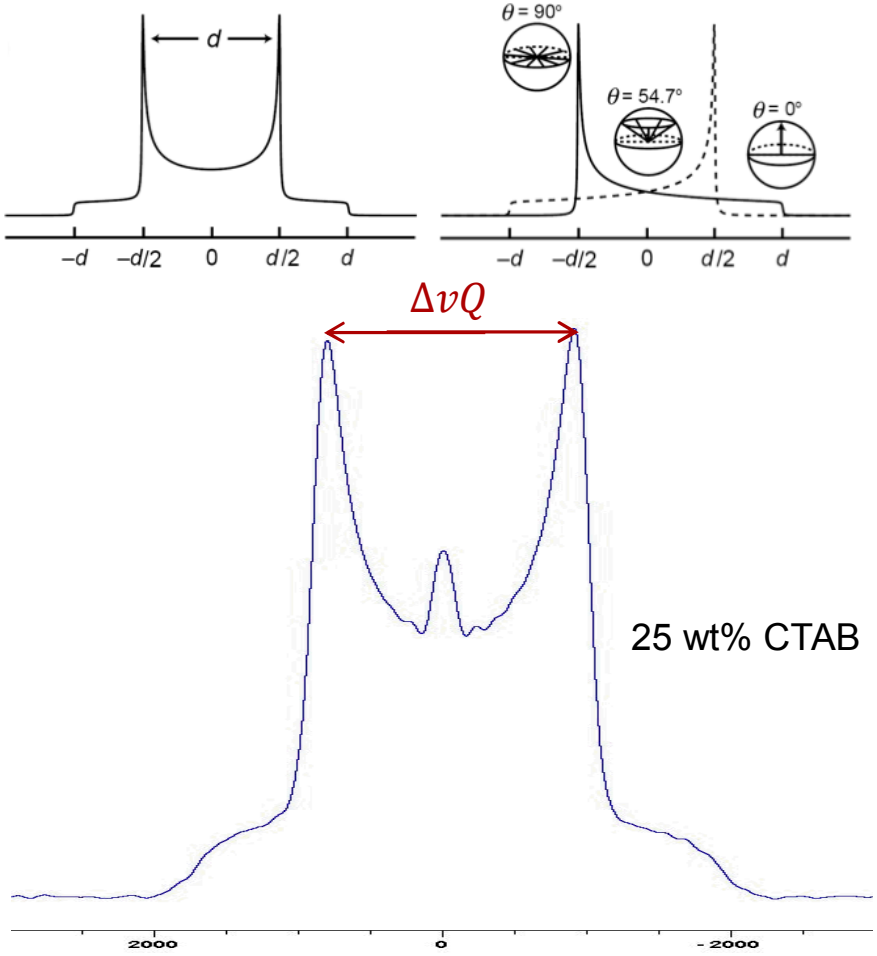
Static Probe



Powder Pattern & Energy Levels

- Powder Pattern in ^{2}H NMR describes the lack of alignment in liquid crystal
- CTAB first put in magnet at room temperature
  - Obtained powder pattern
  - No alignment

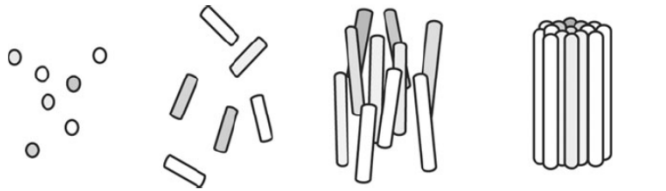
$$\Delta v_Q \sim SCD\left(\frac{3\cos^2\theta - 1}{2}\right)$$

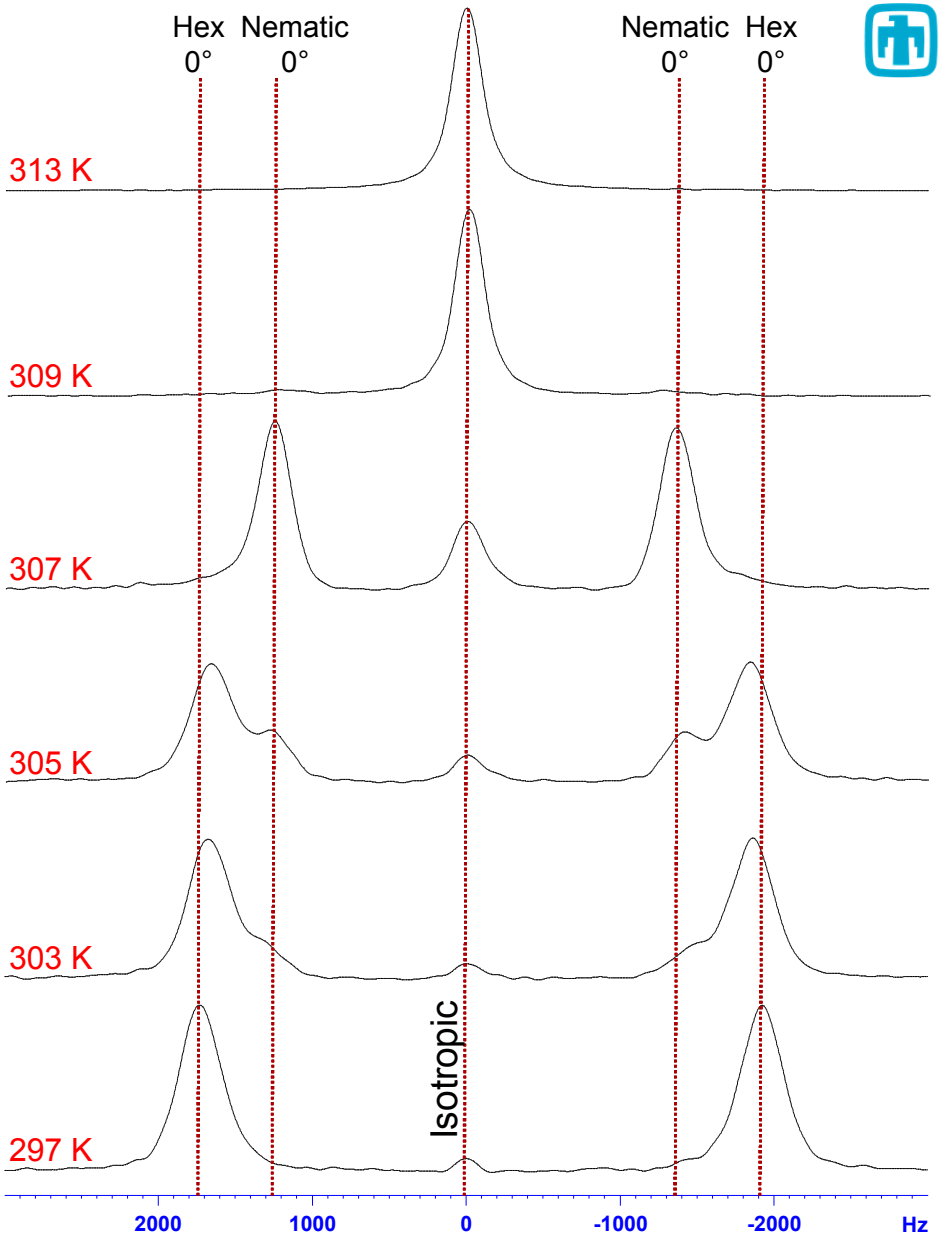


http://www.chemie.uni-hamburg.de/nmr/insensitive/tutorial/en.lproj/solid_state_nmr.html

25 wt. % CTAB Variable Temperature Expt.

- Multiple liquid crystalline phases occurring at once:
  - 0° outer peaks represent the hexagonal phase
  - 0° inner peaks represent the nematic phase
  - Middle peaks represent the isotropic phase
- Relative phase concentration determined by normalized integration of peaks
- In magnetic field:
  - Increase in orientational order
  - Increase in positional order (hexagonal phase)





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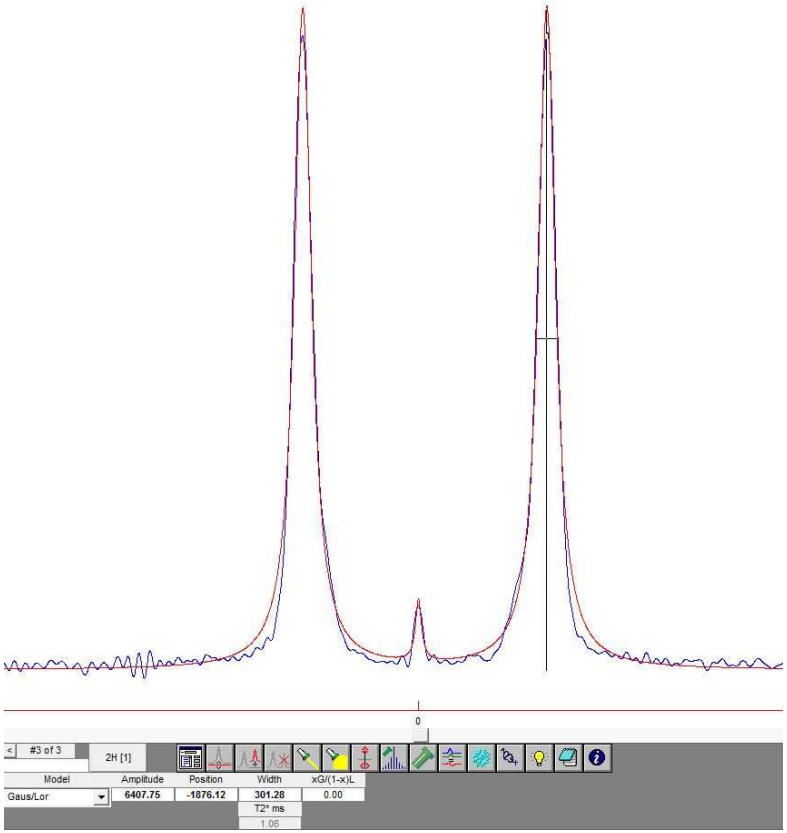
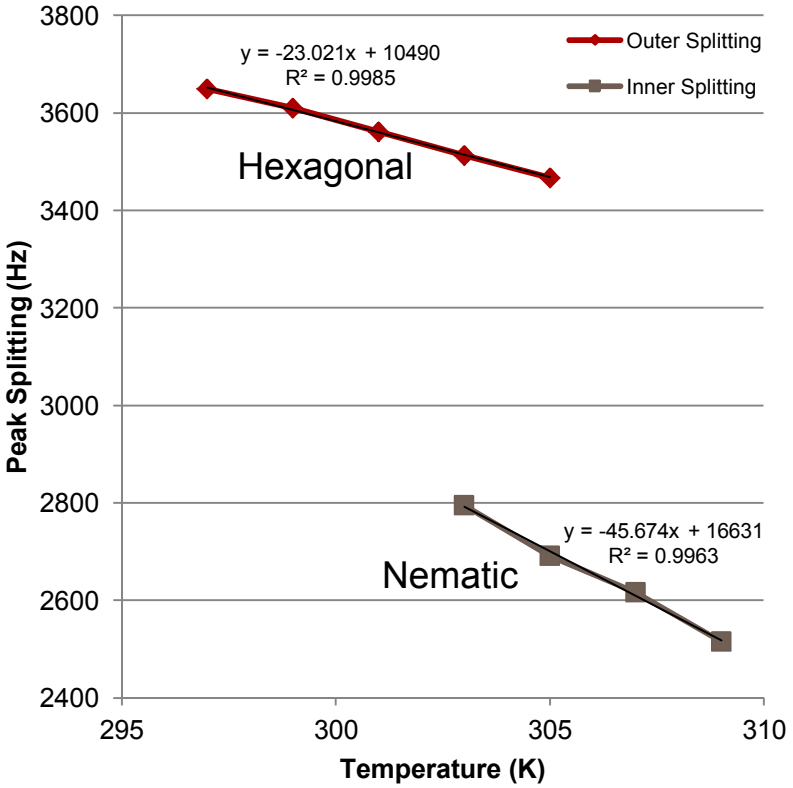
25 wt.% CTAB Splitting

Data gathered from definable peaks through Gaussian modeling using DMFit freeware

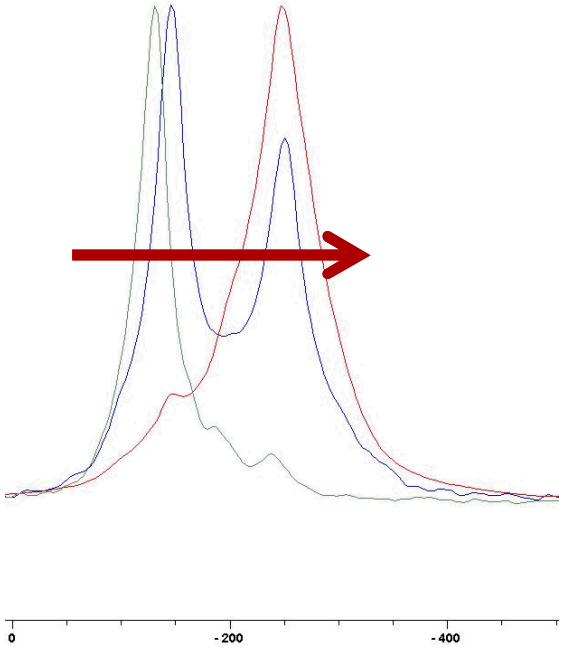


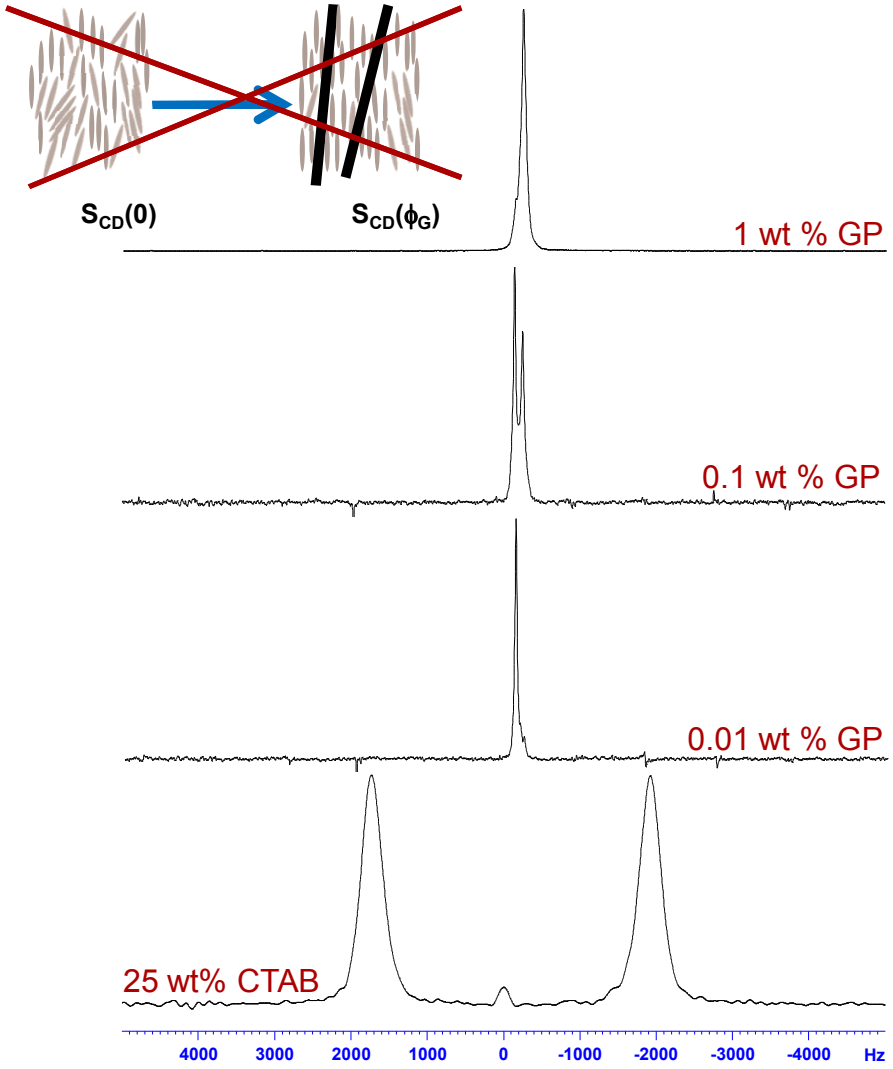
Linear splitting of outer and inner peaks as function of temp.



CTAB vs. GP Spectra

- Graphene doped CTAB samples appear isotropic.
- Conclusion: **Graphene destroys the liquid crystalline phases from forming, even at low concentrations!!**
- Interesting chemical shift in different concentrations of GP samples
  - Increasing surface interaction with GP





Conclusions

- Used ^{2}H NMR to look at LC phases in CTAB
- GP disrupts any of the phase
  - Interaction between GP & surfactant destroys micelle structure
  - Magnetic susceptibility of GP itself different than CTAB

- Thank you:
  - Todd Alam, PhD
  - Staci Dorsey
  - Everyone else in my group

Questions?

Sled champs: The Mountain Goats