

## PROGRESS REPORT (Quarterly)

### 1. DOE Award Number and Name of Recipient

Award number: DE-NT0005287  
Name of recipients: Georgia Tech Research Corporation

### 2. Project Title and Name of Project Director/PI

Title: Reversible Ionic Liquids as Double-Action Solvents for Efficient CO<sub>2</sub> Capture  
PI: Dr Charles. A. Eckert  
Co-PI: Dr. Charles L. Liotta

### 3. Date of Report and Period Covered

Date of report: July 31, 2009  
Period covered: April 1, 2009 – June 30, 2009 (Q3)

### 4. Executive Summary

The objective of this project is to develop reversible ionic liquids as solvents for post-combustion recovery of CO<sub>2</sub> from fossil fuel-fired power plants. These novel solvents are neutral molecules which react with CO<sub>2</sub> to form an ionic liquid, which then dissolves additional CO<sub>2</sub> by a physisorption mechanism. Subsequently modest elevations in temperature reverse the reaction and yield pure CO<sub>2</sub> for disposal. Because of this dual mode, capacity can be large, and we are modifying the precursor structure using structure-property relationships to optimize both physical properties and thermodynamic properties. By incorporating silanes in the molecules we reduce viscosity substantially to augment mass transfer.

We are creating, testing, and optimizing reversible ionic liquids for applications in CO<sub>2</sub> capture, and we shall do the process design and cost analysis for their implementation. In addition we shall develop a process for commodity-scale production of our solvents.

We continue to make substantial progress through the second quarter of this project, meeting or exceeding projected achievements. Our major contributions for the third quarter include:

- We have measured and reported the CO<sub>2</sub> absorption capacities in the ionic liquid form of the following molecular liquids: (3-aminopropyl)trimethoxysilane, (3-aminopropyl)triethoxysilane, (3-aminopropyl)triethylsilane, and (3-aminopropyl)tripropylsilane. The measurement technique utilized attenuated total reflectance (ATR) Fourier transform infrared (FT-IR) spectroscopy and our Generation 3 custom made high pressure reaction vessel at a temperature of 35°C and a pressure of 900 psi.
- Stability tests of (3-aminopropyl)triethylsilane and (3-aminopropyl)triethoxysilane were concluded after a two month period. The results indicate severe degradation of the (3-aminopropyl)triethoxysilane in wet and oxygen-rich environments while the (3-

aminopropyl)triethylsilane showed no degradation, via  $^1\text{H}$  NMR, under any of the conditions studied.

- The viscosities of both the molecular and ionic forms, and densities for ionic form only, have been measured and reported for: (3-aminopropyl)trimethoxysilane, (3-aminopropyl)triethoxysilane, (3-aminopropyl)triethylsilane, and (3-aminopropyl)tripropylsilane.
- We were able to identify several more target molecules to be synthesized and characterized in our laboratory. Based on the data we collected during the first 3 Quarters of the project, we believe these compounds have enhanced properties for  $\text{CO}_2$  capture or their study will provide valuable information that will lead to the development of better candidates.

Our goal remains to minimize the cost and energy requirements of  $\text{CO}_2$  capture to help DOE meet its goal – 90%  $\text{CO}_2$  capture with no more than a 35% increase in cost by 2020.

## 5. Results of Work

### a. Approach

#### 1- Synthesis and Characterization of Custom Reversible ILs

We proposed to investigate the use of a variety of amine and guanidine based materials for the capture and subsequent controlled release of  $\text{CO}_2$ . We have currently synthesized and characterized four candidates: (3-aminopropyl)trimethoxysilane, (3-aminopropyl)triethoxysilane, (3-aminopropyl)triethylsilane, and (3-aminopropyl)tripropylsilane, as previously reported. We have identified three more candidates to be synthesized and characterized in our laboratory (Figure 1): (3-aminopropyl)ethyldimethylsilane, (3-aminopropyl)trihexylsilane, and (3-aminopropyl)diisopropyl(undecafluoropentyl)silane.

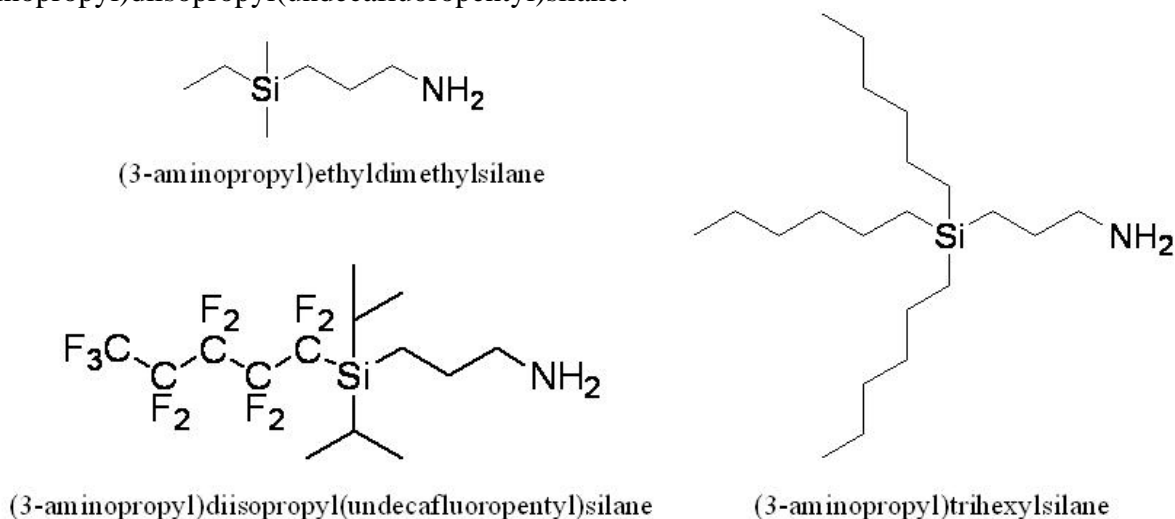


Figure 1. Recently identified candidates for novel  $\text{CO}_2$  capture agents.

*The candidates in Figure 1 were chosen to increase CO<sub>2</sub> capacity of the solvents and, in the case of (3-aminopropyl)diisopropyl(undecafluoropentyl)silane, to show the electronic effect of a fluorinated side chain on the capture and release of CO<sub>2</sub>.* The results from the ATR FT-IR measurements (to be discussed in more detail later in this report) indicate that swelling of the ionic liquids and subsequently the amount of CO<sub>2</sub> absorbed increases as the side chains attached to the Si- group become bulkier. We believe this is due to a decrease in packing efficiency of the ions which will likely be further decreased due to the asymmetry of (3-aminopropyl)ethyldimethylsilane and increased bulkiness of (3-aminopropyl)trihexylsilane. And in an attempt to understand how strong of an influence the side chains on the Si- group have on the thermodynamics of CO<sub>2</sub> capture and release we will examine (3-aminopropyl)diisopropyl(undecafluoropentyl)silane.

As synthesized, each of these candidates will be tested for CO<sub>2</sub> capture as illustrated by the general reaction scheme in Figure 2. The resulting reversible ionic liquids will be fully characterized (NMR, elemental analysis, FT-IR, mass spectroscopy (MS), and solvatochromic polarity measurements). The solvatochromic polarity measurements will be performed using an HP 8453 UV-Vis Spectrophotometer and the polarity probe Nile Red. The wavelength of maximum absorption ( $\lambda_{max}$ ) for the probe in a given solvent is relative to the polarity of the solvent. The  $\lambda_{max}$  of Nile Red has been found and reported for hundreds of solvents, making this an efficient approach for determination of solvent polarity.

The loss of CO<sub>2</sub> upon heating will be explored using NMR and differential scanning calorimetry (DSC). The DSC experiments are performed on a Q20 TA Instruments machine, with a temperature profile of 20°C/min or 30°C/min ramp rates from 20°C initial temperature to 300°C or 400°C final temperature. The first endotherm was taken to represent the loss of CO<sub>2</sub> with the second endotherm representing the evaporation of the molecular liquid.

Although the stability tests confirmed that the trialkyl substituted precursors were stable over a period of two months in both wet and oxygen containing environments, we will still perform the experiment on the precursors that show promising thermodynamic properties or absorption capacities to ensure industrial viability of our candidates produced.

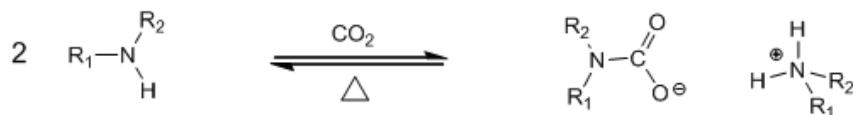


Figure 2. Reaction of custom-made amine with CO<sub>2</sub> to form reversible ionic liquids.

Additionally, we will look to capture <sup>13</sup>C labeled CO<sub>2</sub> to differentiate and quantify the chemisorbed (single or multiple reactions) and physisorbed CO<sub>2</sub> present in the reversible ionic liquid. We anticipate capacities to exceed the 1:2 CO<sub>2</sub> to solvent ratio achieved by single reaction stoichiometry. Quantitative <sup>13</sup>C NMR will be used to perform the analysis and the results will be compared with FT-IR data. Candidates that exhibit favorable properties for use as CO<sub>2</sub> capture agents (such as usable liquid range, stability, capability to release CO<sub>2</sub>, etc.) will then be tested for determination of thermodynamic properties, viscosity, and capacity.

## 2- Thermodynamics of CO<sub>2</sub> Capture

We proposed to exploit our knowledge of molecular design to understand and optimize the chemistry – for example using linear free energy relationships to account for electron donation or withdrawal and related effects (such as neighboring group effects) to increase capacity and modify the thermodynamics. Once promising candidates are identified after undergoing the characterization experiments (as describing in the previous section) we will then start to look at their thermodynamic properties and CO<sub>2</sub> capture capacities. The equilibrium constant  $K$  representative of the capture (and release) of CO<sub>2</sub> can be found by measuring the conversion of the precursor molecule to ionic liquid at a given temperature and CO<sub>2</sub> concentration, and compensation for the non-ideal behavior of the ionic species.

We are using attenuated total reflectance (ATR) Fourier-transform infrared (FT-IR) spectroscopy to determine the conversion under a broad range of conditions. ***This measurement technique allows for the simultaneous measurement of conversion and CO<sub>2</sub> capacity.*** The ATR FT-IR optics bench used for data collection will be the Heated Golden Gate ATR sample accessory supplied by Specac, with a working temperature range up to 300°C and pressure rating for the tungsten carbide embedded diamond being 15,000psi.

Equilibrium measurements are currently being performed by using a custom designed and built ATR FT-IR high pressure reactor. Consultation for the design was offered by Dr. Sergei Kazarian of Imperial College London. ***We are now using the Generation 3 stainless steel reactor, which has been successfully tested at temperatures to 150°C and pressures to 1500psi.***

We are currently studying the reaction of the custom-made (3-aminopropyl)triethylsilane and CO<sub>2</sub> with simultaneous <sup>1</sup>H, <sup>13</sup>C NMR and IR spectra being collected on the same sample. The <sup>1</sup>H, <sup>13</sup>C NMR used is a Bruker AMX 400 located in the School of Chemistry and Biochemistry at Georgia Tech. The purpose of collecting simultaneous spectra on both the NMR and IR will be to correct for changes in molar absorptivity of our samples as they are converted from the molecular liquid form to the ionic liquid form. We will first analyze five different conversions for the same sample to verify that the carbonyl peak intensity is linearly proportional to the conversion determined by <sup>1</sup>H NMR. From this point, we will only need to collect one (1) simultaneous NMR/IR spectra for each unique molecular liquid examined. Previous experiments performed on the reversible ionic liquid N-butyl-N,N,N,N-tetramethylguanidinium methylcarbonate indicated that linearity between conversion and carbonyl intensity holds true.

In addition, we can gather information on the approximate amount of CO<sub>2</sub> that is physically absorbed into the ionic liquids using the FT-IR data that is collected for the equilibrium measurements. The CO<sub>2</sub> that is in solution and not chemically bound to the amine (referred to as “free CO<sub>2</sub>”) has a very distinct absorption band in the mid-infrared region (the  $\nu_3$  band of CO<sub>2</sub> at *ca.* 2335 cm<sup>-1</sup>). Following the Beer-Lambert Law, the absorbance of this band is directly proportional to the concentration of this “free CO<sub>2</sub>” absorbed in solution. A calibration curve relating the absorbance of CO<sub>2</sub> and the concentration was obtained for a methanol/CO<sub>2</sub> system using VLE data found in literature to calculate the concentration of CO<sub>2</sub> at various

temperatures and pressures. For the analysis, density of the ionic liquid is required. This information will be measured using a 2.0 mL pycnometer.

Experimentation has been started for the following custom-made candidates: (3-aminopropyl)triethylsilane and (3-aminopropyl)tripropylsilane using pure CO<sub>2</sub> feed streams. As we determine the equilibrium constants at multiple temperatures, we will be able to determine the heat of reaction for the specific molecular structures. The molecular structures will be systematically altered to allow for the use of structure-property relationships where we can determine the optimal molecular configuration to give us desired capacities and enthalpies for reversing our solvents and expelling the CO<sub>2</sub>. For example, the compound (3-aminopropyl)diisopropyl(undecafluoropentyl)silane will allow for us to determine the effect of fluorinated side chains on the enthalpic properties of the CO<sub>2</sub> capture candidates. The custom reversible ionic liquids that show promising pure CO<sub>2</sub> capacities and reaction enthalpies will be investigated with altered feed streams to examine the effects of mixed N<sub>2</sub>/CO<sub>2</sub> streams, water, SO<sub>x</sub>, NO<sub>x</sub>, and carryover from the scrubbers. This will give us insight into how the solvents behave under “real world” operating conditions. We can then further modify the structures to overcome any problems that arise.

For the evaluation of the equilibrium constants, we are looking at examining the non-ideal behaviors (activity and fugacity coefficients) of our one component ionic liquids. We have started looking at an equation-of-state (EOS) model to account for the non-ideal behavior of the ionic species in the solution, namely the SAFT model. ***Preparation of a modified SAFT model has been initiated, and as data is collected and analyzed from the FT-IR we will start to incorporate the experimental data into the model for evaluation.*** This information will be useful to develop accurate expression for the equilibrium constants and offer insight into how specific molecular structures can advantageously deviate from ideality for the purpose of CO<sub>2</sub> capture and, more importantly, release.

### **3- Viscosity Studies as a function of CO<sub>2</sub> capture**

The change in viscosity as a function of CO<sub>2</sub> capture will be investigated. As will be discussed later in this report, viscosity measurements have been conducted for the four candidates that have been successfully synthesized and characterized ((3-aminopropyl)trimethoxysilane (3-aminopropyl)triethoxysilane, (3-aminopropyl)triethylsilane, and (3-aminopropyl)tripropylsilane). The rheological results indicate that there is a three order of magnitude change in viscosity as they are completely converted from the molecular liquid to the ionic form. Laboratory observations indicate that the change in viscosity is non-linear, with viscosity increasing sharply at high conversions. The viscosity as a function of conversion for each candidate is being measured using a MCR300 controlled stress rheometer supplied by Anton Paar, located in the Complex Fluids Group Laboratory at Georgia Tech. ***We are currently examining the effect of conversion to ionic form on the viscosity of (3-aminopropyl)tripropylsilane.***

## 4- Scrubber Process Design

With the direct involvement of an undergraduate research assistant, an ASPEN simulation to treat a *model coal-fired power plant flue gas stream has been developed and validation with existing literature data is underway*. Initially, the model will be used to evaluate targets for our CO<sub>2</sub> capture agents to meet the goal of 90% CO<sub>2</sub> capture with no more than a 35% increase in cost. We are using the monoethanolamine (MEA) process as a basis for comparison, and are altering the operating conditions to give us targets for the development of one component reversible ionic liquids. The parameters we look to optimize are the enthalpy of capture and release, the capture and release temperatures, CO<sub>2</sub> capacities of the solvent, and viscosity of the solvent. The data acquired in the laboratory for the custom-made reversible ionic liquids will be put into the model and evaluated as it is collected, giving us real-time analysis of the economic viability and performance of our solvents. This information will be used to direct the modifications to molecular structure in order for us to meet the goals set forth by DOE and our previous models.

Additional design issues that we plan to consider in the future are the effects of the presence of SO<sub>2</sub>, NO<sub>2</sub>, and carryover gypsum particles from the scrubber in the gas. We do know that our reversible ionic liquids will also absorb SO<sub>2</sub>, but the thermodynamics and kinetics have not yet been investigated. We suspect that the NO<sub>2</sub> will not affect the process as proposed, but need to verify this. The surface of gypsum particles is ionic, so these will probably adsorb small amounts of the ionic liquid, but it is likely that this is reversible with temperature. All these issues will be considered and verified by experiment as we move forward.

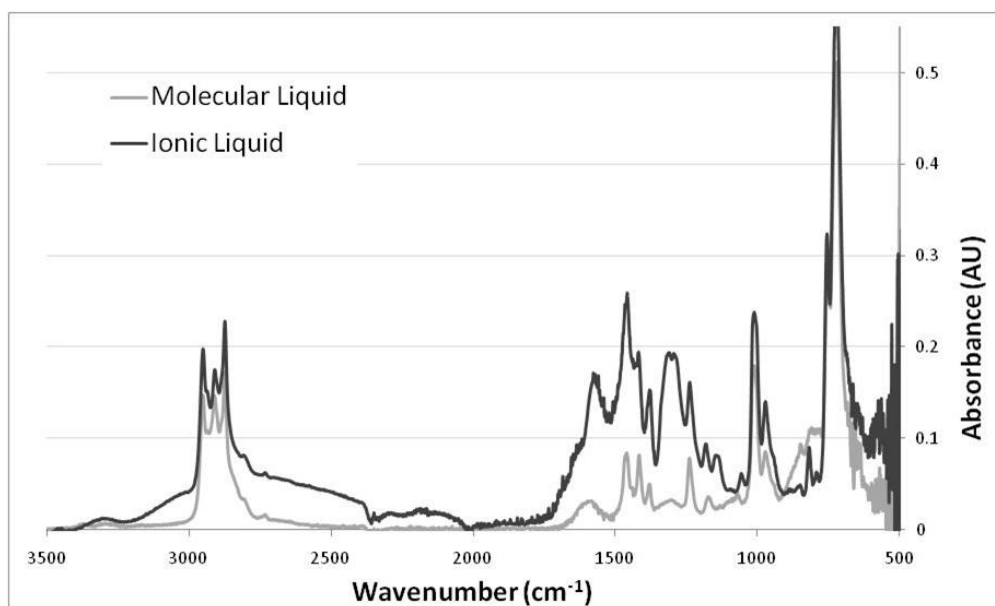
### b. Results and Discussion

#### 1- Synthesis and Characterization of Custom Reversible ILs

The complete characterization of the (3-aminopropyl)trimethoxysilane, (3-aminopropyl)triethoxysilane, (3-aminopropyl)triethylsilane, and (3-aminopropyl)tripropylsilane) and the corresponding ionic liquids was finalized by using solvatochromic polarity measurements, FT-IR, DSC. The DSC experiments indicate that the loss of CO<sub>2</sub> occurs at a temperature significantly different (>100°C) than the loss of the solvent due to evaporation. ***Additionally, the results indicate there is variation in the reversal temperature with respect to the molecular structure of the solvents.*** As more suitable candidates are synthesized and characterized, we can use structure-property relationships to determine the effect of structure on reversal temperature and design optimal compounds for CO<sub>2</sub> capture and release.

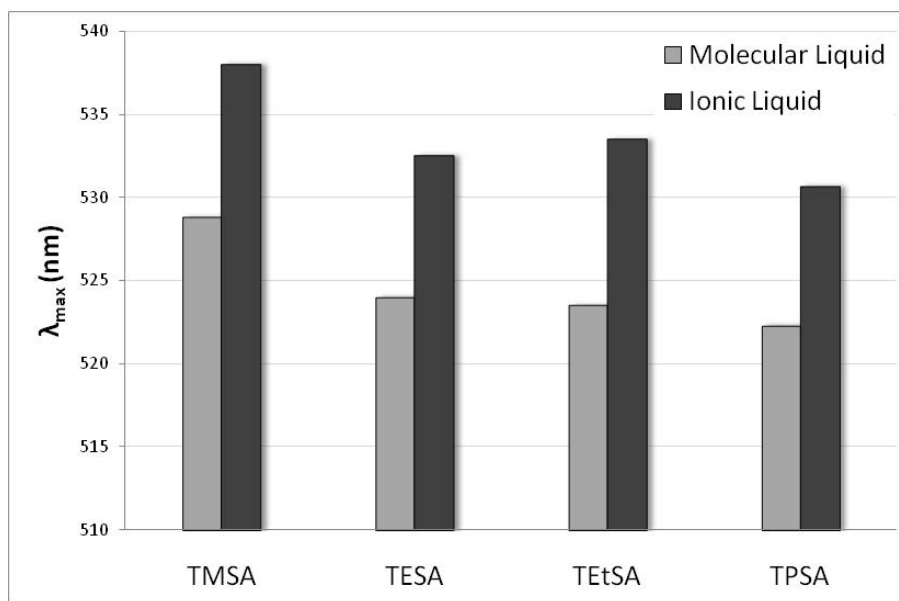
Figure 3 shows the ATR FT-IR spectra of both the molecular liquid and ionic liquid forms of (3-aminopropyl)triethylsilane. The spectral results show the appearance of carbonyl peaks due to the formation of the ionic liquid product. However, carbonyl peaks (located *ca.* 1500 cm<sup>-1</sup>) are generally very sharp and strong signals. When sharp peaks are broadened and split as they appear to be in Figure 3, it suggests there are multiple species present in the ionic liquid. Therefore, we hypothesize that there are multiple CO<sub>2</sub> molecules bound per amine pair. The result would be an increase in capacity from reaction beyond the expected CO<sub>2</sub>:amine of 1:2,

based on well known reaction stoichiometry. To confirm the hypothesis, we will examine the  $^{13}\text{C}$  NMR of the ionic liquids formed from  $^{13}\text{CO}_2$  as well as the  $^{15}\text{N}$  NMR of the ionic liquids.



**Figure 3.** The ATR FT-IR spectra of the molecular liquid and ionic liquid forms of (3-aminopropyl)triethylsilane showing evidence of multiple carbonyl species present.

The solvatochromic experiments were performed using the polarity indicator dye Nile Red (Figure 4). The graph shows that there is a significant change in polarity upon conversion from molecular liquid to ionic liquid. The  $\lambda_{\text{max}}$  value will be used as a parameter in the structure-property relationship study.



**Figure 4.** The polarity of the neutral and ionic forms of the one-component reversible ionic liquid solvents. TMSA = (3-aminopropyl)trimethoxysilane; TESA = (3-aminopropyl) triethoxysilane; TEtSA = (3-aminopropyl)triethylsilane; TPSA = (3-aminopropyl)tripropylsilane.

The stability tests of (3-aminopropyl)triethylsilane and (3-aminopropyl)triethoxysilane concluded after a two month period. The  $^1\text{H}$  NMR results showed that the (3-aminopropyl) triethoxysilane showed signs of decomposition in even in the completely dry argon environment, with the decomposition rate being considerably accelerated under the wet and oxygen-rich environment. *No degradation over the two months was observed for any of the (3-aminopropyl)triethylsilane samples, showing exceptional resistance to degradation in especially wet environments.*

Additionally, we are continuing to make progress towards the synthesis of 1-component silyl guanidine-based reversible ionic liquids. Several candidates have been identified but the preliminary synthetic experiments have shown that the reaction is extremely sensitive to the presence of water. We are modifying the synthetic techniques to accommodate.

## 2- Thermodynamics of CO<sub>2</sub> Capture

The Generation 3 high pressure stainless steel reactor for the ATR FT-IR measurements has been received, and successfully tested at 150°C and 1500psi. We have successfully measured the density and CO<sub>2</sub> capacity at 900 psi and 35°C for ionic forms of (3-aminopropyl)trimethoxysilane, (3-aminopropyl)triethoxysilane, (3-aminopropyl)triethylsilane, and (3-aminopropyl) tripropylsilane. The density was required for the calculation of swelling, and the swelling was needed to calculate the CO<sub>2</sub> capacity. The results (Figure 5) indicate that the swelling and subsequent CO<sub>2</sub> capacity increase as the side chains on the Si- group become longer. These findings lead to the identification of the bulky next generation CO<sub>2</sub> capture agents to be synthesized and characterized (Figure 1). The stoichiometric ratio of CO<sub>2</sub>:amine of 1:2 was used to calculate the CO<sub>2</sub> reaction capacity. It should be noted that if we can confirm the hypothesis that we are exceeding this ratio, the result could lead to a drastic increase in the CO<sub>2</sub> capacity.

Ionic Liquid	Density (g/cm <sup>3</sup> )	Swelling (%)	CO <sub>2</sub> Absorption Capacity (mol CO <sub>2</sub> /kg amine)	CO <sub>2</sub> Reaction Capacity (mol CO <sub>2</sub> /kg amine)	Total CO <sub>2</sub> Capacity (mol CO <sub>2</sub> /kg amine)
TMSA	1.151	17%	10.9	2.79	13.69
TESA	1.060	23%	12.5	2.26	14.76
TEtSA	0.945	16%	12.3	2.88	15.15
TPSA	0.907	31%	17.9	2.32	20.2

**Figure 5.** Density, swelling, physical and chemical capacity, and the total capacity for the four reversible ionic liquids tested. TMSA = (3-aminopropyl) trimethoxysilane; TESA = (3-aminopropyl) triethoxysilane; TEtSA = (3-aminopropyl) triethylsilane; TPSA = (3-aminopropyl) tripropylsilane.



*Experiments are currently underway for the low pressure reaction of CO<sub>2</sub> with (3-aminopropyl)triethylsilane and (3-aminopropyl) tripropylsilane.* At lower pressures, there is less ionic species present which results in a smaller deviation from ideality. This, in turn, makes the thermodynamic analysis simpler and more accurate. The non-ideality still can't be considered negligible, so we are developing a modified SAFT EOS model to deal for the non-idealities of the ionic species. As data is collected and analysis, it will be incorporated into the model.

### 3- Viscosity Studies

The viscosity was measured for both the ionic and molecular forms of (3-aminopropyl)trimethoxysilane, (3-aminopropyl) triethoxysilane, (3-aminopropyl)triethylsilane, and (3-aminopropyl)tripropylsilane at 25°C (Figure 6).<sup>a</sup> The results indicate that there is a significant increase in the viscosity as the molecular liquids are converted to ionic liquids. And although there seems to be a correlation between the viscosity and the nature of the side chains attached to the Si- group, a three order of magnitude change is observed for all compounds. Laboratory observations have indicated that the viscosity change is minor until high conversions. Thus, we are currently measuring the viscosity as a function of conversion.

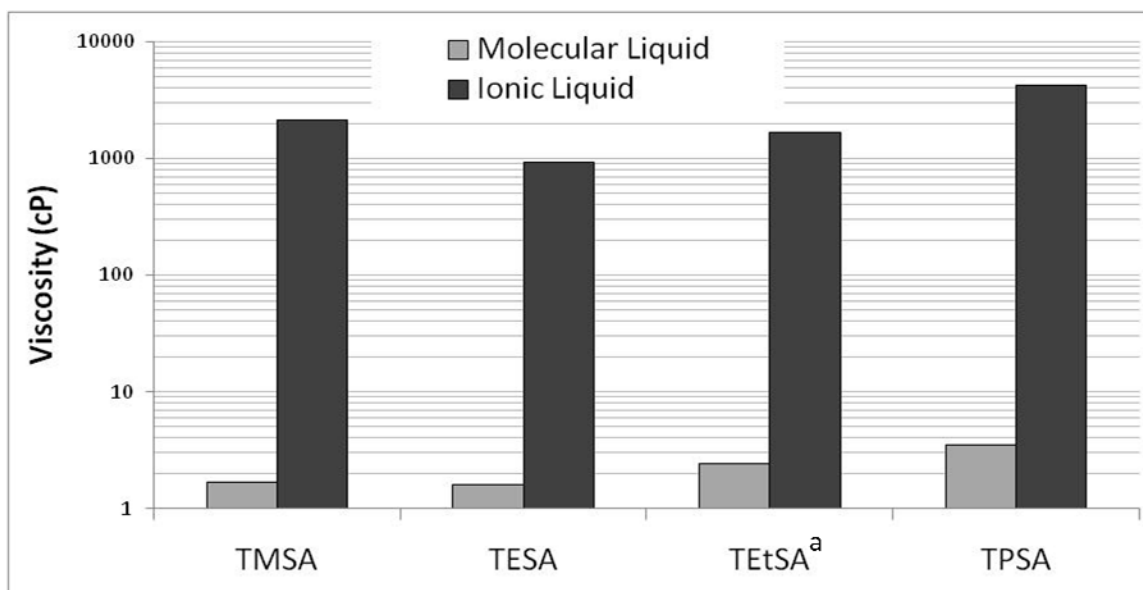


Figure 6. Viscosity of both molecular liquids and ionic liquids. TMSA = (3-aminopropyl) trimethoxysilane; TESA = (3-aminopropyl) triethoxysilane; TEtSA = (3-aminopropyl) triethylsilane; TPSA = (3-aminopropyl)tripropylsilane.

<sup>a</sup> The viscosity of the ionic form of (3-aminopropyl)triethylsilane was measured at 35°C due to difficulty of obtaining an accurate measurement at lower temperatures.

### c. Conclusion

We continue to make substantial progress towards helping the DOE achieve the goal of 90% CO<sub>2</sub> capture with no more than a 35% increase in cost by 2020. The recent advancements in the project have resulted in a submittal for publication in the journal *Fuel*.

Significant accomplishments were made during the 3<sup>rd</sup> Quarter of the project by successfully synthesizing and completely characterizing silyl amine-based reversible ionic liquids. We're ahead of schedule on the thermodynamic analysis, and have used the measurement technique to simultaneously investigate conversion of the molecular liquids and absorption capacity in the ionic liquids for four CO<sub>2</sub> capture solvent candidates. Viscosity measurements are being completed; combined with the characterization data, we are getting the information required for the structure-property relationship analysis. And importantly, the information being collected is giving insight into compounds with enhanced properties for the application to CO<sub>2</sub> capture from fossil fuel-fired power plants.

### 6. Cost Status

This information is being provided independently by the Grants and Contracts department of Georgia Tech Research Corporation.

### 7. Milestone Status

The three milestones listed in the Project Management Plan for Year One are as follows:

ID	Milestone Description	Planned Completion	Verification Method
A	Complete Project Management Plan	10/01/08	PMP approved by DOE COR
B	Complete laboratory synthesis and characterization of one new single-component silyl amine-based reversible ionic liquid.	6/30/09	laboratory synthesis and characterization of single-component silyl amine-based reversible ionic liquid.
C	Complete laboratory synthesis and characterization of one new single-component silyl guanidine-based reversible ionic liquid.	9/30/09	Progress Report describing laboratory synthesis and characterization of one new single-component silyl guanidine-based reversible ionic liquid

At this time, Milestone A has been completed on schedule with the approval of the Project Management Plan.

Also, Milestone B has been completed ahead of schedule, with the complete laboratory synthesis and characterization of four new single-component silyl amine-based reversible ionic liquids.

We fully anticipate that Milestone C will also be completed during Year One.

## 8. Summary of Significant Accomplishments

The significant accomplishments are:

- Prepare, isolate, purify and *fully characterize* four total amine-based reversible ionic liquids for CO<sub>2</sub> capture
- Commence ATR FT-IR studies on the four candidates to get information for thermodynamics and directly measure the absorption capacities
- Successfully measure viscosities for molecular and ionic forms of all four candidates
- Identify promising target molecules for future synthesis and characterization based on evidence collected during the first 3 Quarters of the project
- Completed stability tests that showed our custom-made compounds had superior degradation resistance than the commercially available compounds
- Recent advancements have resulted in a submittal for publication in a scientific journal

## 9. Actual or anticipated problems or delays, and actions taken

We have not had any problems or delays, and because we are able to stay ahead of schedule, we do not anticipate any problems or delay.

## 10. Products produced

### a. Publications

Papers published:

Vittoria Blasucci, Cerag Dilek, Hillary Huttenhower, Ejae John, Veronica Llopis-Mestre, Pamela Pollet, Charles A. Eckert, and Charles L. Liotta, "One Component, Switchable, Neutral to Ionic Liquid Solvents Derived from Siloxylated Amines," *Chem Comm*, 116-119, 2009.

Vittoria Blasucci, Ryan Hart, Veronica Llopis-Mestre, D. Julia Hahne, Melissa Burlager, Hillary Huttenhower, Reginald Thio, Charles L. Liotta, and Charles A. Eckert, "Single Component, Reversible Ionic Liquids for Energy Applications," *Fuel*, submitted (June 2009).

Papers presented:

Charles A. Eckert and Charles L. Liotta, "Reversible Ionic Liquids as Double-Action Solvents for CO<sub>2</sub> Capture," Annual NETL CO<sub>2</sub> Capture Technology for Existing Plants R&D Meeting, Pittsburgh, PA, March 24, 2009.

Vittoria Blasucci, Cerag Dilek, Hillary Huttenhower, Ejae John, Veronica Llopis-Mestre, Pamela Pollet, Charles L. Liotta, and Charles A. Eckert "One-Component, Switchable, Neutral to Ionic Liquid Solvents Derived from Siloxylated Amines," 237<sup>th</sup> National Meeting, ACS, Salt Lake City, UT, March, 2009.

Vittoria Blasucci, Ryan Hart, Cerag Dilek, Hillary Huttenhower, Veronica Llopis-Mestre, Pamela Pollet, Eduardo Vyhmeister, Charles L. Liotta, and Charles A. Eckert, "Reversible Ionic Liquids as Double-Action Solvents for Efficient CO<sub>2</sub> Capture," AIChE Spring National Meeting, Tampa, FL, April 2009

Philip G. Jessop, Michael Cunningham, Charles A. Eckert, and Charles L. Liotta "CO<sub>2</sub> as a Trigger for Switchable Chemistry, International Conference on Carbon Dioxide Utilization, China, May 2009.

Ali Fadhel, Vittoria Blasucci, Cerag Dilek, Ryan Hart, Hillary Huttenhower, Veronica Llopis-Mestre, Pamela Pollet, Eduardo Vyhmeister, Charles A. Eckert, and Charles L. Liotta "Designer Reversible Ionic Liquids for CO<sub>2</sub> Capture," 13<sup>th</sup> Annual Green Chemistry & Engineering Conference, Washington, DC, June 2009.

Papers to be presented:

Ryan Hart, Vittoria Blasucci, Charles A. Eckert, and Charles L. Liotta, "Development of One-Component Reversible Ionic Liquids for Energy Applications," 2009 Annual AIChE Meeting, Poster, Nashville, TN, November 2009.

Invited paper:

Charles A. Eckert, Ryan Hart, Vittoria Blasucci, and Charles L. Liotta, "'Smart' Solvents for Extractions and Purifications", 2009 Annual AIChE Meeting, "New Developments in Extractive Separations," Nashville, TN, November 2009.

#### **b. Websites**

Webpages have been prepared and posted within the Eckert/Liotta group website (<http://www.chbe.gatech.edu/eckert/projects.html>).

#### **c. Networks or collaboration fostered**

The DOE grant has fostered an intracampus collaboration between the Eckert-Liotta Joint Research Group and the Breedveld Complex Fluids Group. Dr. Victor Breedveld is very talented regarding the flow behaviors of complex fluids, and has the equipment necessary for the evaluation of the viscosity change as a function of conversion for our reversible ionic liquid systems. Following his recommendations and direction, we have been able to properly select, validate, and test a method using his rheometer to obtain information that is quite valuable for the design of a CO<sub>2</sub> capture facility utilizing liquid sorbents for capture.

#### **d. Technologies/Techniques**

We designed and developed custom stainless steel reactors that will fulfill our experimental needs: it will hold high pressure (up to 2,000 psi), high temperature (up to 300°C) with a volume of about 5 ml and adapt easily onto the heated golden gate ATR cell. This set-up is user-friendly: as it allows for fast and accurate measurements, easy set-up and easy cleaning between runs (limiting potential cross-contamination).

#### **e. Inventions/Patents**

Patent filing for the one-component reversible ionic liquids is in process.