# Effect of Water on Physicochemical and Electrochemical Properties of Ionic Liquids Containing Aprotic Heterocyclic Anions

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## ABSTRACT

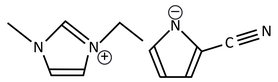

- Ionic liquids (ILs) have many properties that make than an attractive candidate for replacing organic solvents in ion-lithium batteries. ILs are highly conductive, have negligible vapor pressure and thermally stable to high temperatures. This work investigates the effect of water on the electrical conductivity of select ILs while monitoring the density and viscosity. ILs readily absorb water and will likely contain water in any practical application. For the ILs investigated, water had no impact on the conductivity up to 1 weight percent water. Additional water after 1 weight percent up to about 10 weight percent water increased the conductivity as the viscosity dropped according to the expected trend described by the Walden rule. Additional water after 10 weight percent significantly dropped performance.


## OBJECTIVES

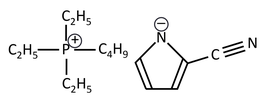
- Study effect of water on conductivity, viscosity and density of ionic liquids (ILs)
- Develop a project that connects STEM research to classroom objectives

## EXPERIMENTAL METHODOLOGY

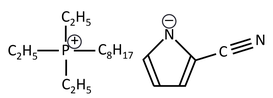
- Ionic Liquids Prepared
  - 1-ethyl-3-methylimidazolium 2-cyanopyrrolide [emim][CNpyr]



  - butyltriethylphosphonium 2-cyanopyrrolide [$P_{2224}$][CNpyr]

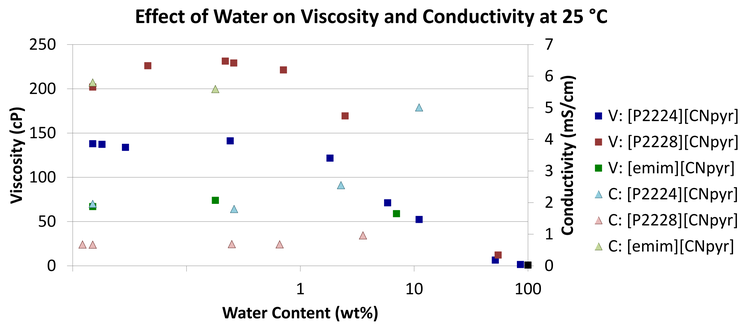


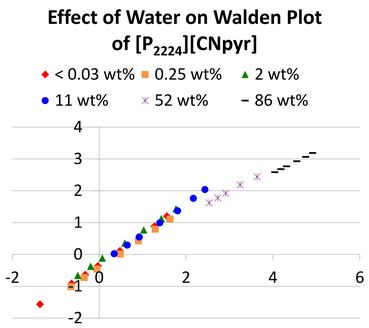
  - octyltriethylphosphonium 2-(cyano)pyrrolide [$P_{2228}$][CNpyr]

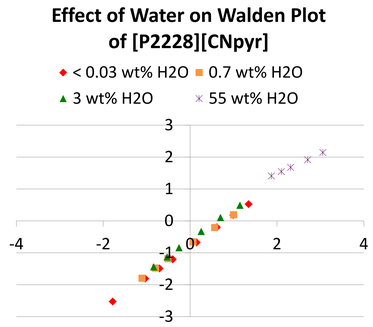


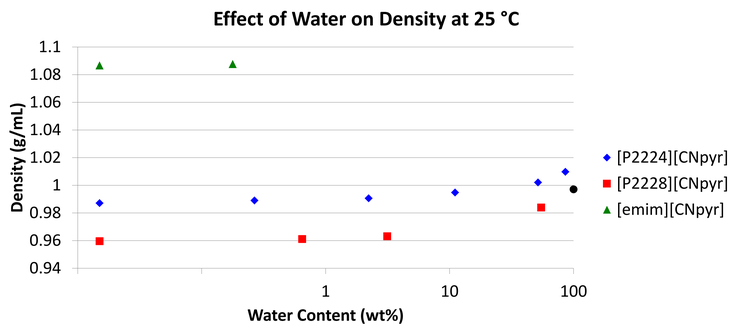
- Density Measurements: DMA 4500 Anton Paar oscillating U-tube densitometer
  - Uncertainty $10^{-3}$ g/cm$^3$
  - Temperature uncertainty ± 0.01 K
- Viscosity Measurements: Brookfield DV-III Ultra (cone and plate) rheometer
  - 50 to 1,000 cP
  - Uncertainty of ± 5%.
  - Temperature uncertainty ± 0.1 K
- Viscosity Measurement: AMVn automated microviscometer from Anton-Paar
  - Uncertainty of ± 3%
  - Temperature uncertainty of ± 0.01 K
  - 5 to 70 cP: MS 1.8 mm tube
  - 0.5 to 10 cP: MS 1.6 mm tube
- Electrical Conductivity Measurements: Solartron SI 1260 Impedance / Gain-phase analyzer connected to a Solartron 1287 electrochemical interface
  - Uncertainty of ±3%
  - Temperature uncertainty ± 0.1 K

## RESULTS




## CONCLUSIONS

- Water had little impact on the conducity and viscosity of [$P_{2224}$][CNpyr] and [emim][CNpyr] up to 1 wt% which resulted in little impact on the performance of the IL on the Walden plot.
- [$P_{2228}$][CNpyr] had an initial increase in viscosity while maintaining the same conductivity, which created a slight increase in performance on the Walden plot.
- The performance of [$P_{2224}$][CNpyr] on the Walden plot was relatively constant up to 10 wt% water, after which a decrease in performance was observed.

## STATISTICS ASSESSMENT PROJECT

***Prior Knowledge*:**

- Quantitative Single-Variable Analysis (Measures of Center: Median & Average, Measures of Spread: Interquartile Range & Standard Deviation, Z-score and Outlier Identification)
- Proper Graphing Techniques
- Regression (Correlation Value, Identifying Trends, Principle of Least Squares, and Deviation Plot)
- Using software (MS Excel) to perform the above statistical analysis techniques

***Project*:**

Each student is assigned a different chemical compound so that each student will be doing the same analysis on individualized numbers. For that compound the student is given 5 density and dynamic viscosity measurements made of that specific compound over 5 different temperatures (20, 25, 30, 40, 50 °C).

1st Project Deadline:

- Identify any outliers in their data set.
- Report the average density and viscosity at each temperature after outliers have been removed.

2nd Project Deadline:

- Graph the density and viscosity averages separately, each as a function of temperature.
- Perform linear regression on the density data.
- Fit an exponential and quadratic function to the viscosity data.

3rd Project Deadline:

- Determine which fit is better for the viscosity data.
- Using the regressions models, determine the kinematic viscosity at a random temperature which is calculated by dividing the dynamic viscosity by the density.

## ACKNOWLEDGEMENTS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## REFERENCES


1. C. Shi, M. Quiroz-Guzman, A. DeSilva, and J. F. Brennecke, *J. Electrochem. Soc.*, 2013, **160** (9), A1604-A1610
2. C. Shi, 2013, Doctoral Dissertation, University of Notre Dame