



THE UNIVERSITY OF TEXAS AT EL PASO



NANOMATERIALS, INTERFACES, AND CONFINEMENT
FOR ENERGY & THE ENVIRONMENT LABORATORY



U.S. DEPARTMENT OF
ENERGY

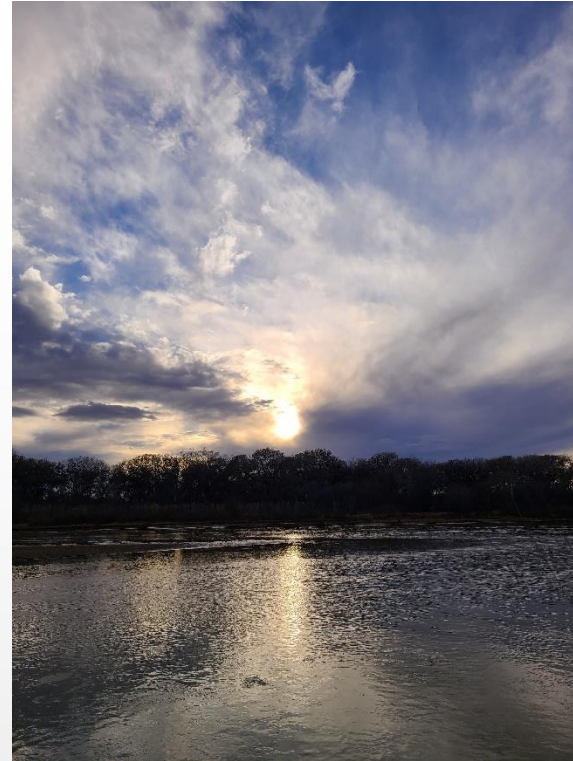
Water Effects on Clustering and Reverse Micelle Formation of CO₂ Capture Solvents

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About Myself

- Born in the Philippines
- Settled in Albuquerque, NM
- Enrolled at The University of New Mexico to study Mechanical Engineering
- Like to play guitar, longboard, and play sports with friends



Why Capture CO₂?

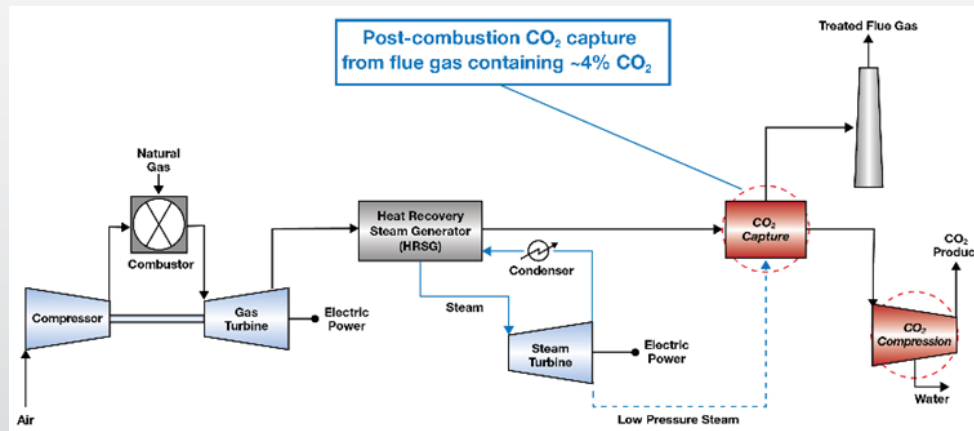
- Carbon Dioxide traps heat that bounces off the Earth's surface₁.
 - Rise in global temperature
 - Rise in sea levels
 - Change in weather patterns
 - Droughts
 - Acidification of Oceans
 - Death of marine life
- Why is there CO₂ in the first place?



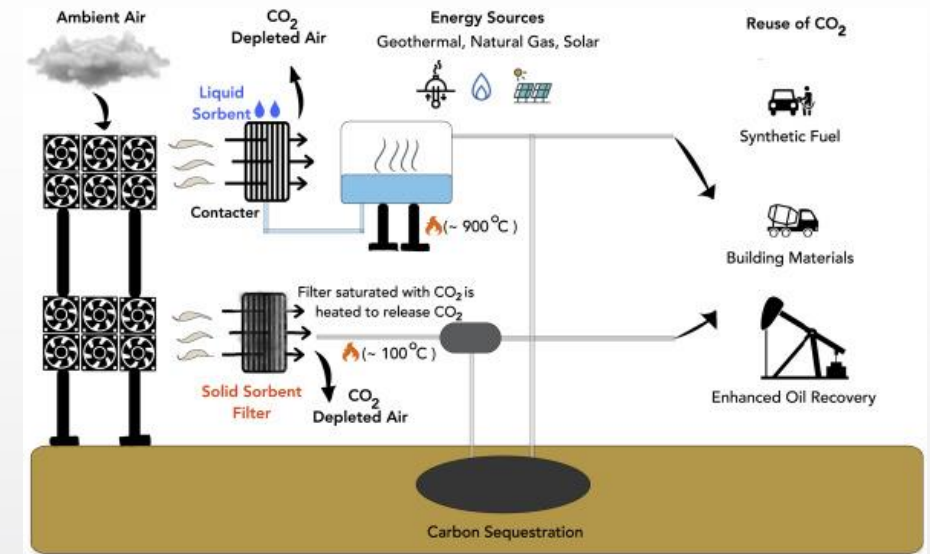
[Business Insider](#)

Motivation and Applications

- Need better molecular understanding to improve
 - Point Source Capture
 - Captures CO₂ from a power plant's flue gas stream to prevent its release into the atmosphere
 - Direct Air Capture
 - Captures CO₂ directly from the atmosphere and is then stored or used for other purposes



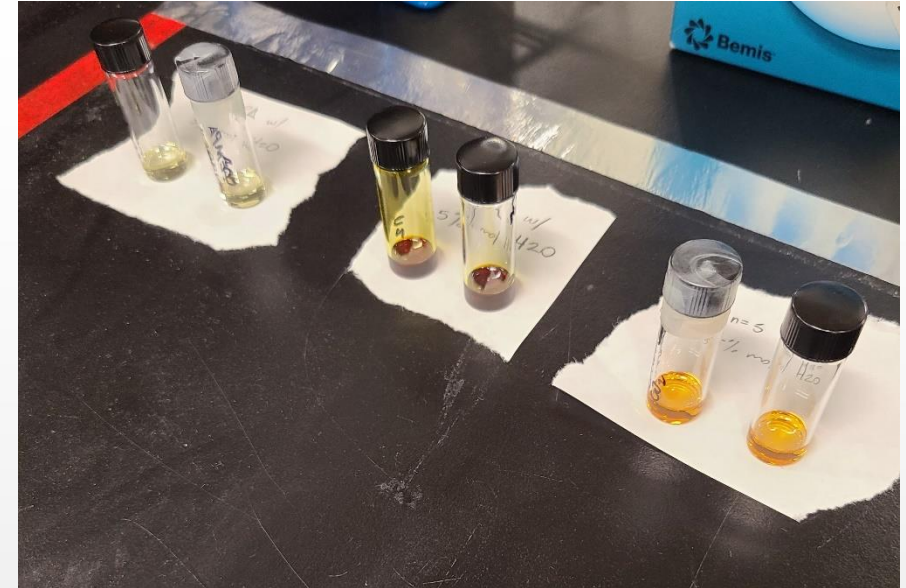
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Science Direct

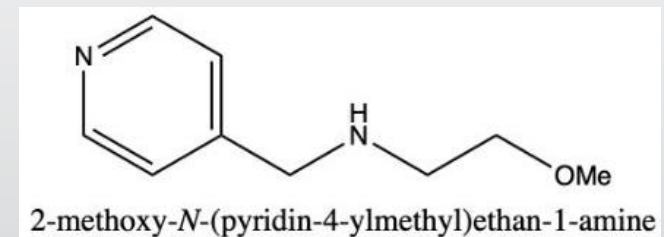
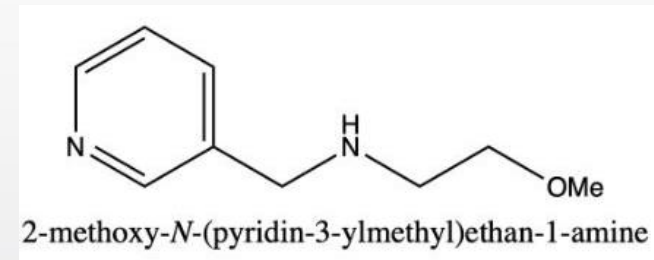
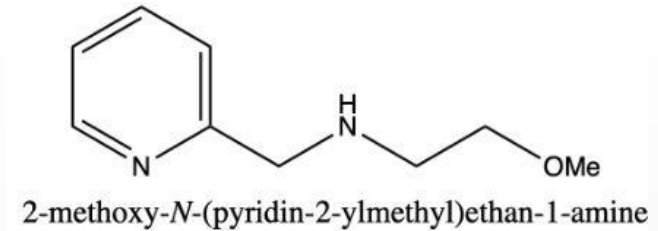
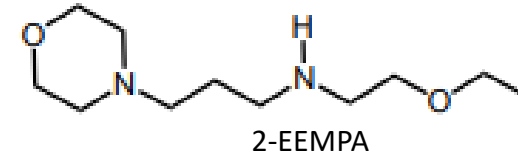
Carbon-Capturing Water Lean Solvents (WLS)

- What does “water lean” mean?
 - Why use them?
- Properties
 - Nonpolar
 - Hydrophobic
- Benefits₂
 - High capture efficiency
 - Lower regeneration energy
 - Minimized use of water
 - Overall lower cost



WLS Continued

- WLS used in study
 - 2-EEMPA
 - 2-Aminopyridine
 - 3-Aminopyridine
 - 4-Aminopyridine
- Other Properties
 - High viscosity increase with CO₂
 - Increase in polarity with CO₂
 - Reversible with the removal of CO₂
 - Reusable

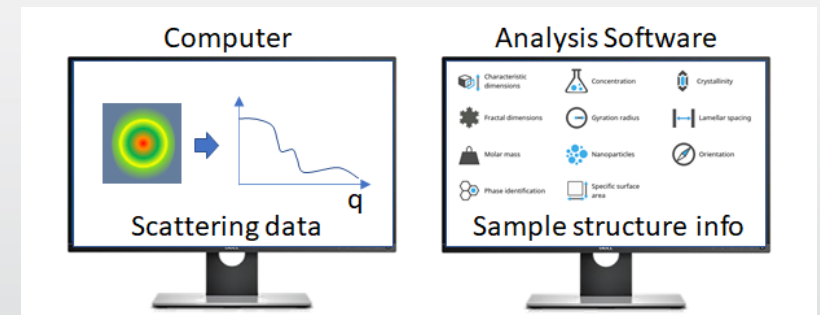
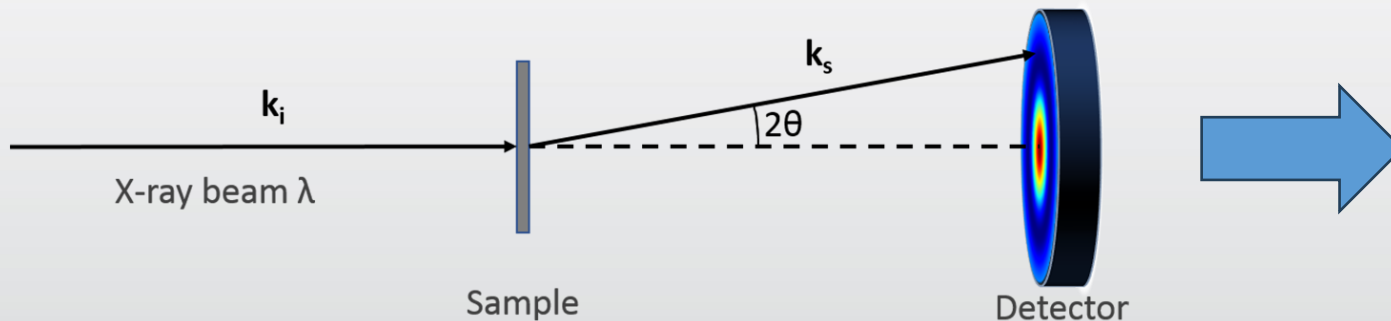


Ways to Study Structure

- Small Angle X-Ray Scattering₃
 - Provides information about larger structures in a sample
- Wide Angle X-Ray Scattering
 - Provides more precise information to the spacing between atoms

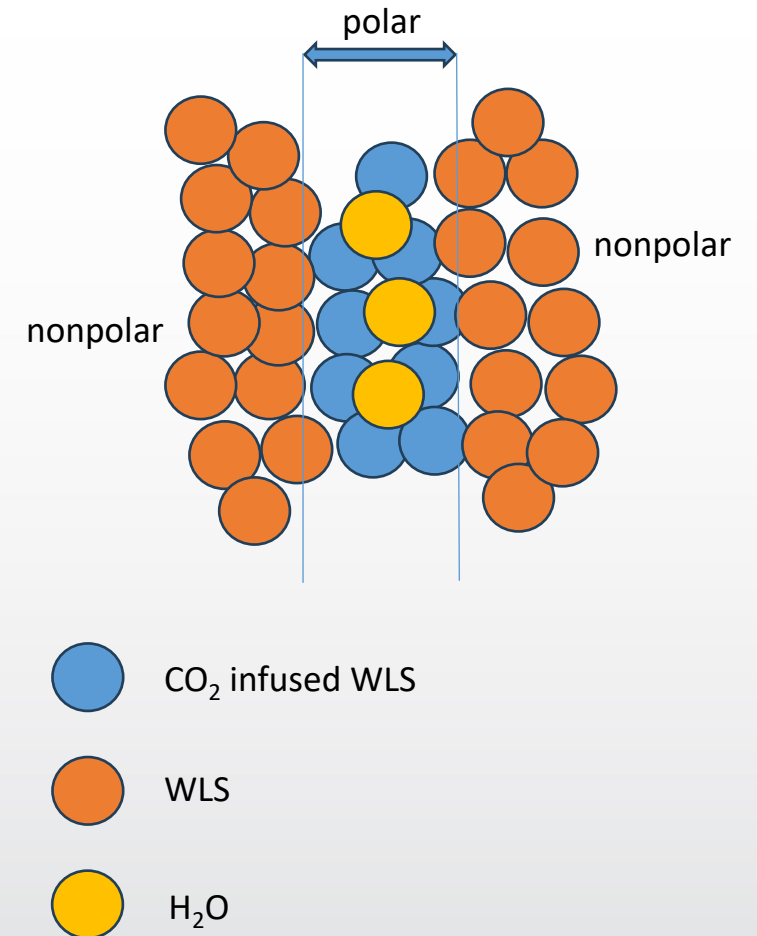
$$Q = k_f - k_i$$
$$Q = \frac{4\pi \sin \theta}{\lambda}$$

$$d \sim \frac{2\pi}{Q} \quad 2\theta \sim \frac{\lambda}{d}$$



My Study

- 2-EEMPA, 2-Aminopyridine, 3-Aminopyridine, and 4-Aminopyridine were introduced with H₂O and CO₂
 - Samples of "5%" mol H₂O without CO₂
 - Samples of "5%" mol H₂O with CO₂
 - Samples of 40% mol H₂O with CO₂
- Form small micelle-like clusters
 - Will later become reverse micelles once Pluronic F-127 is introduced



DISCLAIMER

	EEMPA	N=2	N=3	N=4
Water Mass (g)	Insufficient Data*	0.0205	0.01557	0.00583
Actual Water mol %	~12-15**	15.9	12.5	5.12

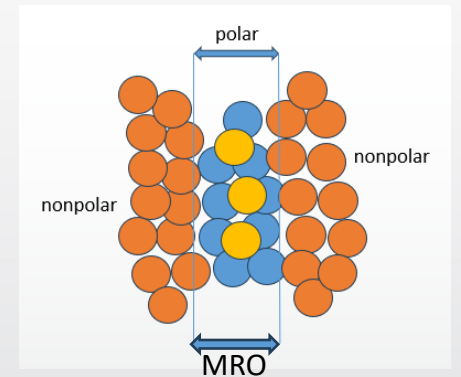
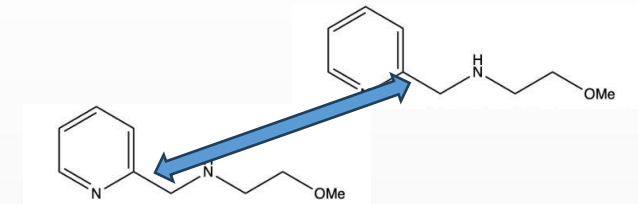
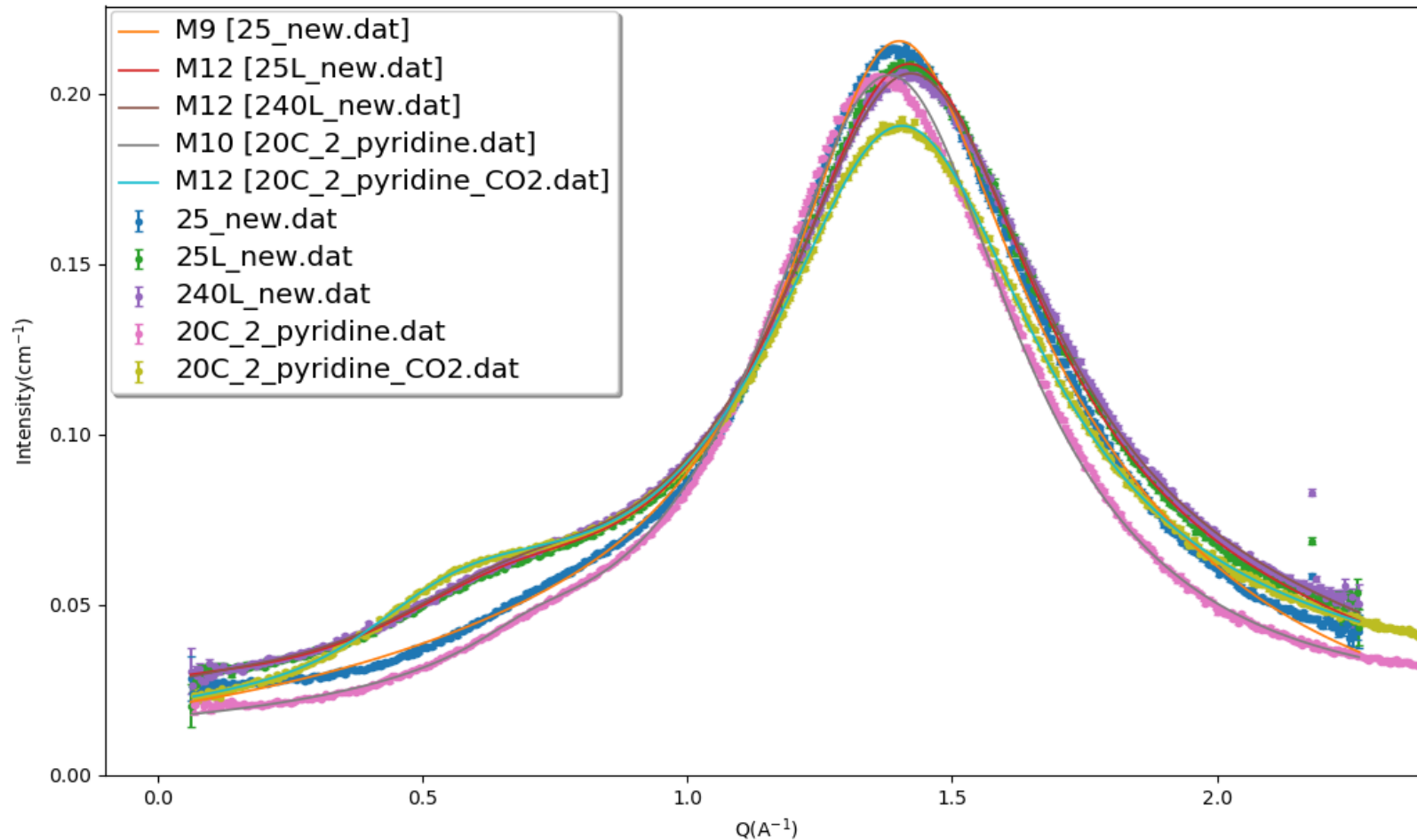
*actual water mass was not recorded, only calculated mass

**one droplet of water was dropped for EEMPA, N=2, and N=3 so the estimate is around the water mol % of N=2 and N=3

Interpreting the Results

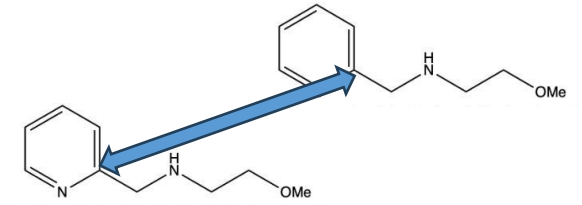
Intensity: higher=higher concentration, lower=lower concentration
 Q value: higher=smaller distance, lower=bigger distance
 Peak width: narrow=higher degree of order, broad=lower degree of order

$$d \sim \frac{2\pi}{Q}$$

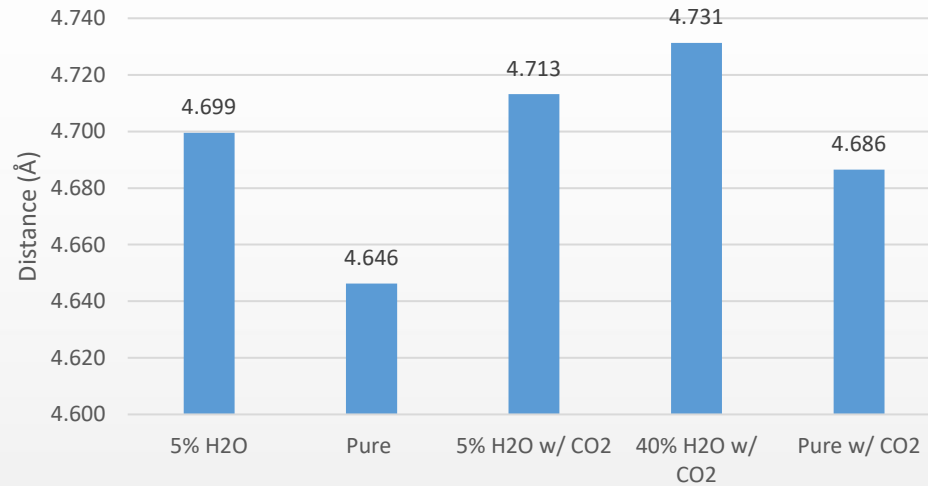


Results and Analysis

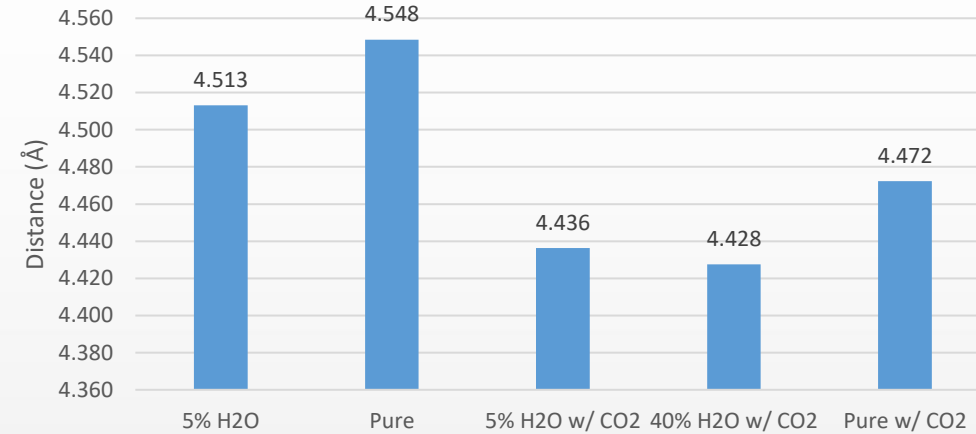
Nearest Neighbor Distance Between Center of Mass of Each EEMPA/Aminopyridine Molecule



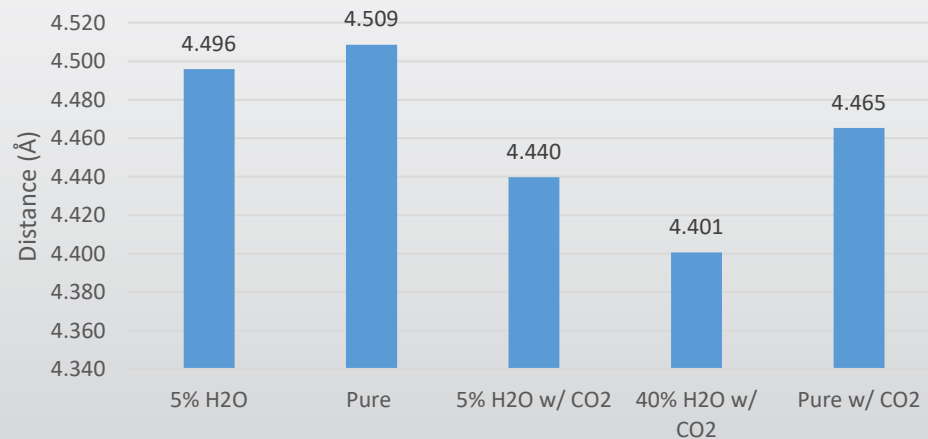
EEMPA



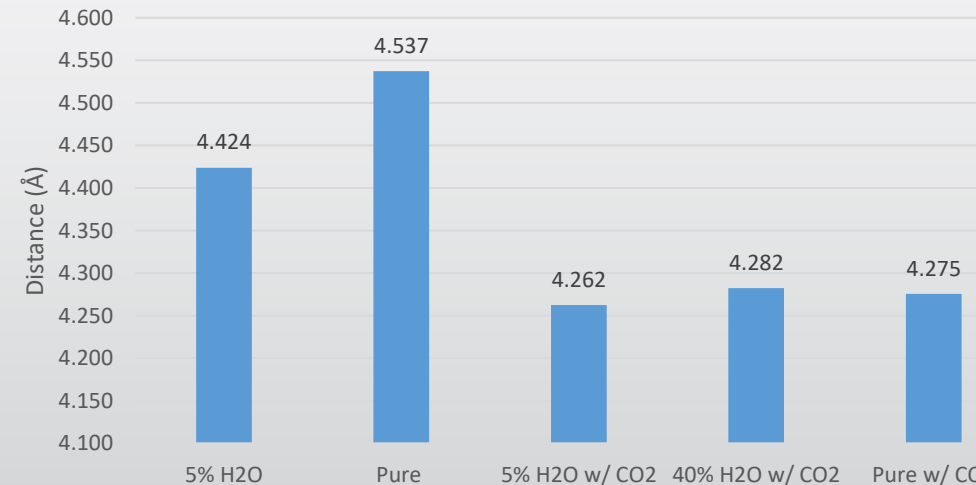
2-Aminopyridine



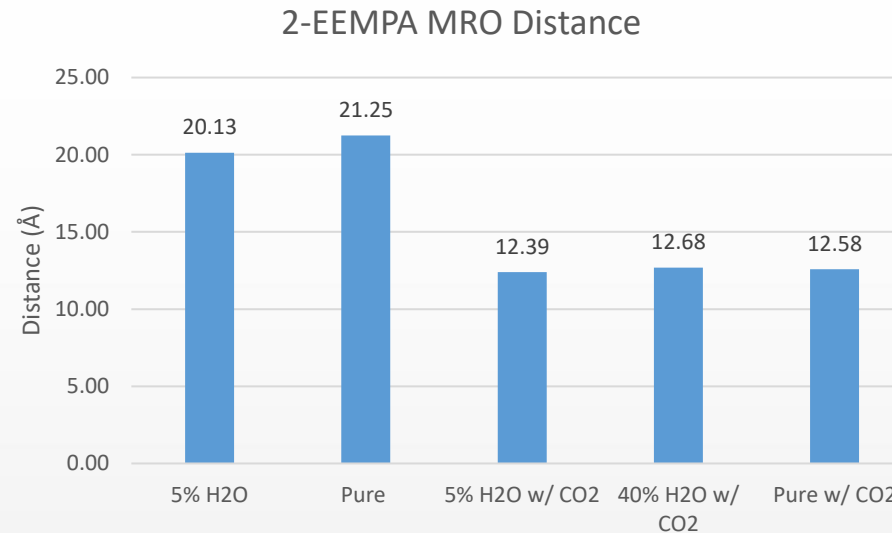
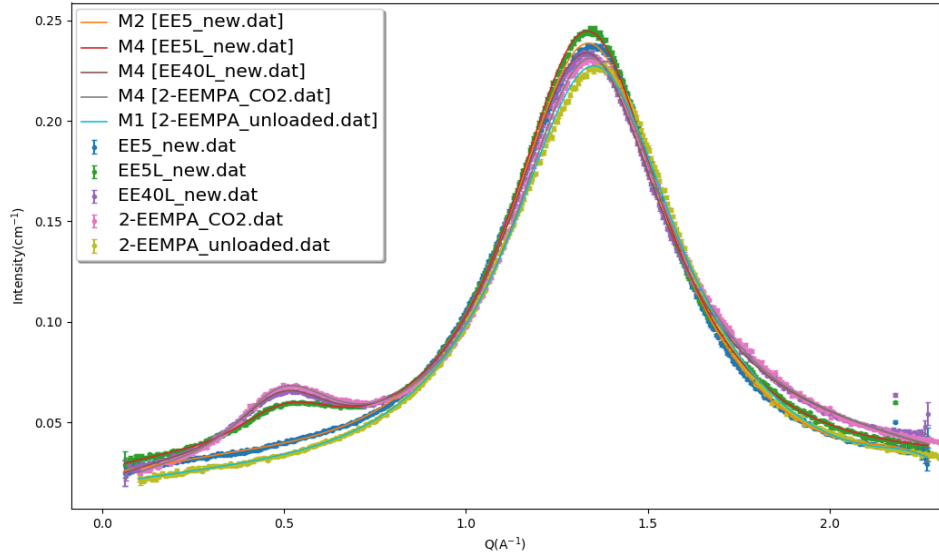
3-Aminopyridine



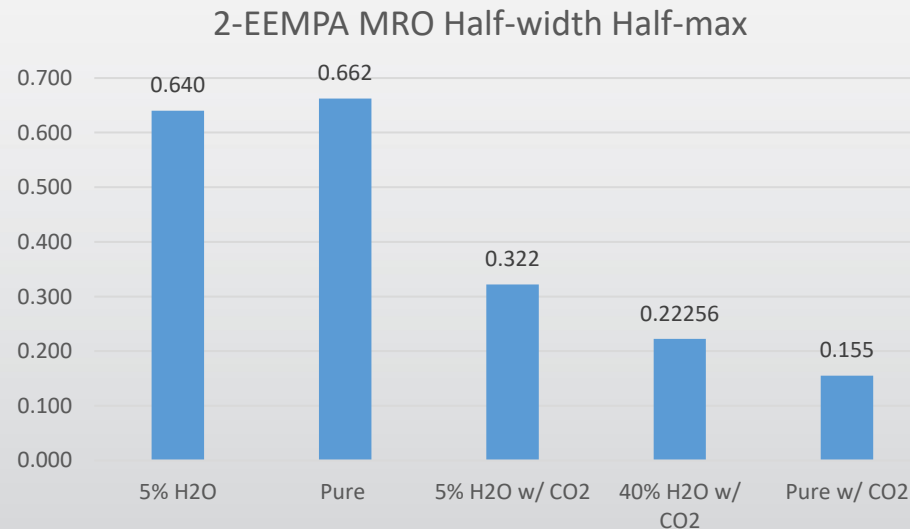
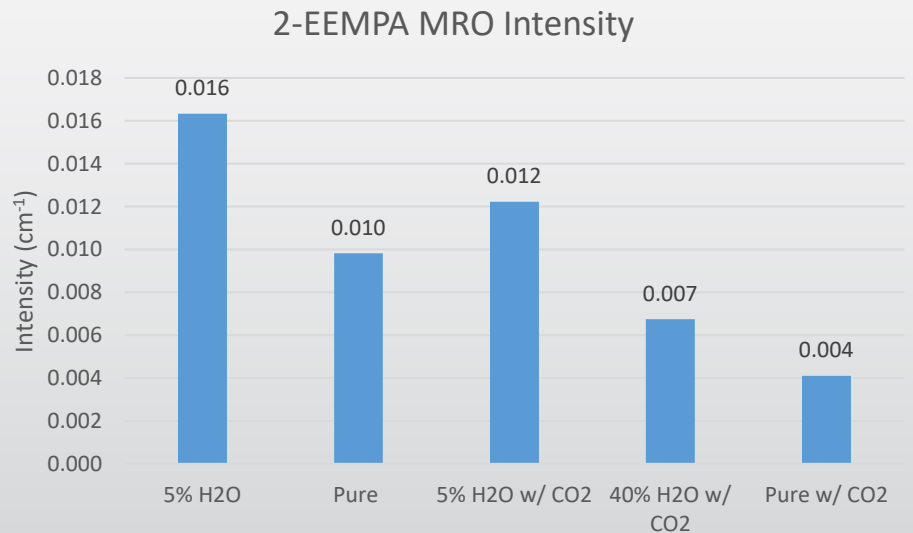
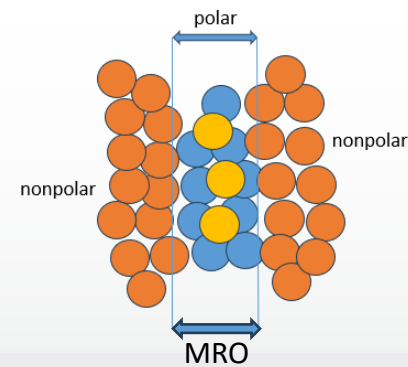
4-Aminopyridine



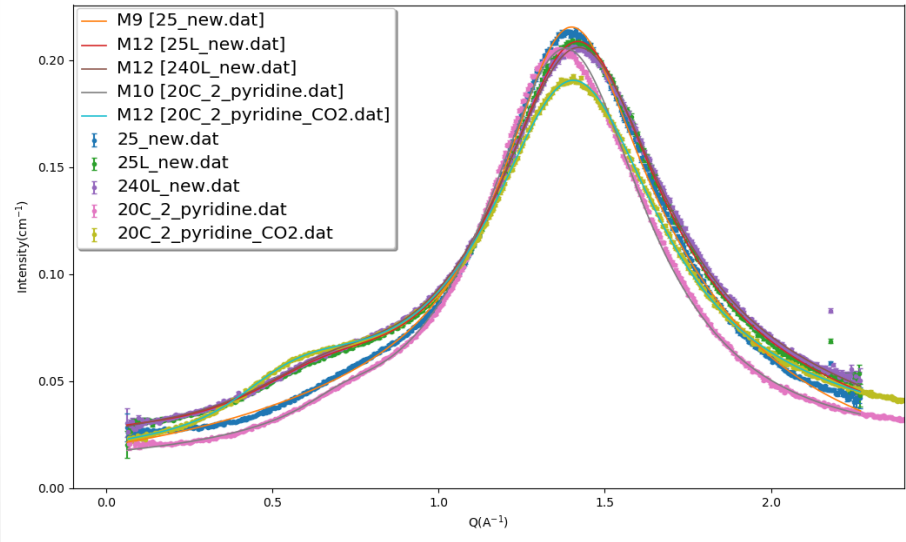
2-EEMPA Medium Range Order



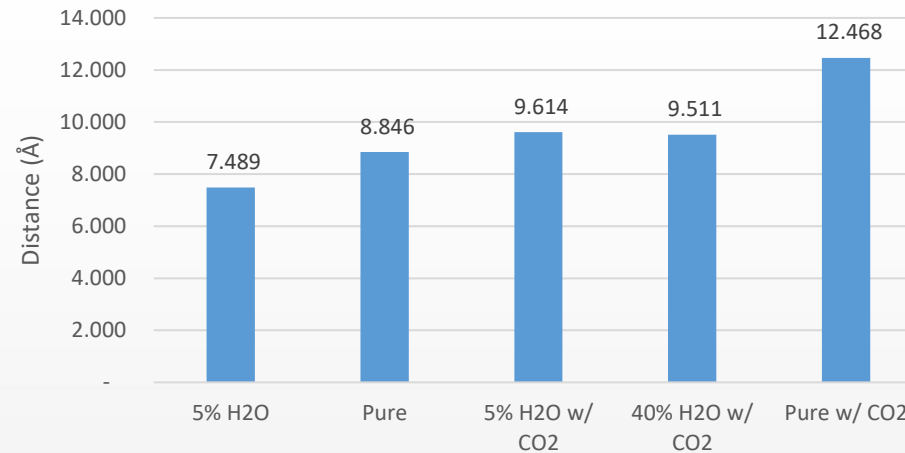
Intensity: higher=higher concentration, lower=lower concentration
 Half-width, Half-max: lower=higher degree of order, higher=lower degree of order



2-Aminopyridine Medium Range Order

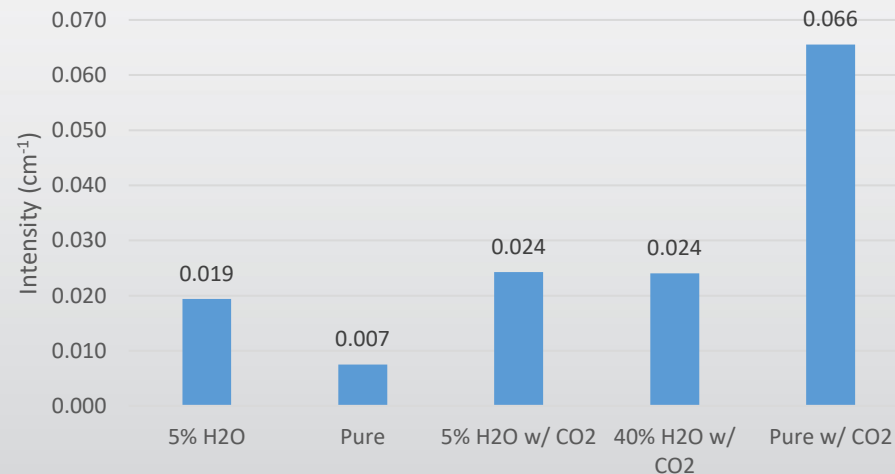


2-Aminopyridine MRO Distance

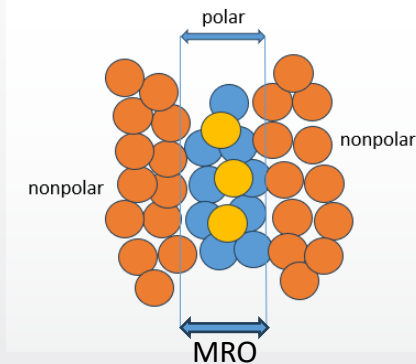
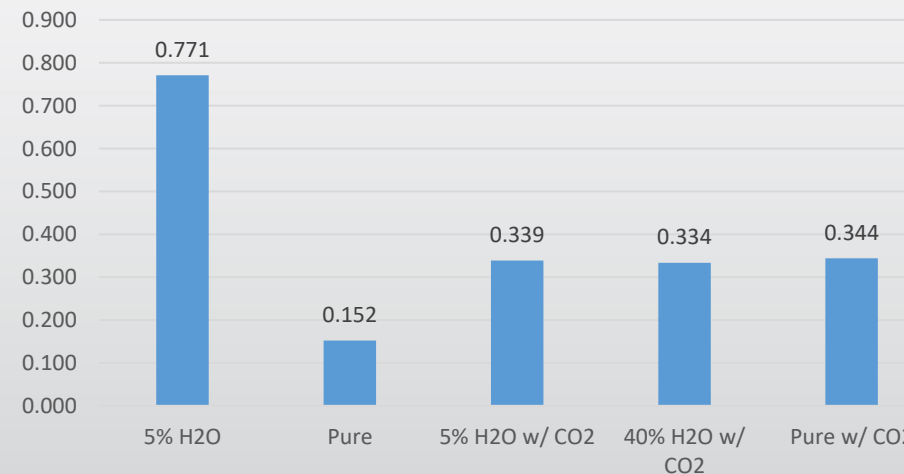


Intensity: higher=higher concentration, lower=lower concentration
 Half-width, Half-max: lower=higher degree of order, higher=lower degree of order

2-Aminopyridine MRO Intensity



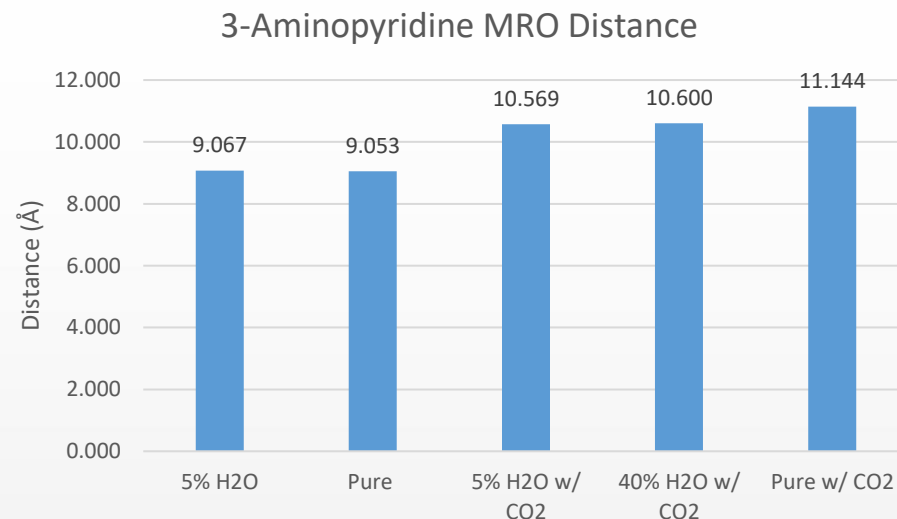
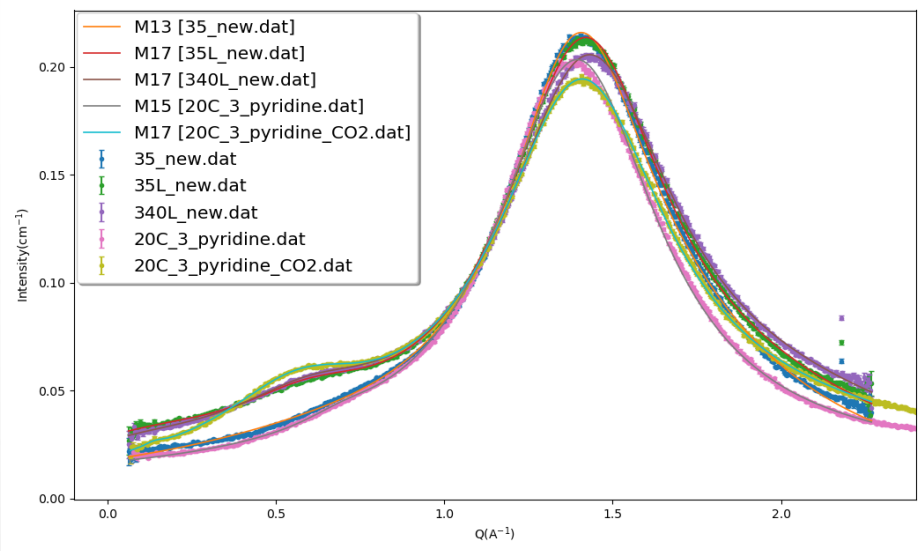
2-Aminopyridine Half-width Half-max



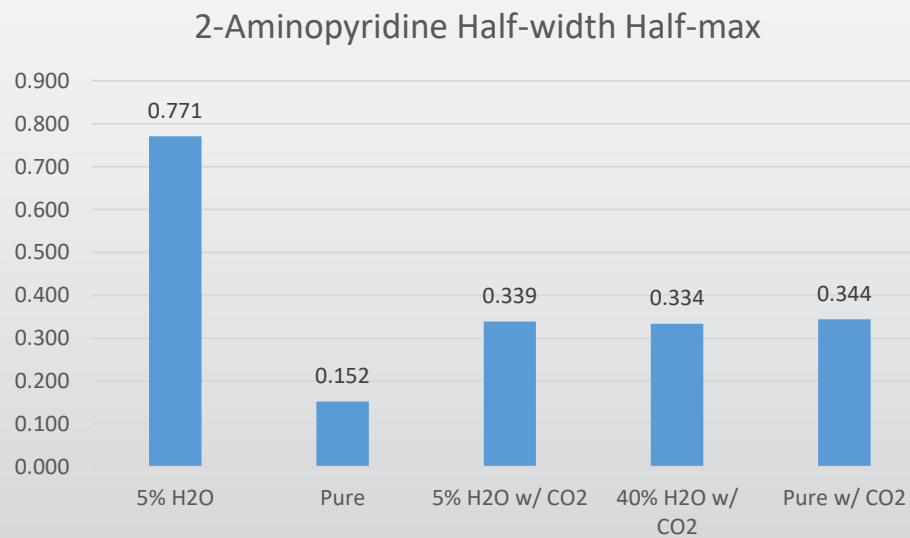
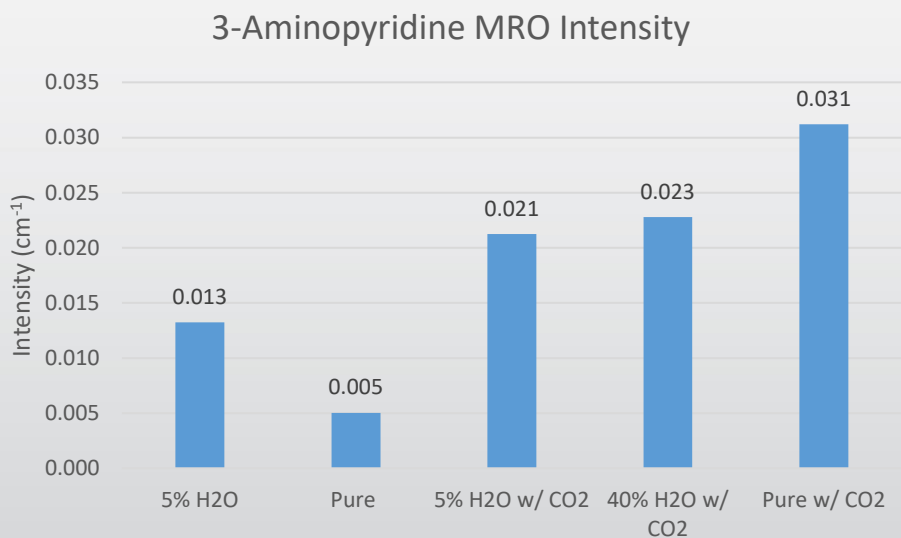
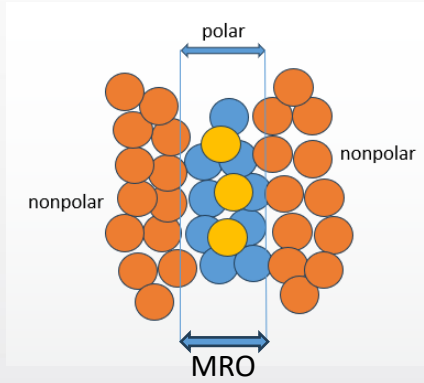
*Samples without CO₂ have a relatively high fitting error



3-Aminopyridine Medium Range Order



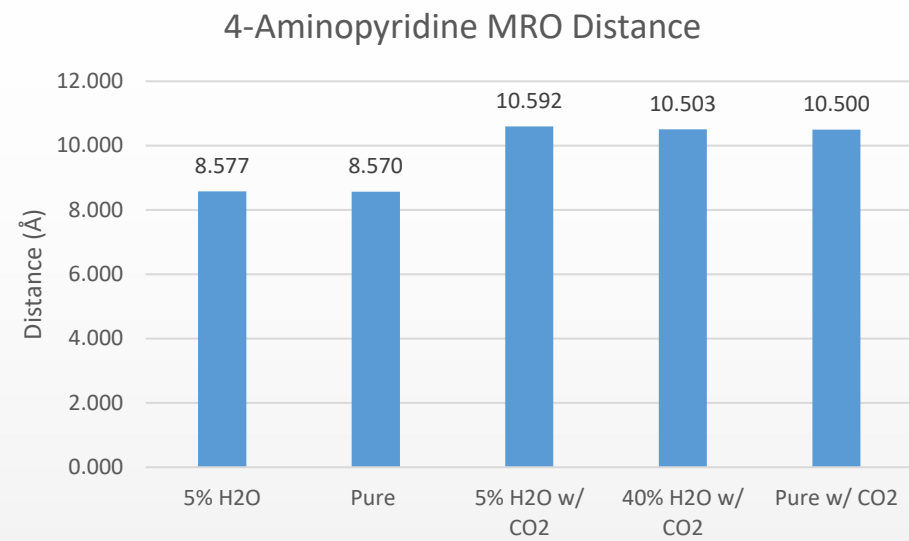
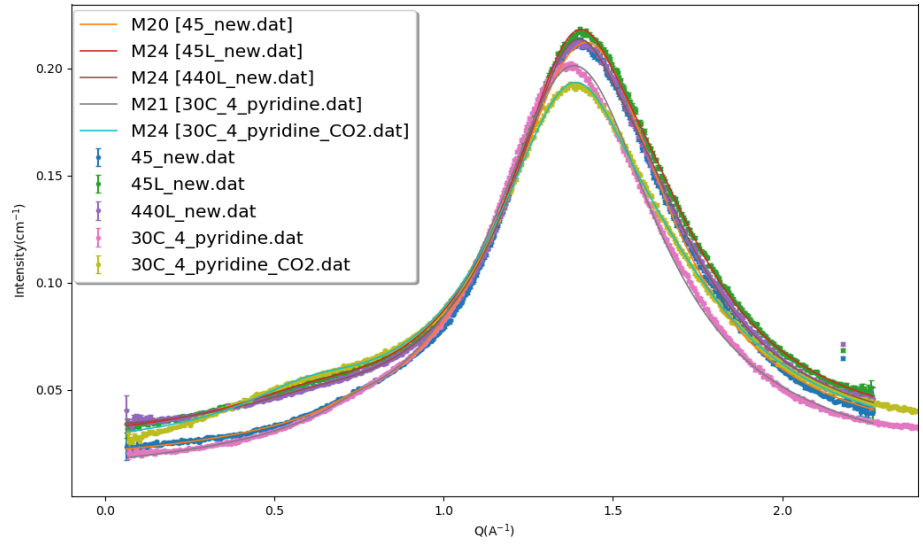
Intensity: higher=higher concentration, lower=lower concentration
 Half-width, Half-max: lower=higher degree of order, higher=lower degree of order



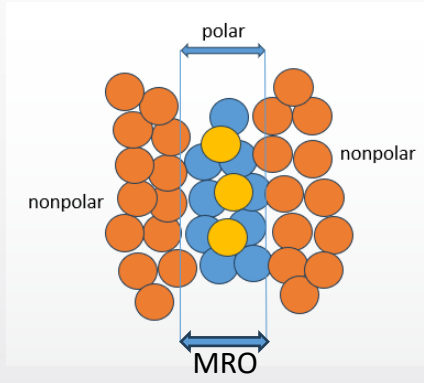
*Samples without CO₂ have a relatively high fitting error



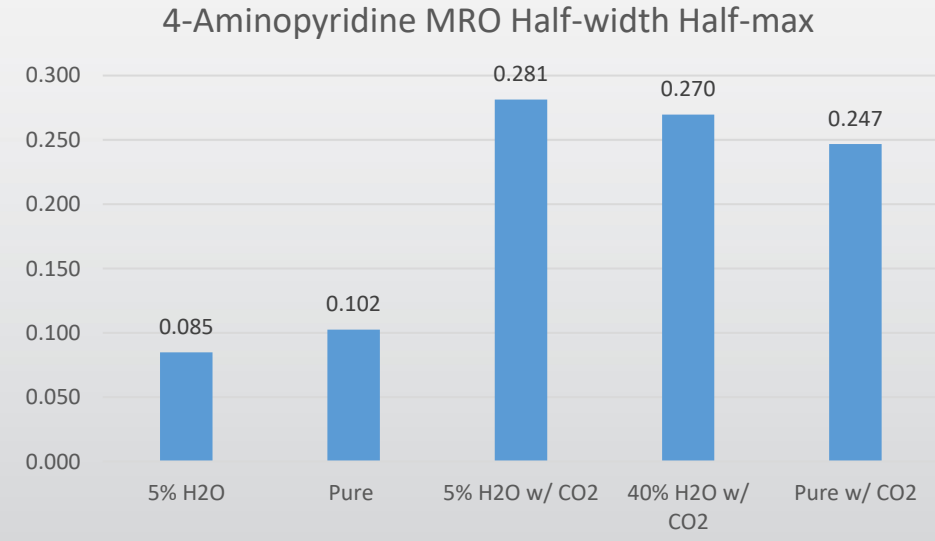
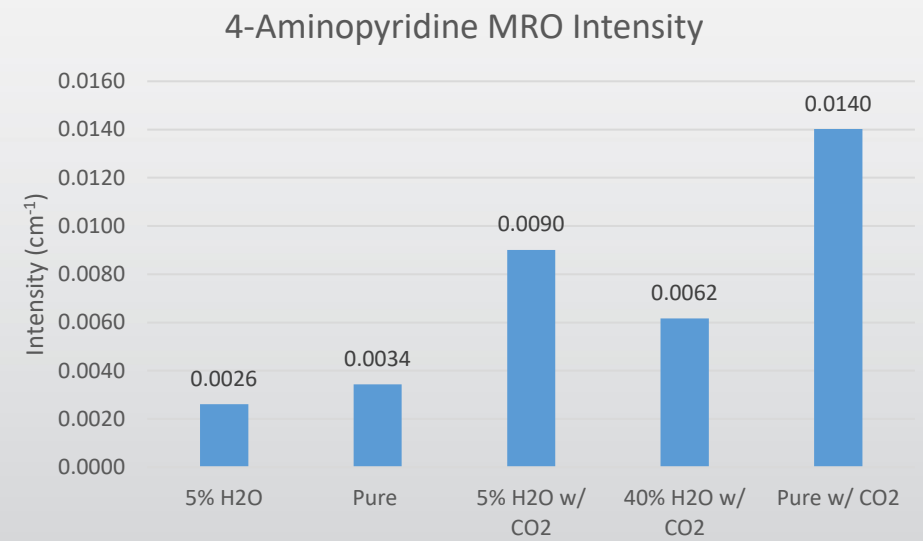
4-Aminopyridine Medium Range Order



Intensity: higher=higher concentration, lower=lower concentration
 Half-width, Half-max: lower=higher degree of order, higher=lower degree of order

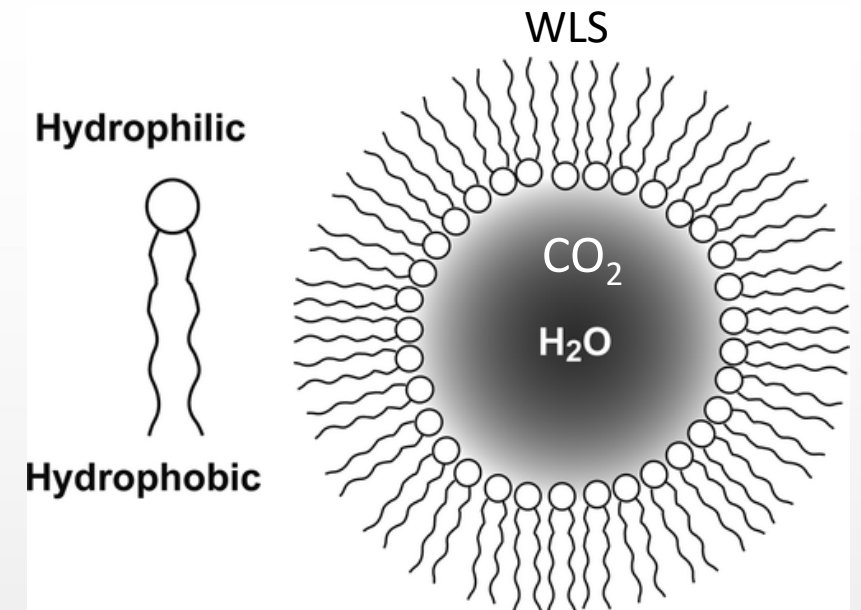


*Samples without CO₂ have a relatively high fitting error



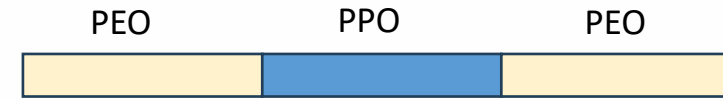
Overview of Reverse Micelles

- What is a reverse micelle?
- How is it made?
 - Made new samples of CO₂ infused 2-EEMPA and water
 - Mixed with Pluronic F-127
- In theory, all the CO₂ and H₂O should go into the core



Pluronic F-127

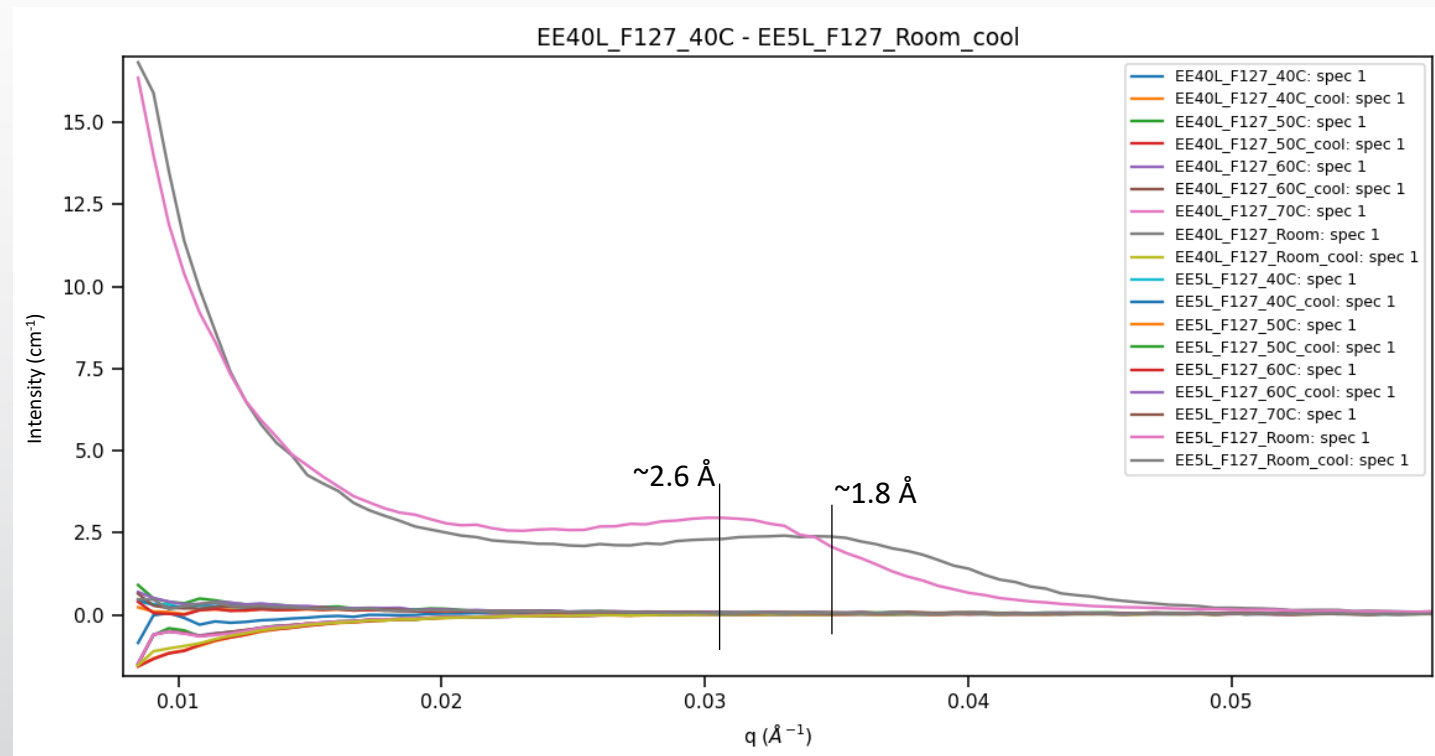
- Amphiphilic Triblock copolymer
 - PEO blocks
 - PPO block
- Took a temperature dependent SAXS scan



Hydrophilic



Hydrophobic



Conclusion

Acknowledgements

- This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Chemical Sciences, Geosciences, & Biosciences (CSGB) Division
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 - Dr. Jose L. Banuelos, Department of Physics, The University of Texas El Paso



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Thank You!

Contact: ryndecastro22@unm.edu

References

1. Climate.gov <https://www.climate.gov/news-features/understanding-climate/climate-change-atmospheric-carbon-dioxide#:~:text=Carbon%20dioxide%20is%20Earth's%20most,includin%20back%20toward%20Earth's%20surface.>
2. David J. Heldebrant, Yuan Jiang, Richard Zheng, Dushyant Barpaga, Charles Freeman, Phillip K. Koech, Deepika Malhotra, Greg Whyatt, and Andy Zwoster (2021). Performance and cost predictions of 2-EEMPA, and future opportunities for water-lean post-combustion capture solvents. *15th International Conference on Greenhouse Gas Control Technologies.*
3. Xenox.com <https://www.xenocs.com/knowledge-base/saxs/#waxs>