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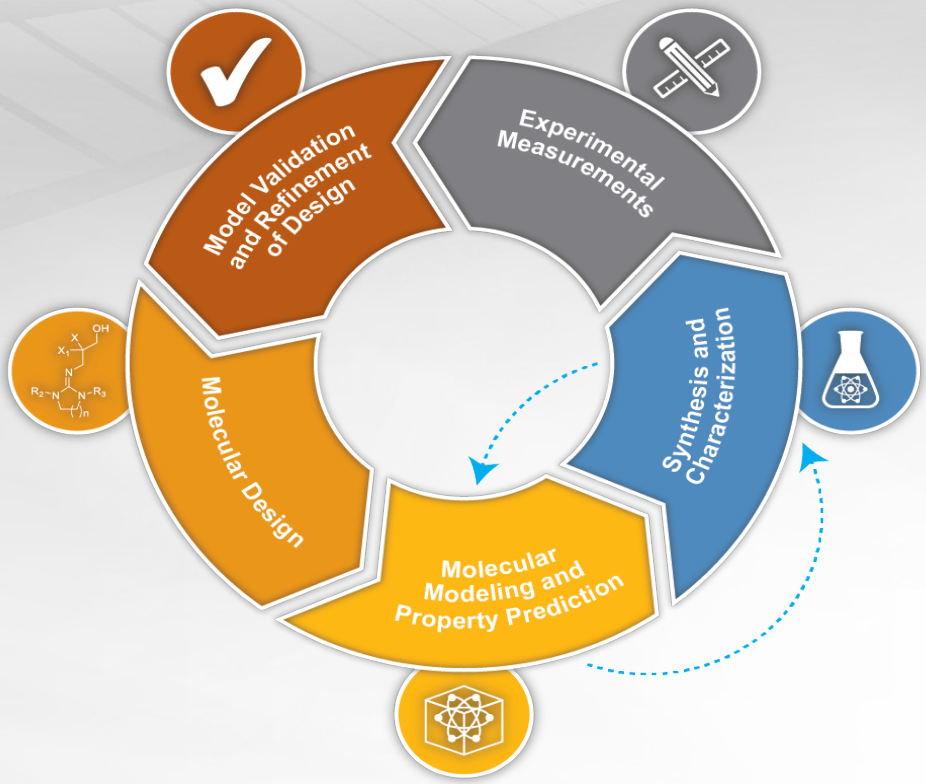

Accelerating the development of transformational solvent systems for CO_2 separations

DAVID J. HELDEBRANT
NETL, MORGANTOWN, WV
JUNE 20, 2017

U.S. DEPARTMENT OF ENERGY | NATIONAL ENERGY TECHNOLOGY LABORATORY

Objectives of This Talk

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Update DOE-FE/ NETL & FE on Solvent Development Program

- Solvent development approach for primary properties
- Results from testing of new aqueous amines (Fluor)
- Review development work/progress
  - CO_2BOLs
  - Aminopyridines
  - 3rd generation amines (Company previously known as GE)
- Remaining FY17 scope & recommendations for FY18 scope
  - DOCCSS spinoff
  - Need and approaches for 2˚ and 3˚ properties

Integrating Molecular Design, Synthesis & Testing For Multiple Platforms

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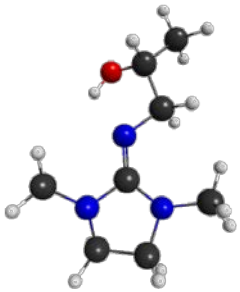
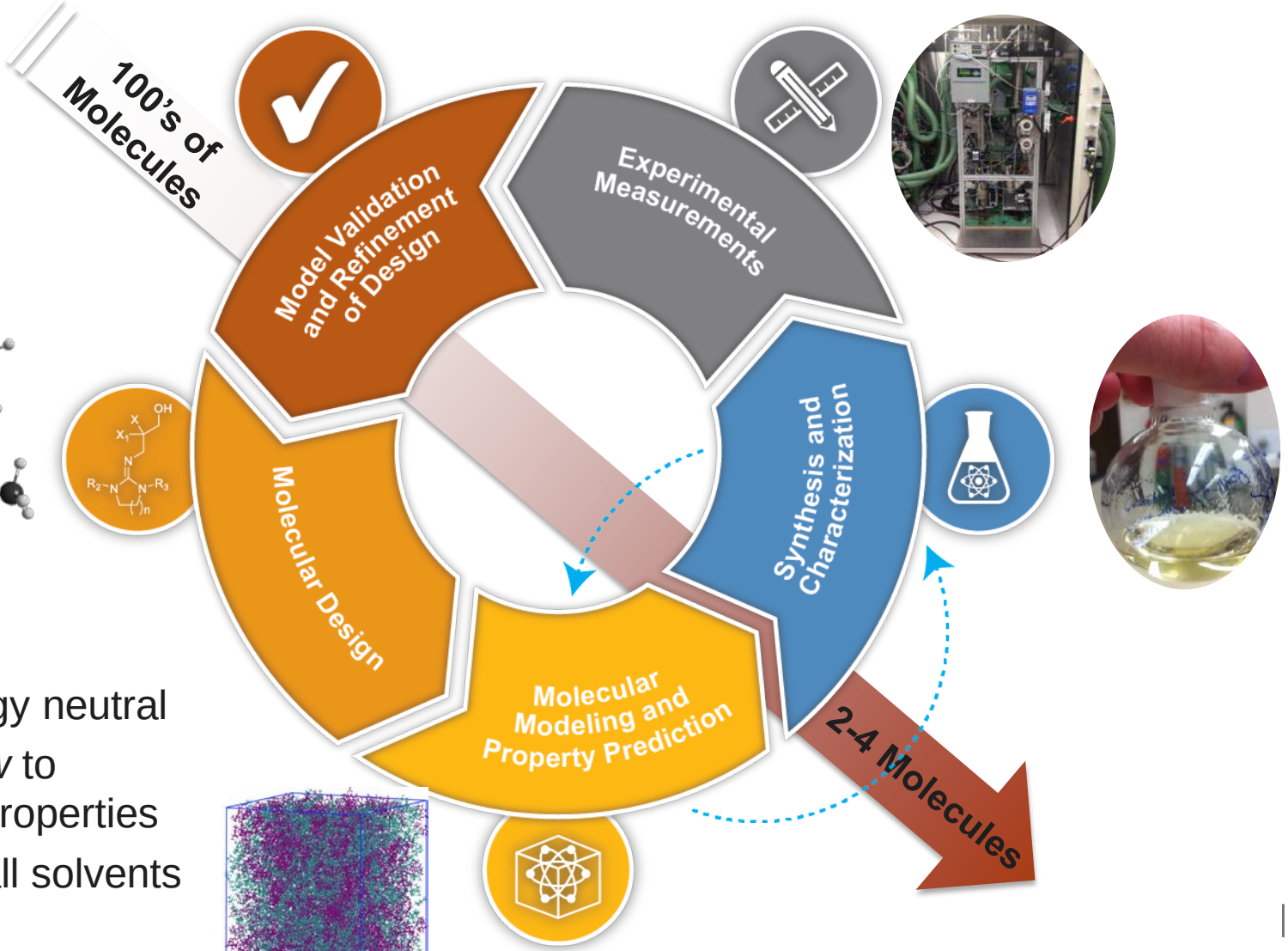
***Aiding DOE's solvent portfolio by controlling properties of solvents at the molecular level.**





- Technology neutral
- Learn *how* to improve properties
- Apply to all solvents

Milestones

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Milestone Number	Milestone Description BP2 (FY16)	Actual or Revised Completion Time
1	Updated project management plan	June 2014
2	Construct physical property model	December 2014
3	Synthesize &characterize 13 candidate CO_2BOL molecules	May 2015
4	Viscosity reduction of 200 cP demonstrated	April 2014
5	Go no-go presentation at NETL	May 2015
6	Synthesize and characterize second round of 13 candidate CO_2BOL molecules	June 2016
7	Viscosity reduction of 400 cP demonstrated	December 2015
10	Construct first-generation molecular dynamics (MD) model for carbamates. Initial assessment of viscosity reduction for GE aminosilicones via additives & blends	December 2016
11	Model 50 carbamate derivatives and identify 3 new candidate molecules for synthesis & characterization	December 2016
12	Synthesis & characterization of 3 carbamate solvent variants from MD simulations	September 2016
8	Synthetic methodology of optimal CO_2BOLs at $10/kg	May 2016
10	Final report provided to NETL	October 2017

Milestones Cont…

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Milestone Number	Milestone Description BP3 (FY17)	Actual or Revised Completion Time
1.1	Updated Project Management Plan	September, 2016
1.2	Go-No Go Presentation at NETL	June, 2017
1.3	Milestone 1.3 Delivery of final report to NETL	October, 2017
8.1	Screen 3rd Solvent Class Derivatives and Identify 2-4 Candidate Molecules (With ≥200 cP Reduction) for Synthesis & Characterization	June, 2017
8.2	Synthesize & Characterization of 2-4 3rd Solvent Class Derivatives Identified From MD Simulations	September, 2017
9.1	Up to 100 GAP Derivatives or Additives Down-Selected to 2-4 Candidate Molecules for Synthesis & Characterization	March, 2017
9.2	Synthesis & Characterization of 2-4 GAP Solvent Variants From MD Simulations	June, 2017
9.3	GAP Solvent Viscosity Reduction of ≥400 cP Demonstrated	September, 2017
10.1	Wetted Wall Testing on CO_2BOL Derivative Completed	June, 2017
10.2	Continuous Flow Testing on CO_2BOL Derivative Completed	August, 2017
11.1	Wetted Wall Testing on Fluor Solvents Completed	February, 2016

Current FY17 Program Output

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Publications

- "Reinventing Design Principles for Developing Low-Viscosity Carbon Dioxide-Binding Organic Liquids for Flue Gas Clean Up" *ChemSusChem*, **2017**, | DOI: 10.1002/cssc.201601622
- "Phase Change Aminopyridines as Carbon dioxide (CO_2) Capture Solvents." *Ind. Eng. Chem. Res.,* **2017**, DOI: 10.1021/acs.iecr.7b00874 .
- "Toward Neutral Capture: Reconfiguring the Speciation of Amines for CO_2 Capture." *Energy Environ Sci.,* **2017**, *In Review*.
- "Dynamic Acid/Base Equilibrium in Single Component Switchable Ionic Liquids and Consequences on Viscosity." *J. Phys. Chem. Lett.*, **2016**, 7, pp 1646–1652.
- "Measuring Nitrous Oxide Mass Transfer into Non-Aqueous CO_2BOL." *Ind. Eng. Chem. Res.,* **2016**, DOI:10.1021/acs.iecr.6b00390.

Patent Applications

- Capture and Release of Acid Gasses Using Tunable Organic Solvents with Aminopyridines, Provisional US Patent application Filed Nov 14th, 2016

Expected FY 17 Program Output

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Publications In Preparation

- PVT cell for comprehensive property measurements of CO_2 capture solvents." ***Frontiers in Energy***
- "Deliberate solvent design for low-viscosity CO_2BOL derivatives." ***Science***
- "Reduced model for viscosity predictions for carbon capture solvents." ***J. Phys. Chem. Lett.***
- "Molecular modeling of AminoSilicone Capture Solvents." ***Green Chem.***

Patent Applications

- Low-viscosity CO_2BOL Derivatives
- Legacy 3rd generation diamines

Program Budget

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Budget Details	Federal Share	Cost Share (Cooperative Agreements)
Total Project (Award Value)	$4,061,000	$0
Total FY17 Budget Period (planned)	$1,500,000	$0
Monthly Expenditures (planned)	$125,000	$0
Total Project (cumulative)	$3,087,934	$0
Total BP (cumulative)	$695,992	$0
Monthly Expenditures (actual, DEC)	$100,393	$0
Remaining Funds	$232,199	

Aqueous Amine Solvent Class

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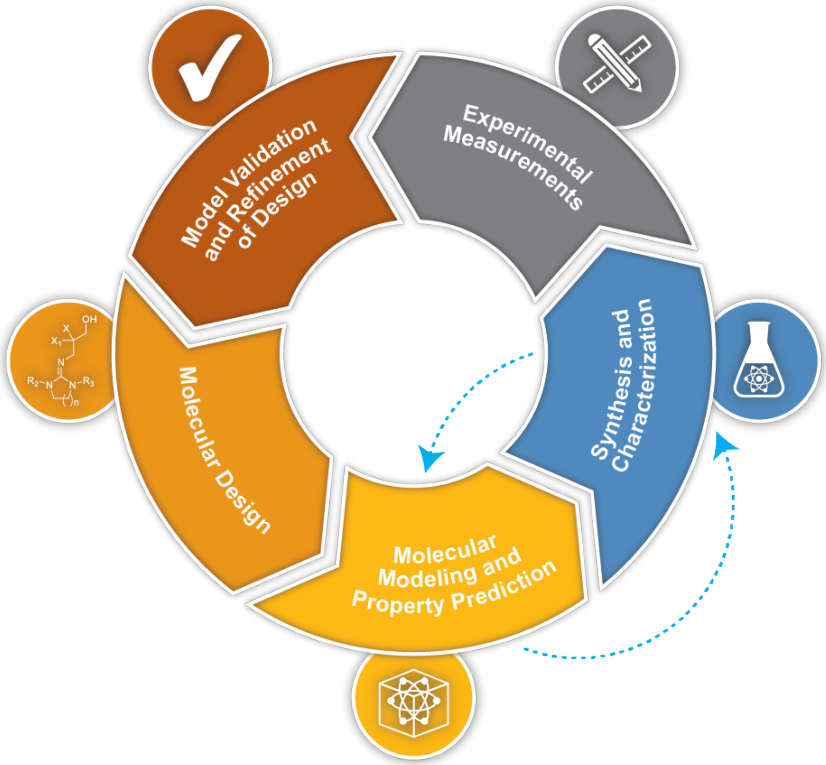
Goal: Advanced amine solvent testing. Added scope for FY17.



- **Objectives:**
  - Test individual compounds P* and k'g and cP
  - Test blend P* and k'g and cP
- **Milestone 10.1**

(2 months – FY17)

Aqueous Amine Highlights

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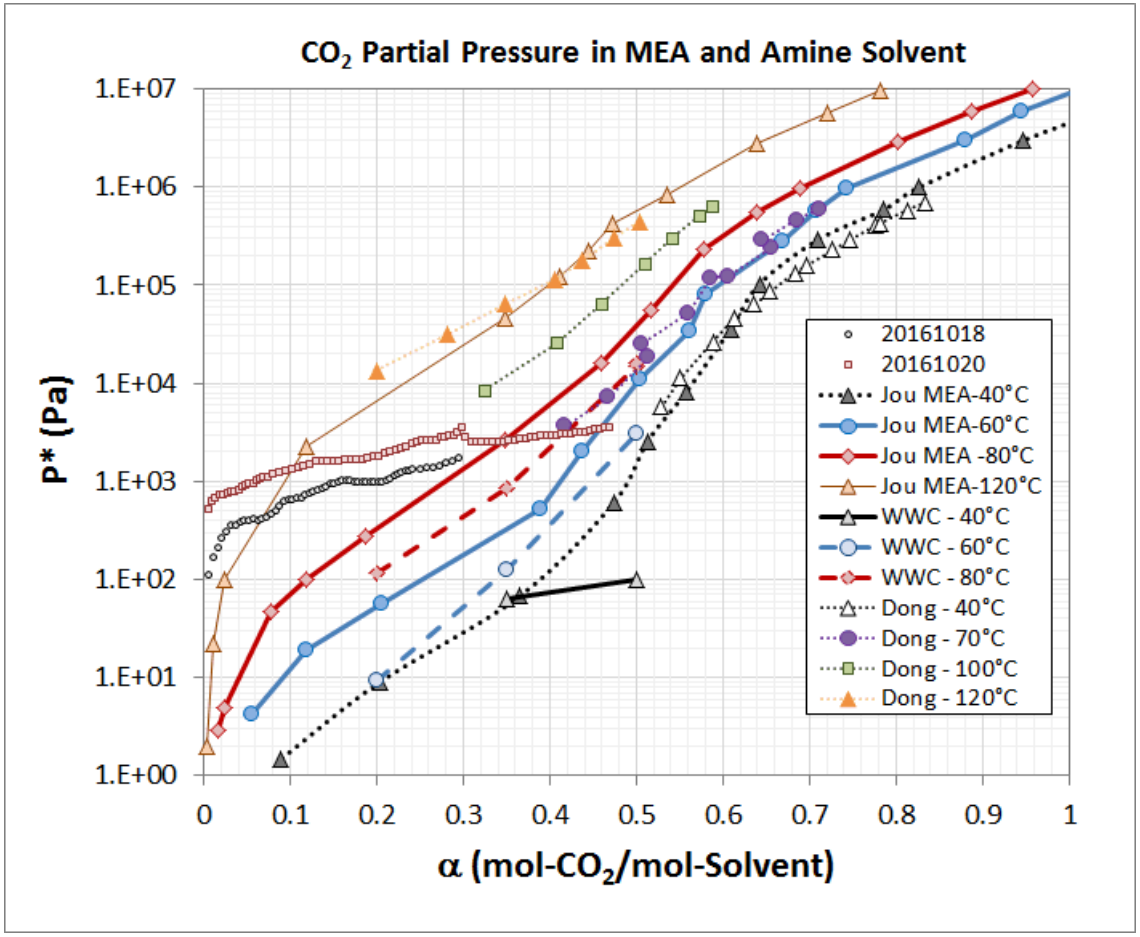
Wetted-wall and PVT testing on compounds A & individually



- PVT data P* data did not match published data
- WWC P* data matched published data

Aqueous Amine Highlights

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Wetted-wall and PVT testing on compounds A & individually.

- *Candidate amine (A) shows stronger complexation of CO_2 than MEA
- *Liquid film mass transfer coefficients comparable to MEA

Run	Temp target, C	loading target	p*, Pa	KG, [mol/m2/s/Pa]	kg_Bishnoi, mol/(s*m2*Pa)	kg'_mol/(s*m2*Pa)
F1	40	0.35	64.7	1.793E-06	1.125E-05	2.133E-06
F2	60	0.35	124.9	1.229E-06	1.242E-05	1.364E-06
F3	80	0.35	869.6	6.918E-07	1.582E-05	7.234E-07
F4	40	0.20	-2.7	2.592E-06	1.122E-05	3.370E-06
F5	60	0.20	9.48	1.648E-06	1.247E-05	1.899E-06
F6	80	0.20	114.7	6.473E-07	1.619E-05	6.743E-07
F7	40	0.50	99.7	3.495E-06	1.134E-05	5.051E-06
F8	60	0.50	3114.6	2.260E-06	1.239E-05	2.764E-06
F9	80	0.50	15131.6	4.215E-07	7.875E-06	4.453E-07
F10	80	0.50	15855	4.146E-07	5.229E-06	4.503E-07

Aqueous Amine Highlights

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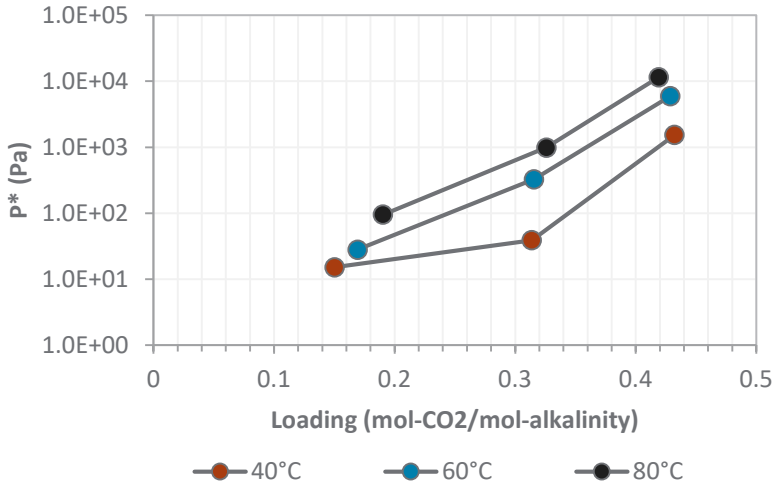
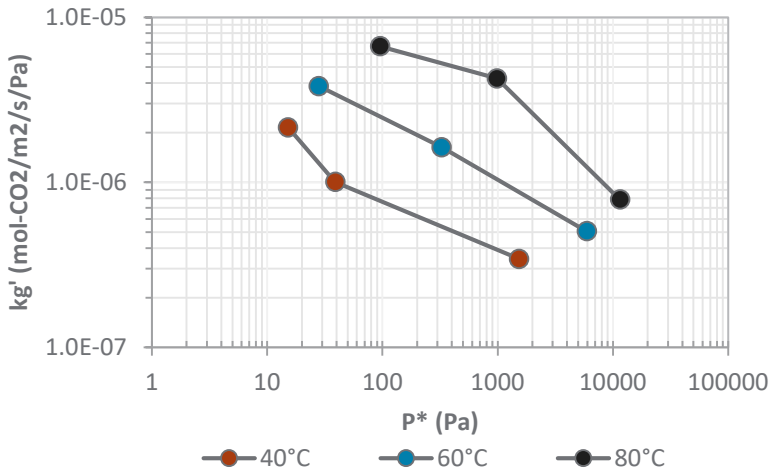
Wetted-wall and PVT testing on a proprietary blend of compounds A & B





Run	T_ave_liq	T_ave_gas	P_total	α_target	α_analyzed	P*	KG	kg_Bishnoi	kg'
[-]	[°C]	[°C]	[psia]	[mol/mol-alkalinity]	[mol/mol-alkalinity]	[Pa]	[mol/m2/s/Pa]	[mol/m2/s/Pa]	[mol/m2/s/Pa]
Test_F28	40.09	43.41	14.70	0.200	0.150	15.2	1.807E-06	1.130E-05	2.151E-06
Test_F22	40.24	41.06	14.90	0.350	0.314	38.9	9.223E-07	1.112E-05	1.006E-06
Test_F25	40.52	42.40	14.36	0.490	0.432	1533.9	3.335E-07	1.158E-05	3.434E-07
Test_F29	58.90	63.18	14.96	0.200	0.169	28.0	2.925E-06	1.241E-05	3.827E-06
Test_F23	58.42	59.14	14.82	0.350	0.316	326.3	1.444E-06	1.252E-05	1.632E-06
Test_F26	59.38	59.19	14.22	0.49	0.429	5913.2	0.0	0.0	5.049E-07
Test_F30	77.29	76.56	14.83	0.20	0.190	95.3	0.0	0.0	6.667E-06
Test_F24	77.45	76.25	14.64	0.35	0.326	984.8	0.0	0.0	4.260E-06
Test_F27	77.57	74.92	14.72	0.49	0.419	11518.3	0.0	0.0	7.853E-07

A + B shows stronger complexation of CO_2 (low P) than MEA

*A + B has comparable mass transfer of CO_2 (*kg'*) to MEA

Aqueous Amine Blend

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- Conclusions:
- Viable solvent blend with superior performance to MEA
  - Blend has a lower P* than MEA
  - Comparable mass transfer rates

Remaining FY17 work:

- Further WWC testing and testing at TCM on another program

Critical Findings From FY16 & FY17

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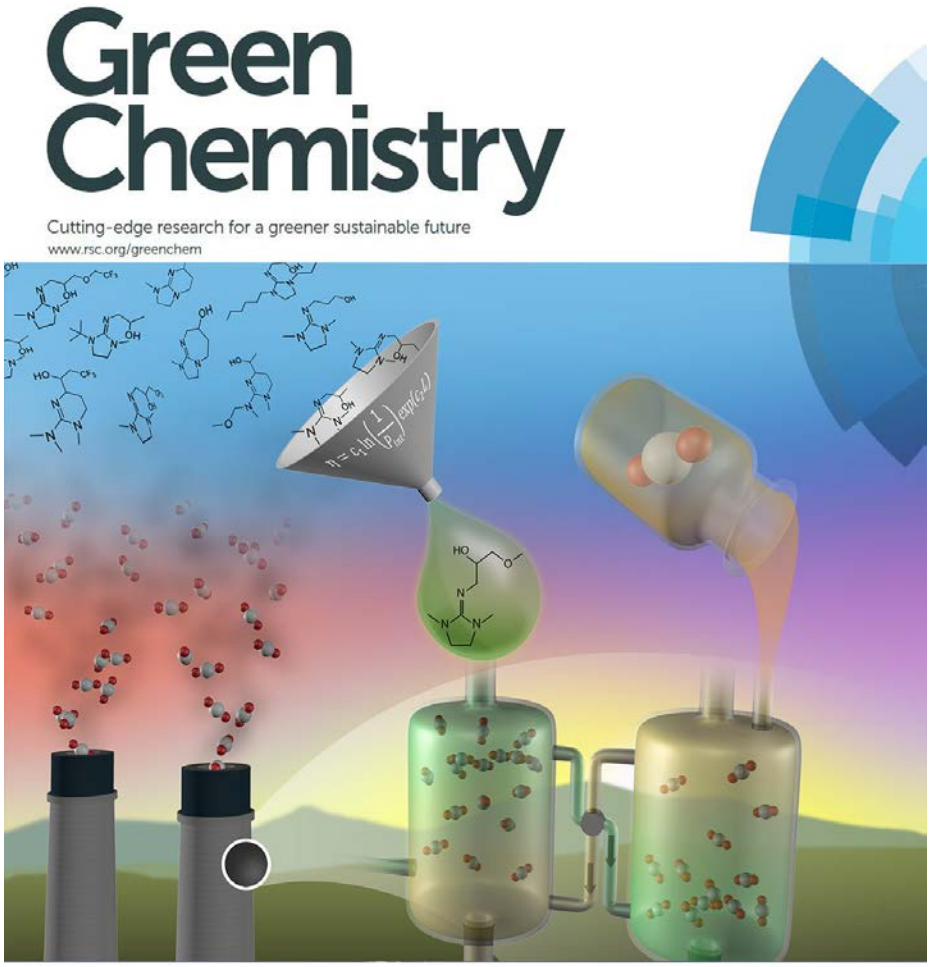

ROYAL SOCIETY OF CHEMISTRY

*Cantu et. al. *Green Chem.* **2016**, **DOI:** 10.1039/C6GC02203K

Viscosity Depends on Hydrogen Bonds Orientation

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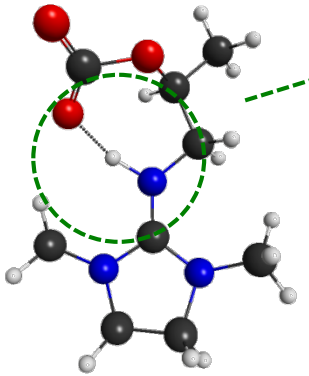
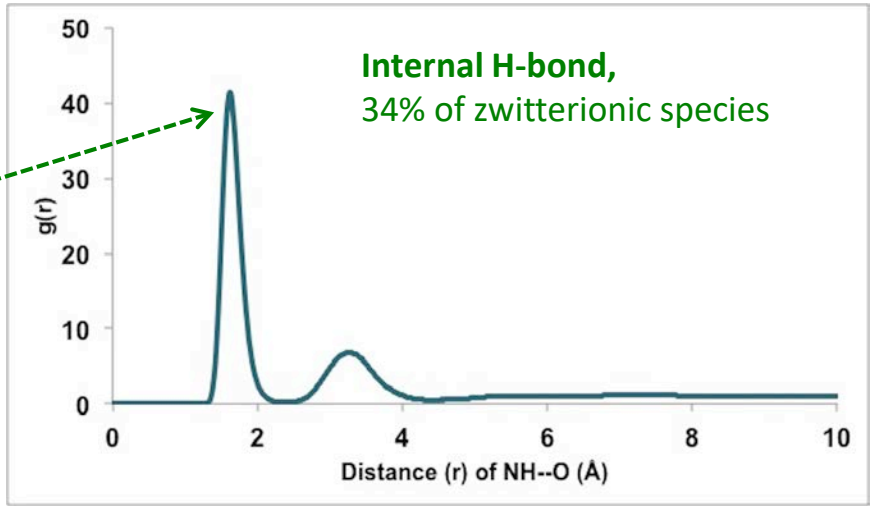
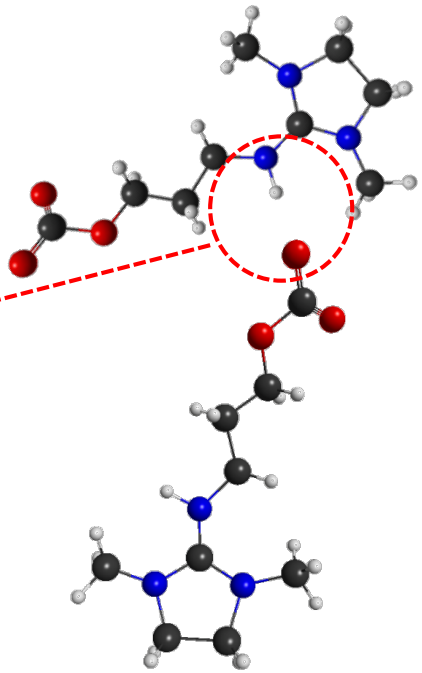
% of internal H-bonding (P_{int}) is the biggest descriptor of viscosity.

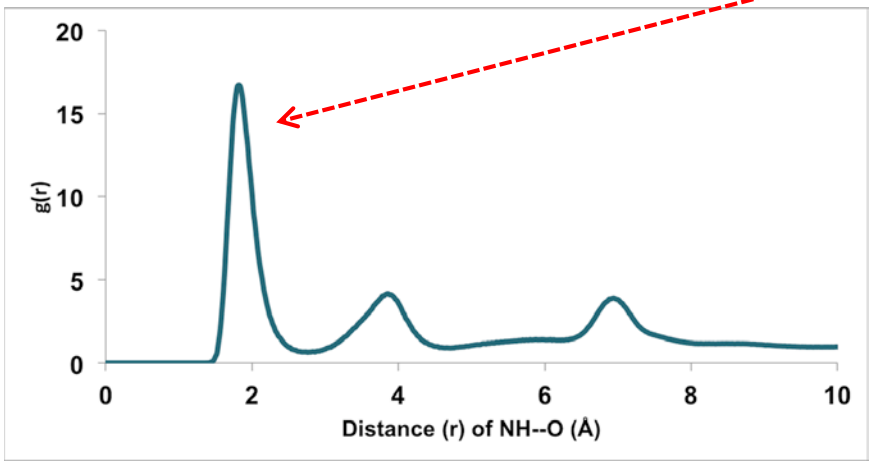




Higher viscosity > 1000 cP at 25% mol loading



Lower viscosity ~110 cP at 25% mol loading



J. Phys. Chem. Lett., 2016, 7, pp 1646–1652

Viscosity and the % of CO_2-Bound Molecules That Have an Internal Hydrogen Bond (P_{int})

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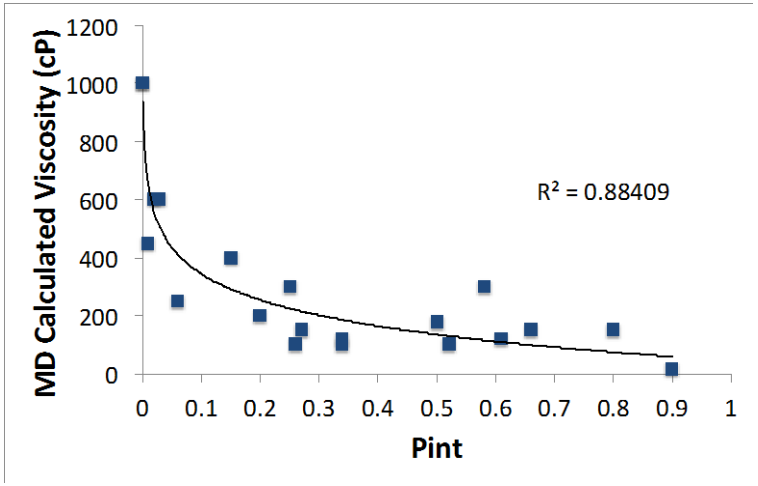
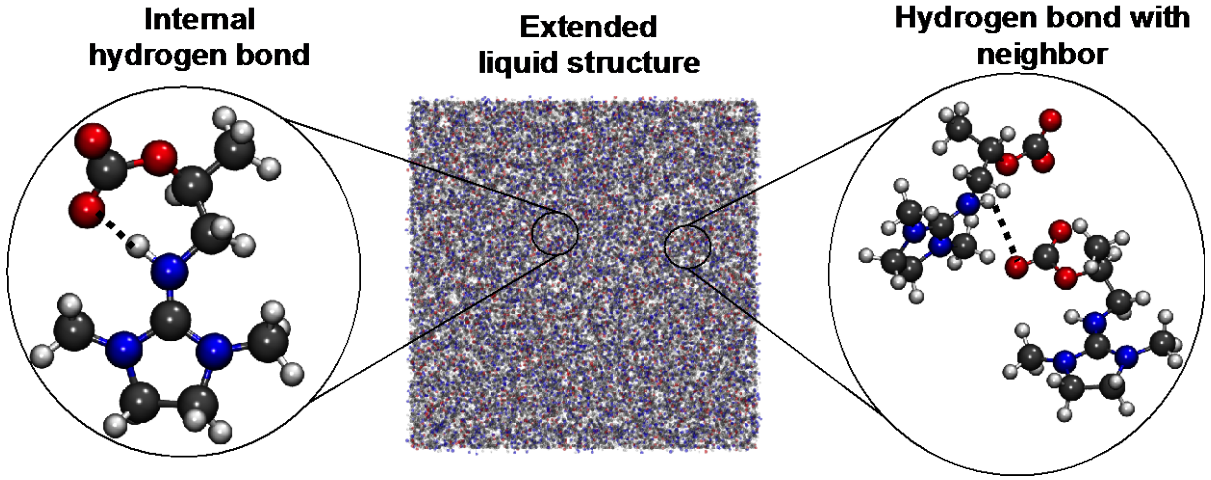
As P_{int} increases, viscosity follows a logarithmic decay.

25% mol loading	100% zwitterion	
system	viscosity (cP)	% internal H-bond
EODM-2-BOL	45.5	92
IPADM-2-BOL	149.5	34
IPATFMM-2-BOL	328.5	13



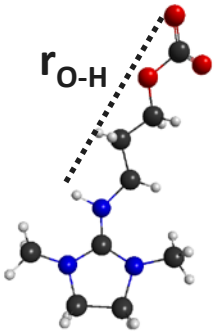


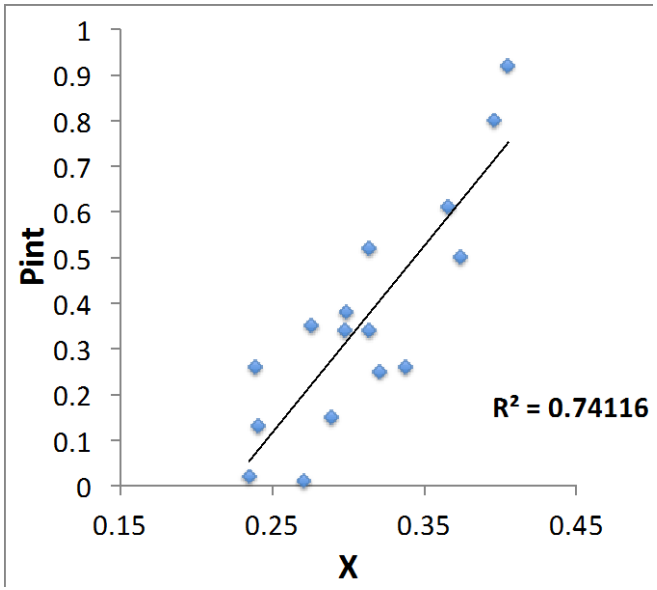
J. Phys. Chem. Lett., 2016, 7, pp 1646–1652

P_{int} From an Optimized Structure

Viscosity can be predicted without time intensive synthesis or modeling.

- If $r_{O\text{-}H} > 2.0$ Å, then $P_{int} = 0.001$

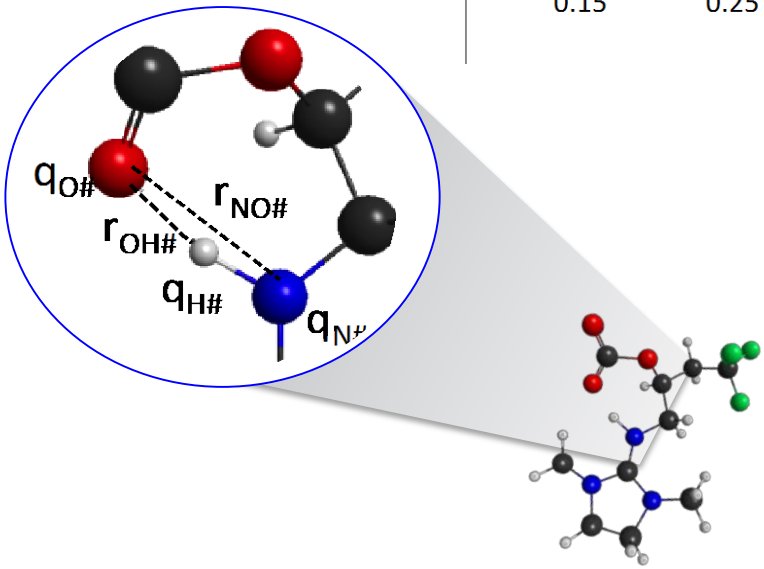




- If $r_{O\text{-}H} < 2.0$ Å, then
- Difference between electrostatic repulsion (NO) and attraction (OH)

$$P_{int} = c_1 X + c_2$$

$$X = \frac{q_N q_O}{r_{NO}} - \frac{q_O q_H}{r_{OH}}$$



J. Phys. Chem. Lett., 2016, 7, pp 1646–1652

Aminosilicone Solvent Class

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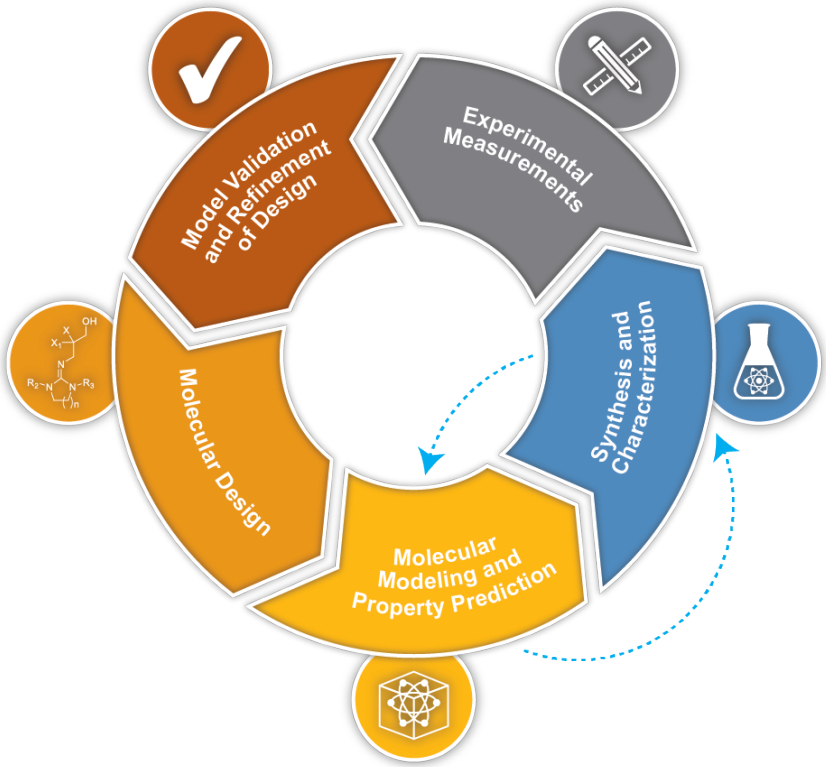
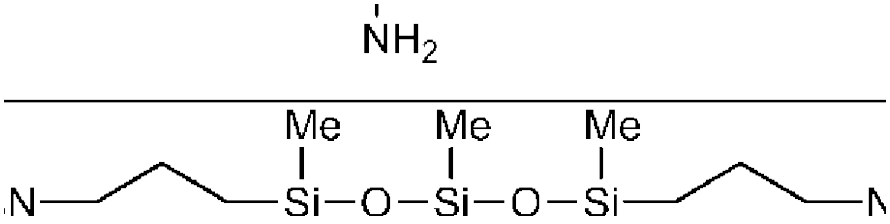
Goal: To form molecular-level insights to GAP-1 solvents.





- **Objectives:**
  - Characterize solvent structure
  - Reduce viscosity by >400 cP
  - Impact of diluents and additives
  - Mechanisms of degradation
    - Water
- **Milestones 9.1, 9.2, 9.3**

(12 months – FY17)

Aminosilicones/Triethylene Glycol Molecular Structure

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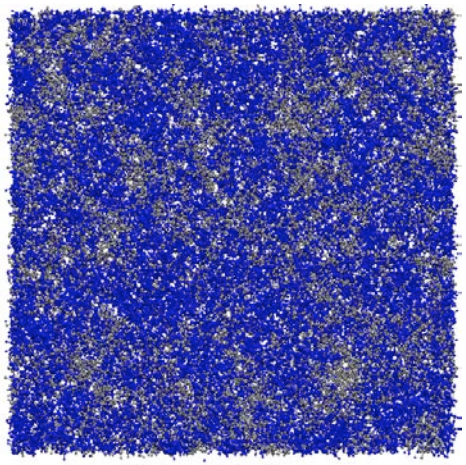
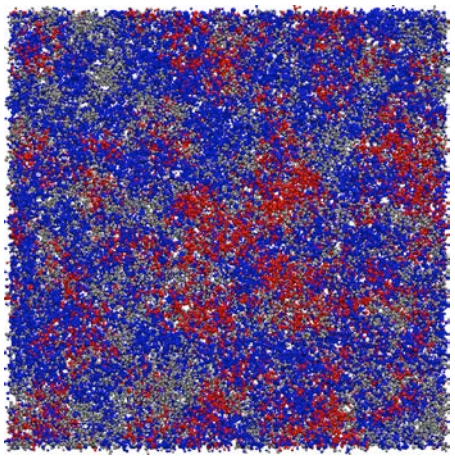
GE Global Research

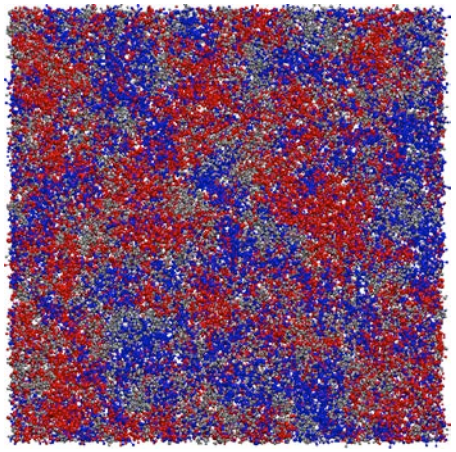
Aminosilicone Solvent Class: (Triethylene Glycol co-Solvent)[2]



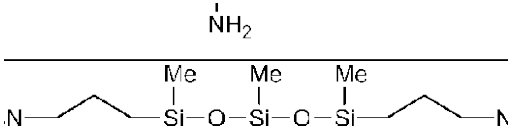
0% CO_2



25% CO_2



50% CO_2



CO_2-GAP-0: red

GAP-0: blue

TEG: silver

- TEG may not be dissolving GAP carbamates
- Co-solvent not needed

1) Cantu et al. *in preparation*

Aminosilicones/Triethylene Glycol Molecular Structure

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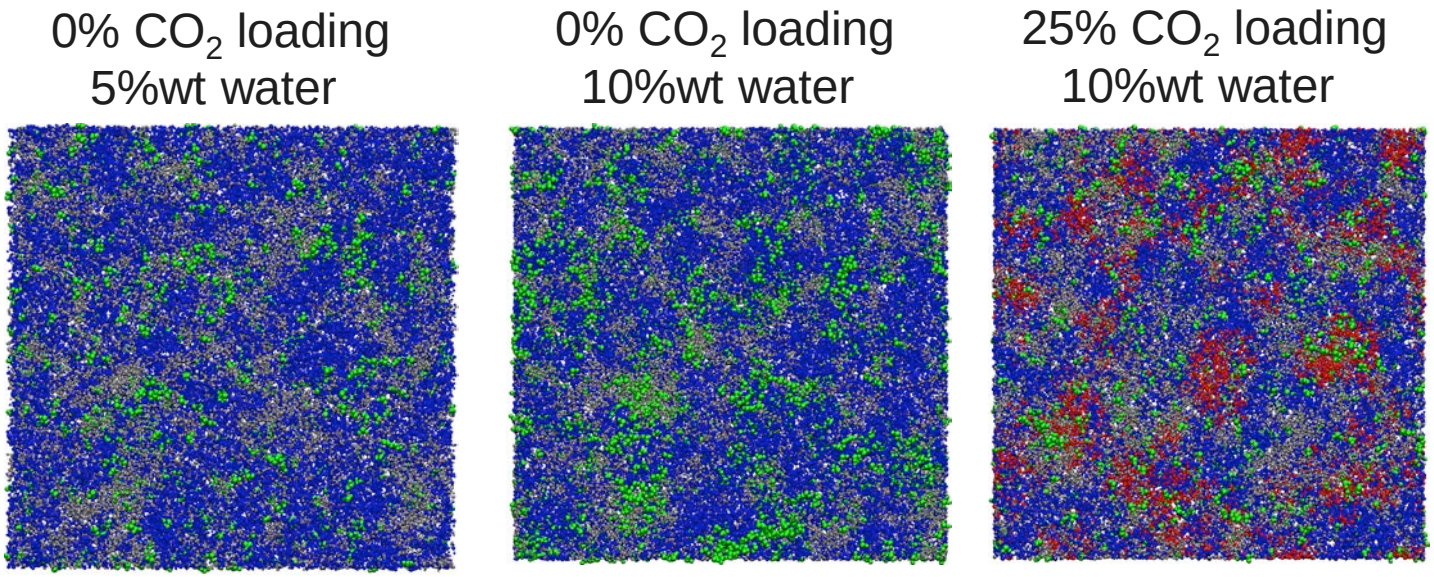
Mixtures of water and and GAP-1/TEG are being simulated to determine the impacts of additives such as water.

KEY:
CO_2-GAP0: **red**
GAP0: **blue**
TEG: **silver**
Water: **green**



- Water acts as a diluent by solvating carbamate clusters
  - (matching experimental observations)
- Comparable solvation seen with ethylene glycol and other diluents
- Diluents do reduce viscosity at low mole fractions
  - (matching experimental observations)

Heterogeneous Molecular Structure May Account for Similar Performance

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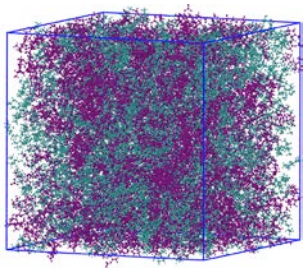
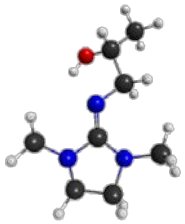
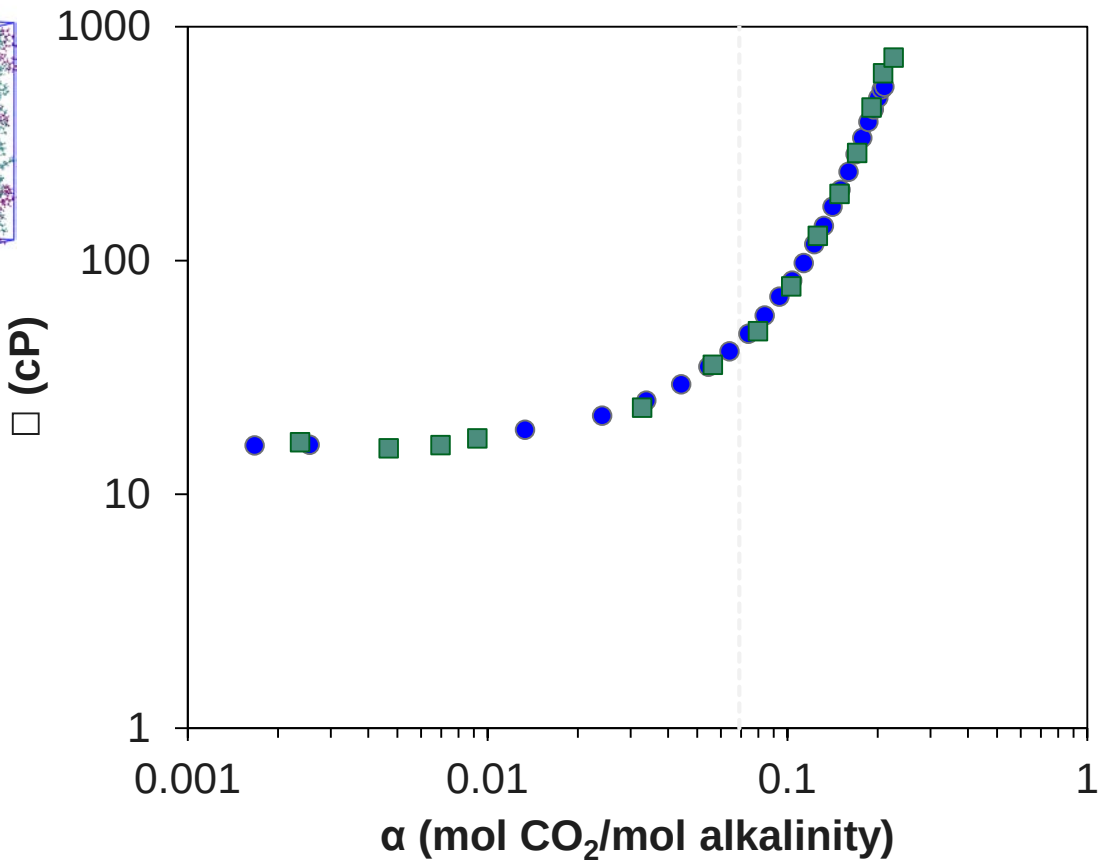
GE Global Research

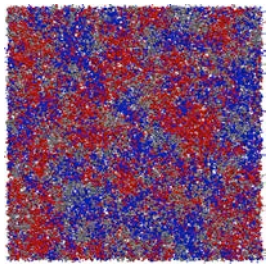
CO_2BOLs and aminosilicones show similar predicted solvent structure and viscosity profiles as a function of CO_2 loading





IPADM-2-BOL





GAP-1/TEG

1) Mathias et al *Energy Procedia,* **2015***;* Cantu *et al. J. Phys. Chem. Lett.* **2016**, *7,* 1646. 2) Malhotra *et al. Manuscript in preparation*

Heterogeneous Molecular Structure May Account for Similar Performance

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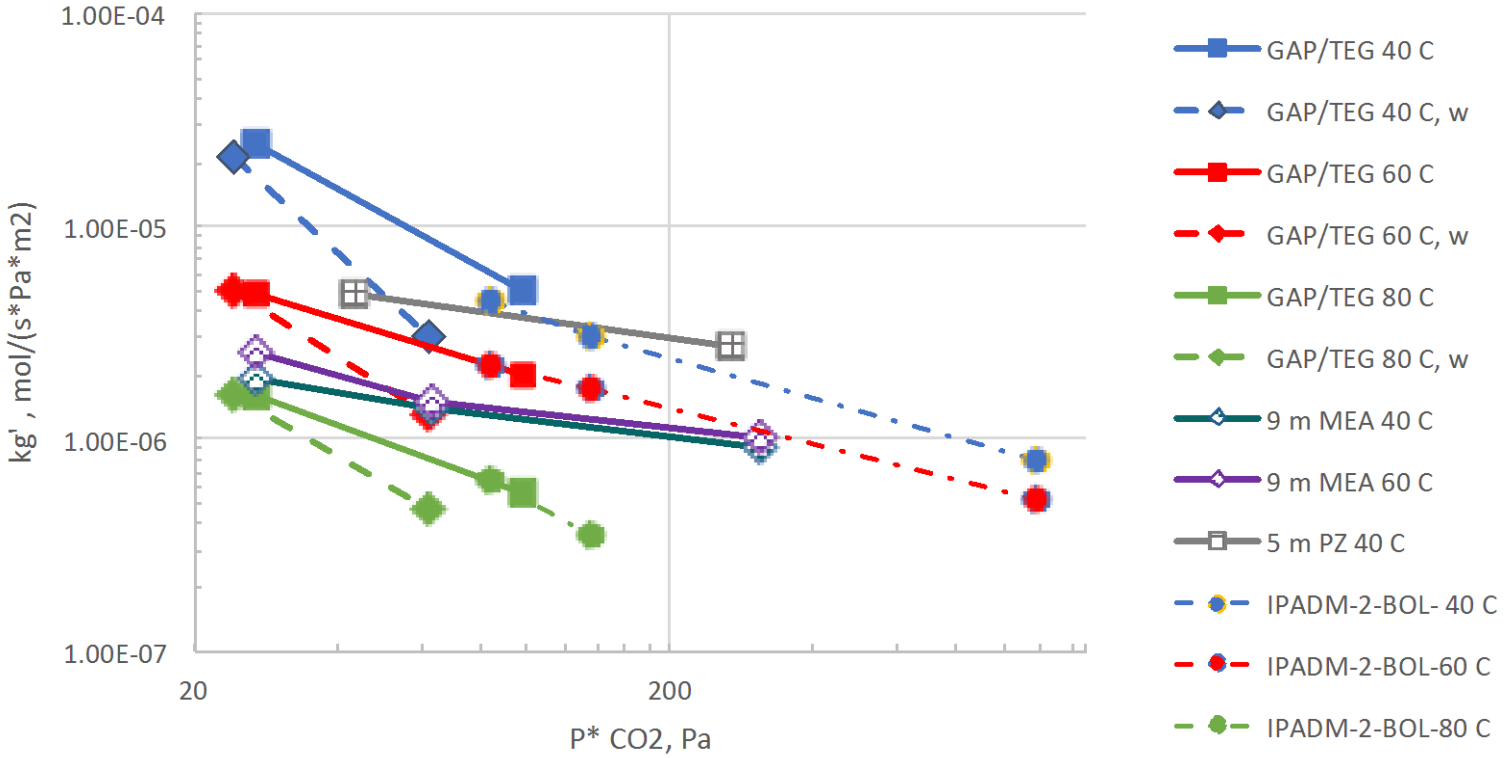
CO_2BOLs and aminosilicones show higher than expected mass transfer.



- k'_g vs. P* are comparable to MEA and piperazine under similar driving force
- Viscosity's impact of CO_2 mass transfer is less than anticipated
- IPADM-2-BOL and GAP/TEG fall on the same curve

*MEA/Piperazine data from UT Austin

Heterogeneous Solvent May be Good for Diffusion and Reactivity

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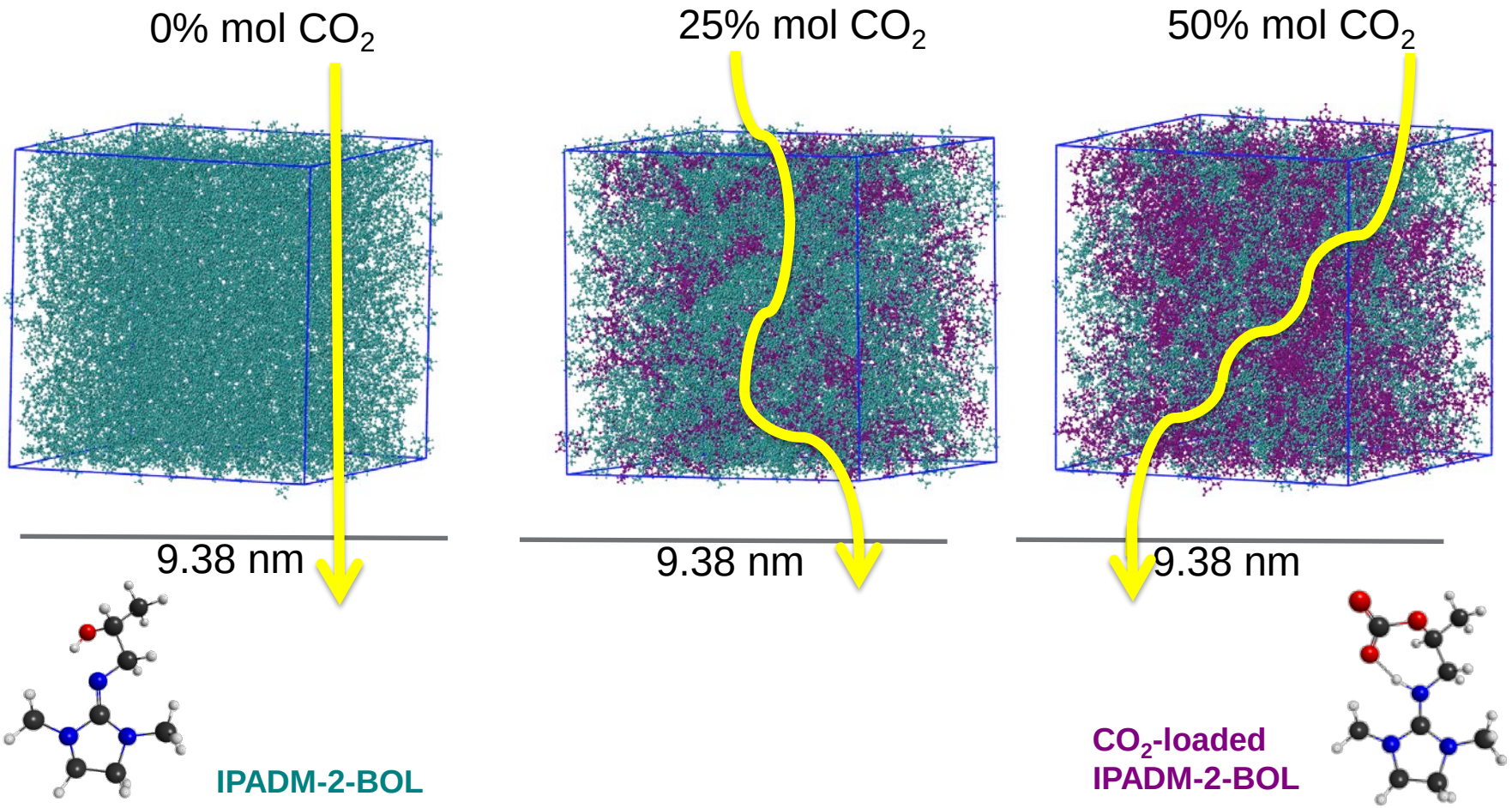

- Open solvent "pores" may provide channels for CO_2 diffusion
- High physical solubility in low CO_2 loaded regions
- Unreacted solvent always available to react with CO_2

Probing the Acid/Base Equilibrium

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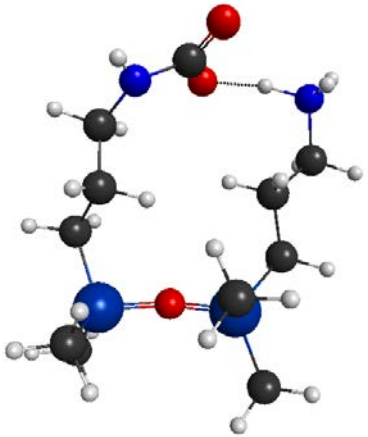
Probing the acid/base equilibrium in aminosilicones.

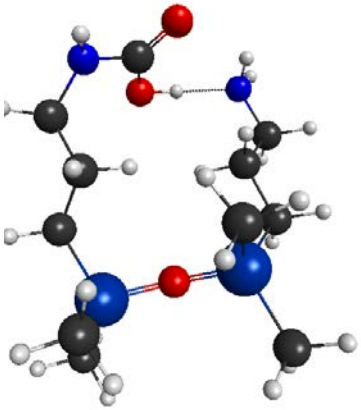
- GAP-0 and GAP-1 with implicit solvent: both isoenergetic (~0.001 kJ/mol)
  - Equilibrium likely observed in solution
- GAP-0 gas phase: Acid state is ~ 35kJ/mol lower in energy
- GAP-1 gas phase: Zwitterion is ~15 kJ/mol lower in energy

GAP-0

Zwitterion

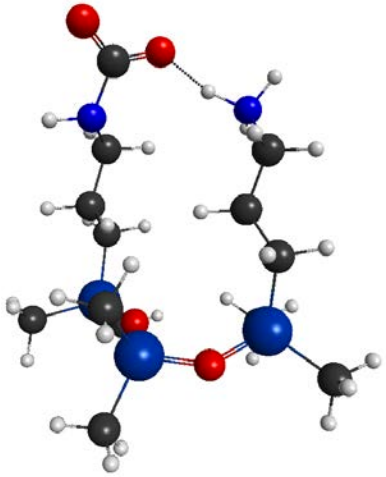


Acid

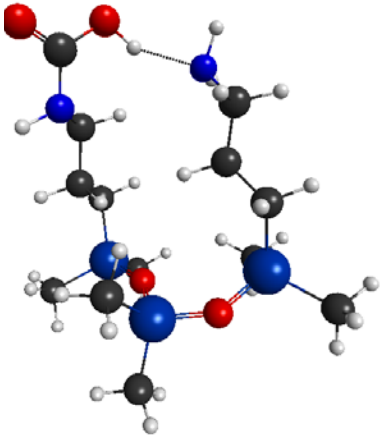


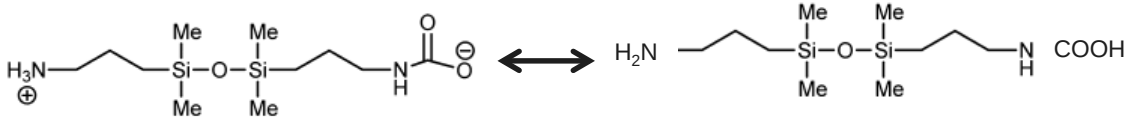
GAP-1

Zwitterion



Acid





Legacy Solvents: 3rd Generation Molecules Currently Being Modeled

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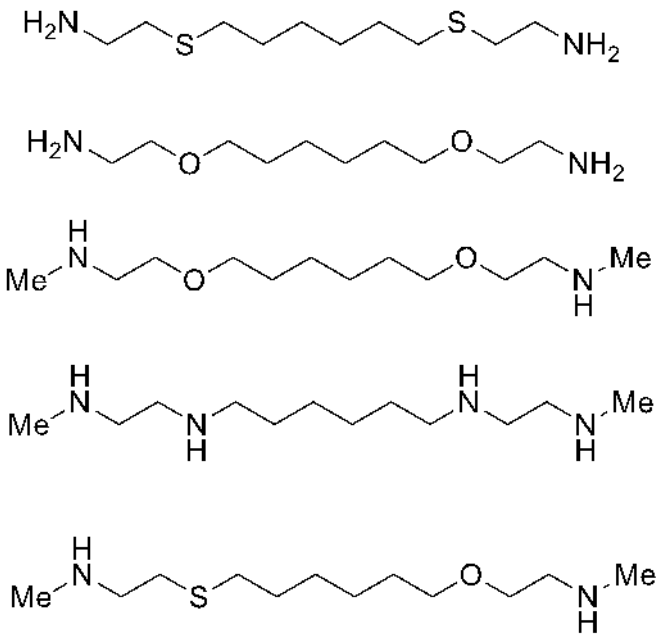
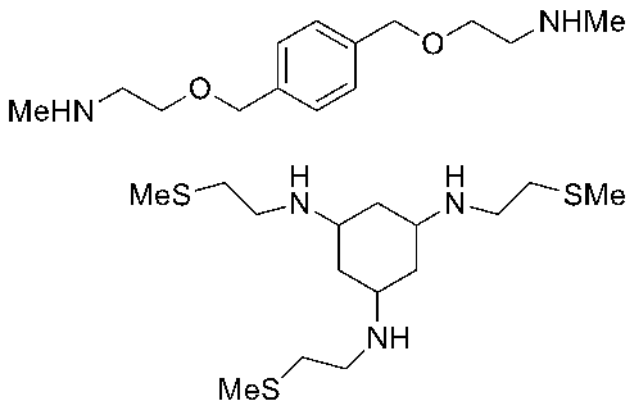
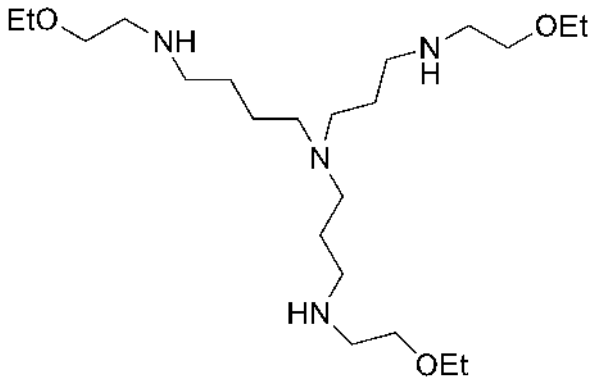
New 3rd generation derivatives designed with high P_{int} for low viscosity.







- 100% concentrated, can utilize PSAR
- Moieties promote internal H-bonding
  - Low viscosity
  - favor “acid” form
  - No hydrolysis or disproportionation
- Cheaper

Legacy 3rd Generation Solvents

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Conclusions:

- Key descriptors of viscosity identified
- Co-solvents do not reduce viscosity
- New derivatives identified
  - More durable
  - Cheaper
- 100% concentrated
  - May use PSAR

Remaining FY17 work:

- Model molecules to determine viscosity of 3rd generation
- Make and test cP/P* and k'g for a 1-2 derivatives

Amino Pyridine Solvent Class

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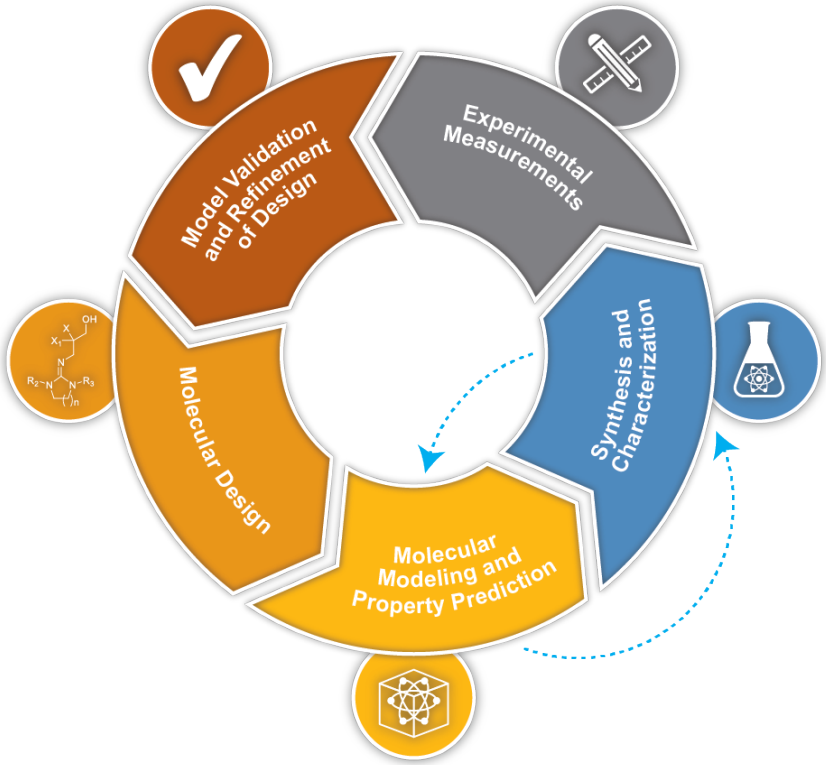
Goal: To form molecular-level insights of this newly discovered amine solvent class.



- **Objectives:**
  - Test individual compounds P* and k'g and cP
  - Reduce volatility while retaining low viscosity
- **Milestones: 8.1, 8.2**

(12 months – FY17)

New Solvent Class Derived From CO_2BOL & GAP-1 Findings

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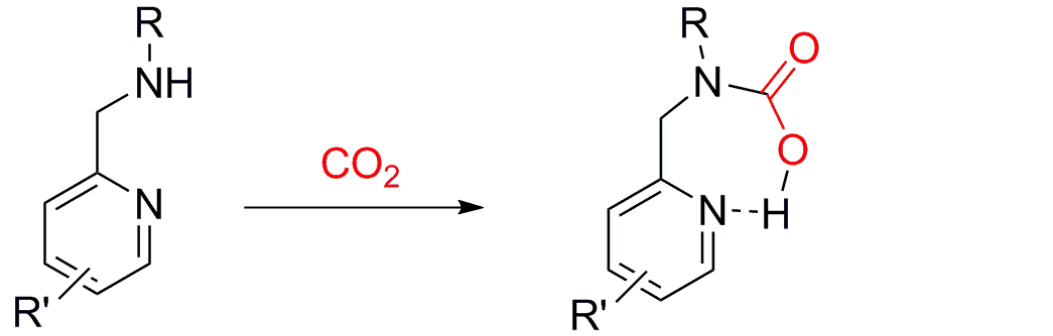
Switchable carbamate ionic liquid with similar properties as CO_2BOLs.



Pyridine-based Amine

R= H, Alkyl, Me, Et, Pr, iPr etc, EWG, CH_2CF_3, CH_2OMe etc
R' =Alkyl, OMe, NO_2, F etc

- 100% concentrated, can utilize PSAR
- Pyridine moiety can be added to GAP-1 derivatives to promote internal H-bonding
  - Low viscosity
- Unique Acid/base equilibria predicted to favor “acid” form
  - Low regeneration temperature

Changing the Speciation of Amine Chemistry

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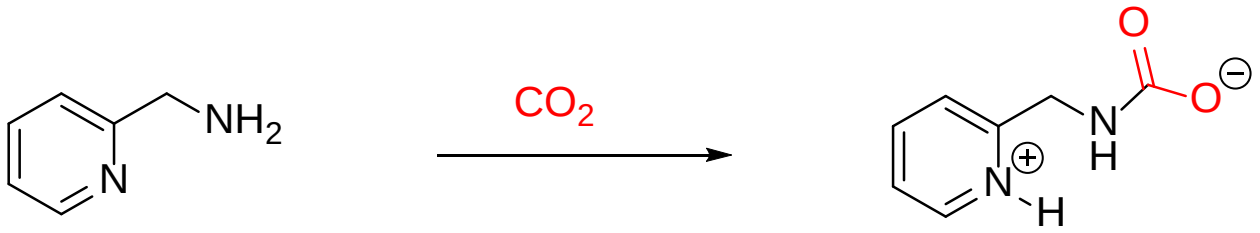
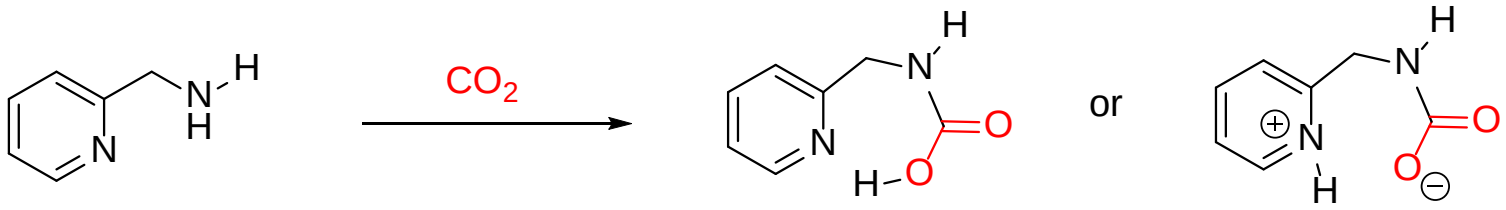
CO_2 Uptake of 2-Picolylamine Shows 1:1 Chemistry Is Achievable



Compound	CO_2 Wt%	CO_2 Mol%	Product state
neat	18	44	Solid
1:1 DMSO:	32 (15)	78.5	Liquid
Koechanol	9	44	Liquid

High P_{int} promotes a high degree of carbamic acid.



- Carbamic acid and zwitterionic carbamate salt equilibrium
- Standard 2:1 amine : binding mode

CO_2 Capacity of AP Derivatives

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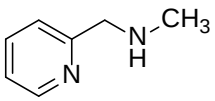
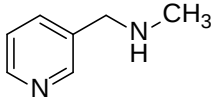
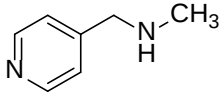
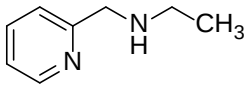
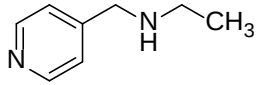
CO_2 Gravimetric Uptake of AP Derivatives at 40 ℃ Show High Capacity.

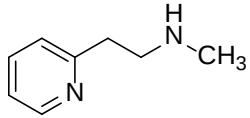

2-MAMP


3-MAMP


4-MAMP


2-EAMP


4-EAMP


2-MAEP

	CO_2 capacity at 25 °C		CO_2 capacity at 40°C	
Compound	Wt%	Mol%	Wt%	Mol%
2-MAMP	19.7	54.8	21.1	58.5
3-MAMP	19.5	54.1	20.0	54.9
4-MAMP	19.7	54.8	18.6	51.5
2-EAMP	18.2	56.5	14.0	43.3
4-EAMP	18.3	56.7	16.7	51.8
2-MAEP	17.8	55.2	19.2	59.8

- Six non-aqueous amines have high CO_2 capture capacity
- CO_2-rich solvents are liquids at room temperature
- Heat of amine reaction with CO_2 is ~75 KJ/mol

Regeneration of AP Derivatives

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CO_2 Release Profiles Show Low Regeneration Temperatures W/WO PSAR

Compound	60 °C PSAR	70 °C	80 °C	100 °C	120 °C
2-MAMP		33.8	60.5	90.3	-
3-MAMP		31.1	51.0	77.5	-
4-MAMP		35.1	51.3	93.8	-
2-EAMP	81	85	95.8	-	-
4-EAMP		71.4	85.1	98.8	-
2-MAEP		-	34.6	76.4	90.3

- Applying PSAR to 2-EAMP lowers regeneration temperature to 60 °C
- Lower regeneration energy enables more net power, low evaporative losses and minimizes thermal degradation

Viscosity Profiles for AP Derivatives

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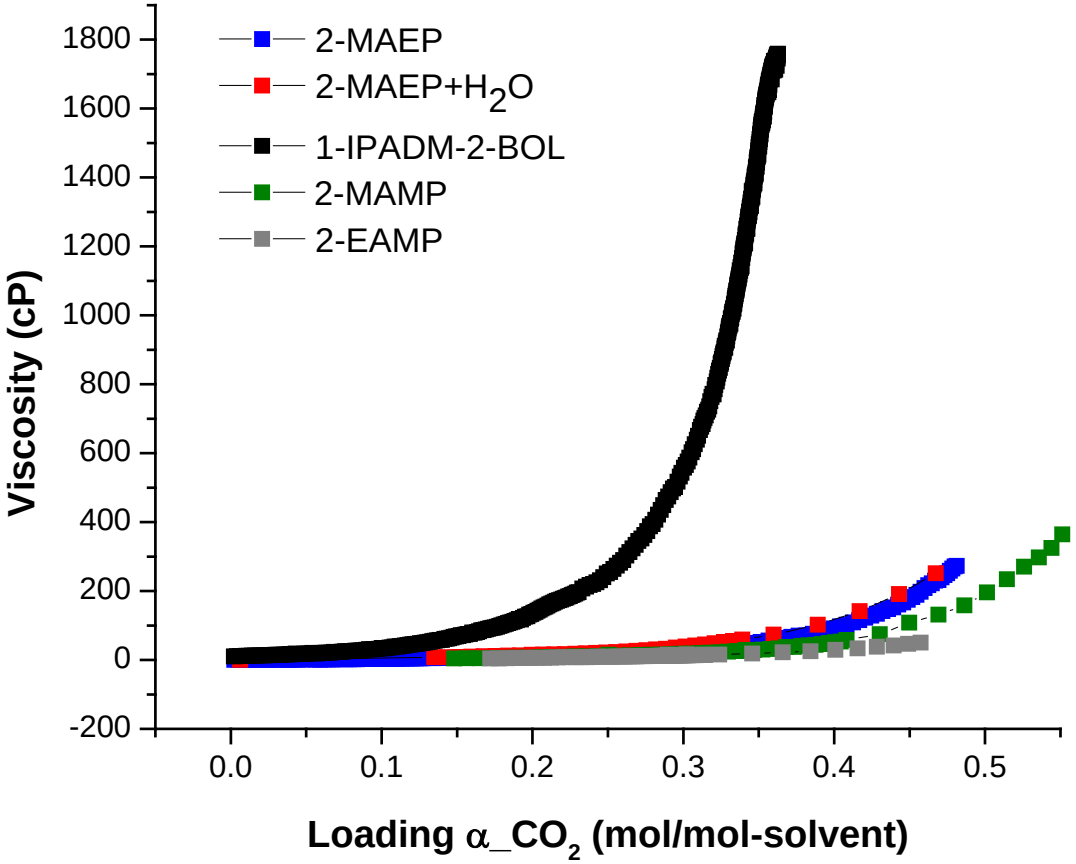
High P_{int} reduces viscosity ~90% over IPADM-2-BOL.



- 2-MAEP has 90% lower viscosity than CO_2BOL IPADM-2-BOL
- Viscosity of 2-MAEP at 40 °C almost matches that of IPADM-2-BOL at 75 °C

Kinetic Profiles for AP Derivatives

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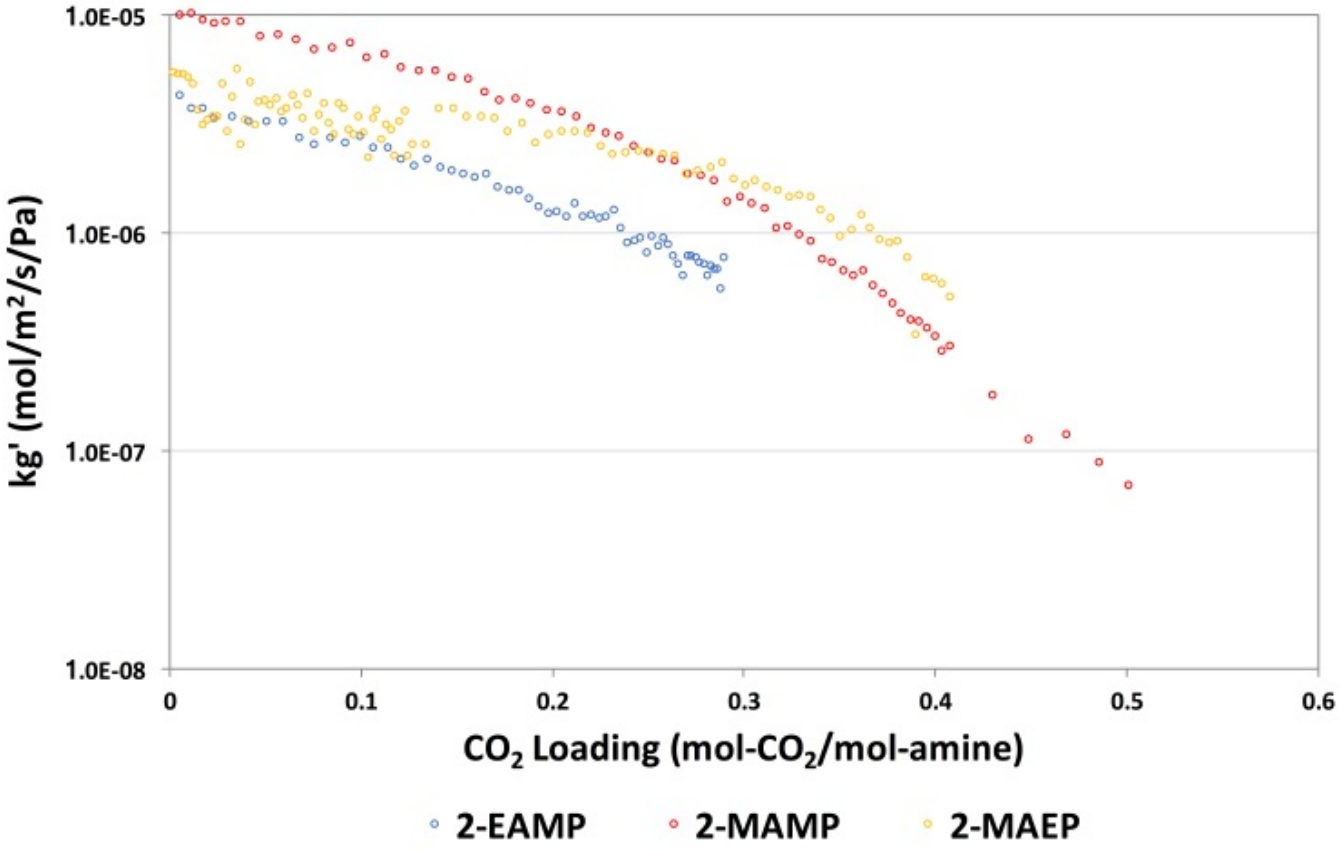
Comparable mass transfer to IPADM-2-BOL.



- 2-MAEP has 90% lower viscosity than CO_2BOL IPADM-2-BOL
- Viscosity of 2-MAEP at 40 °C almost matches that of IPADM-2-BOL at 75 °C

Designing 2nd Generation Aminopyridines

Reducing volatility while retaining low viscosity.

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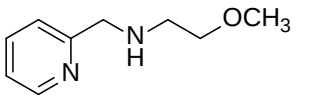
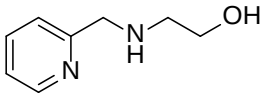
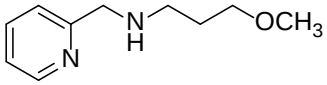
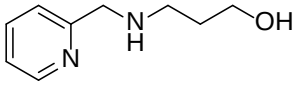
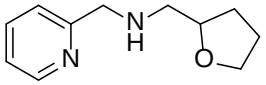
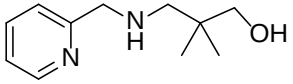
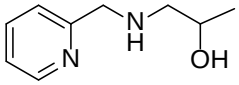
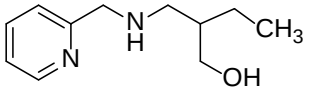
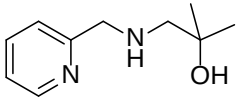
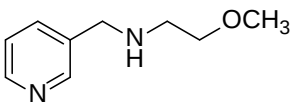
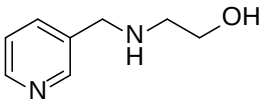
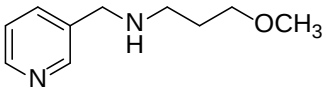
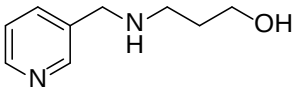
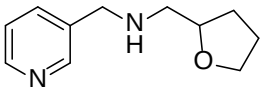
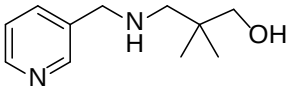
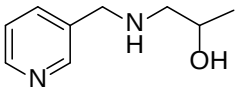
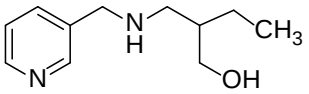
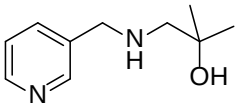
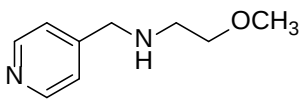
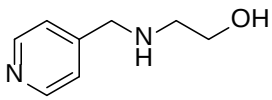
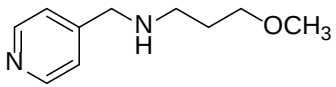
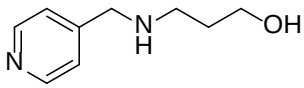
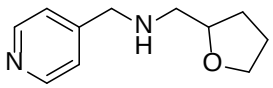
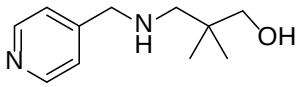
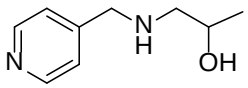
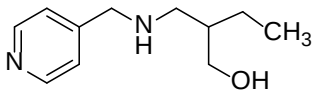
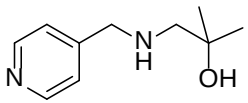
2-Pyridine

3-Pyridine

4-Pyridine

2nd Generation Aminopyridines

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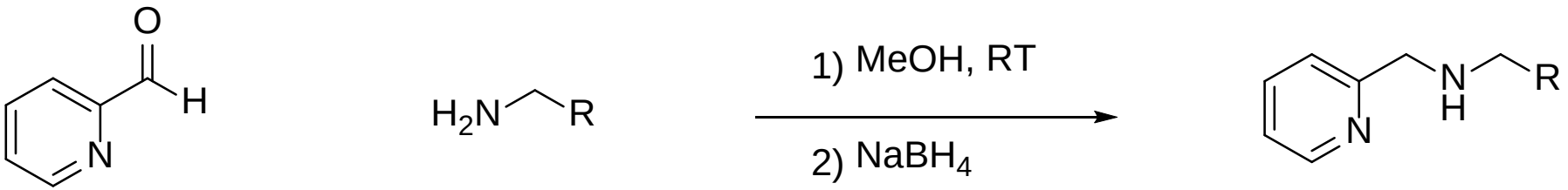
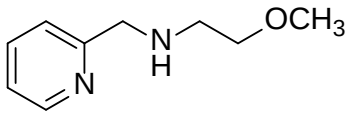
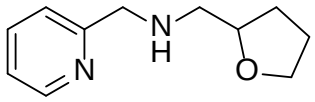
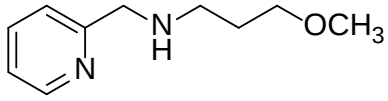
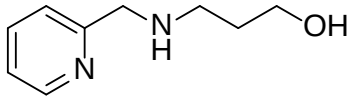
Show reduced volatility while retaining CO_2 capacity and low viscosity.



Compound	MW	BP* (°C)	Vapor Pressure* (Torr @ 25 °C)	CO_2 wt%	CO_2 mol%
	166.2	238.9 ± 20	0.0414	15.2	57.4
	192.3	304.4 ± 17	0.000935	9.4	41
	179.3	261.9 ± 20	0.0112	14.2	57.7
	204.3	315 ± 27	0.000432	7.0	32.7

AP Molecular Structure

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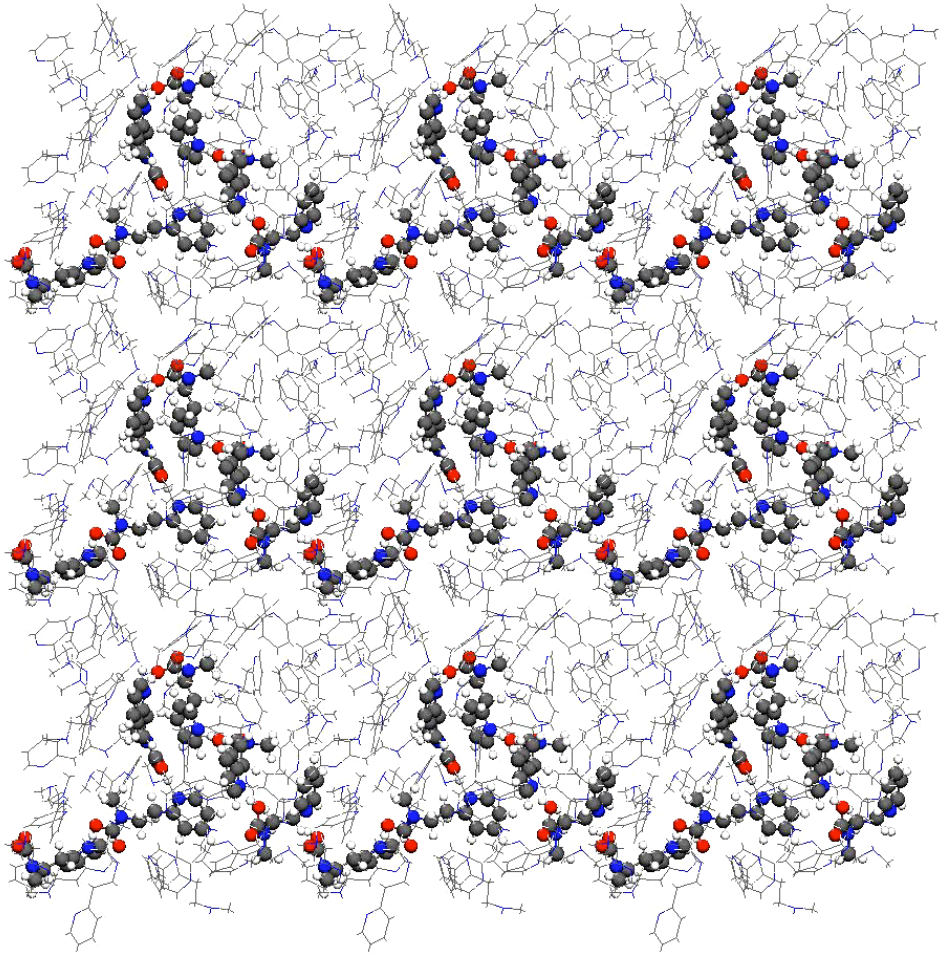
Insights into molecular structure indicate new reactivity mesoscale ordering.



- Carbamate channels show different CO_2 binding mechanisms pending location of pyridine N
- Potential CO_2 diffusion channels

Amino Pyridine Solvent Class

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Conclusions:

- AP solvent class shows promising viscosity though high volatility
- Tunable acid/base equilibria
- Low regeneration temperature (20 ˚C swing)

Remaining FY17 work:

- Reduce volatility while retaining low cP
- WWC testing and PVT to confirm testing
- Explore channels in solvent with respect to mass transfer

CO_2BOL Solvent Class

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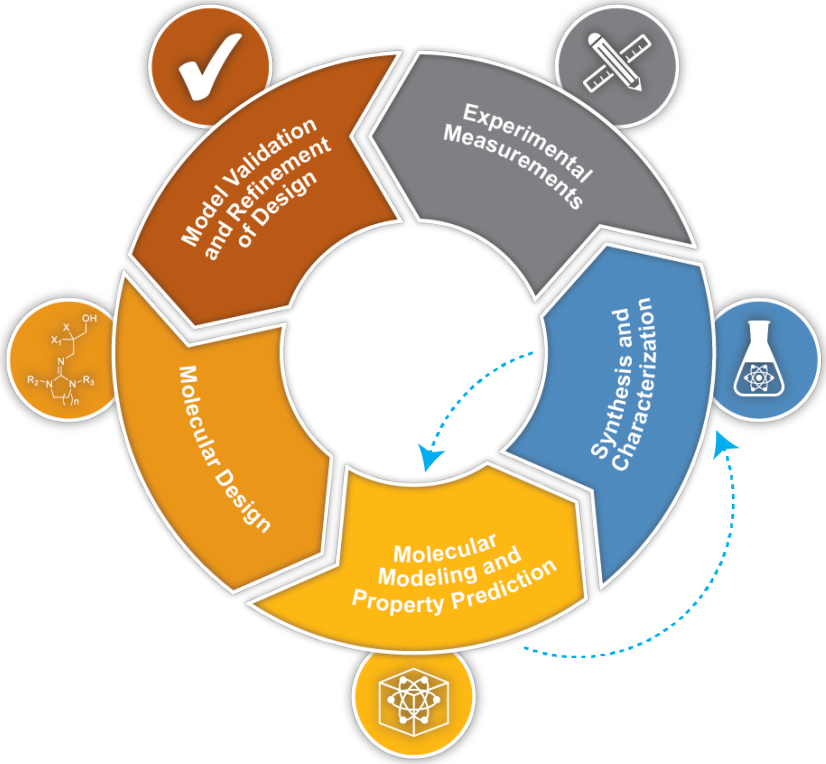
Goal: To continue optimizing molecular structure to reduce viscosity while retaining material performance.



- **Objectives:**
  - Cost target $10/kg
  - Reduce rich viscosity >400 cP
  - Refine viscosity with high P_{int}
  - Refine molecules to promote high acid:base equilibria
- **Milestones: 8, 10.1, 10.2**

(12 months – FY17)

Viscosity Profiles for CO_2BOL Derivatives

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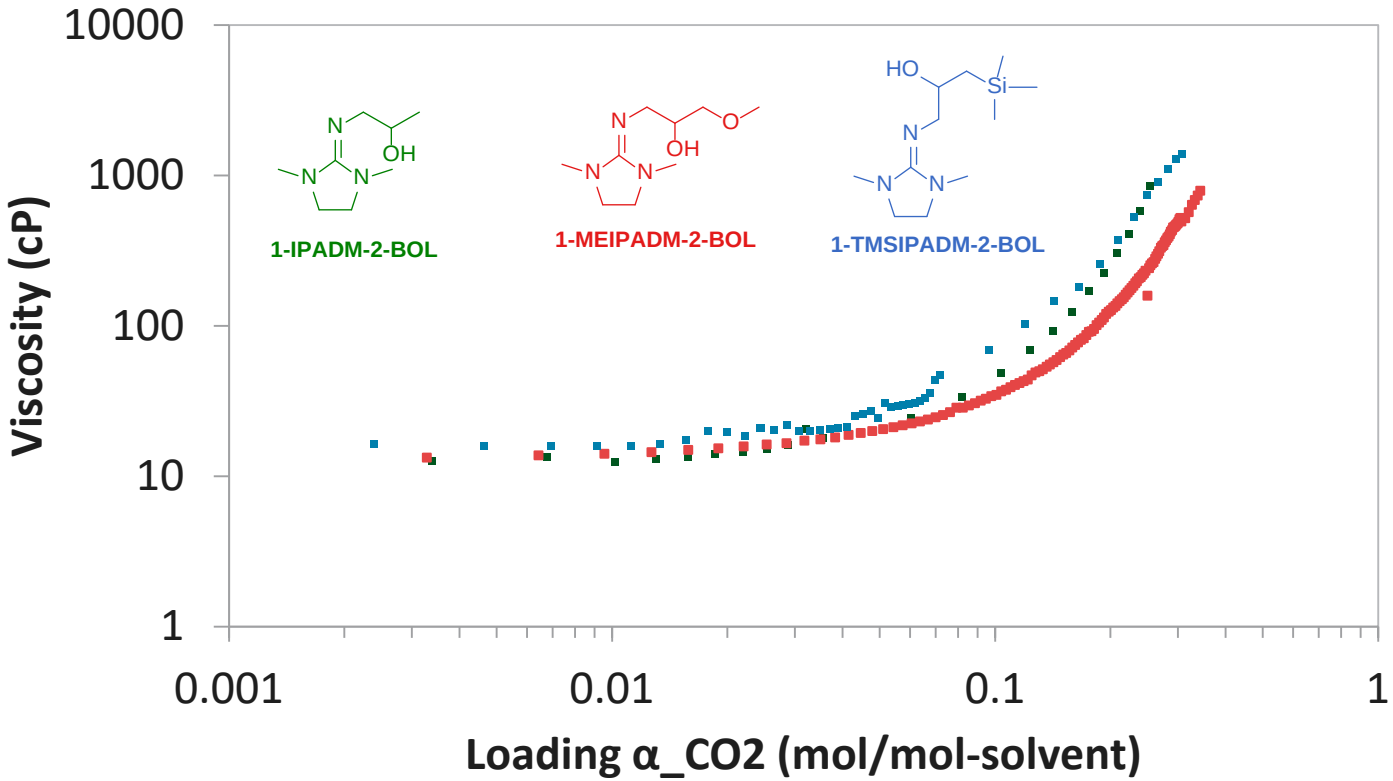
- 13 variants made from each viscosity reducing factor
- Internal H-bond and cation charge solvation (ether) show most promise
- 60% reduction in viscosity for MEIPADM-2-BOL



3,000 cP for IPADM-2-BOL @ 50% CO_2 loading
1,100 cP for MEIPADM-2-BOL @ 50% loading

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3rd Generation CO_2BOL Derivatives

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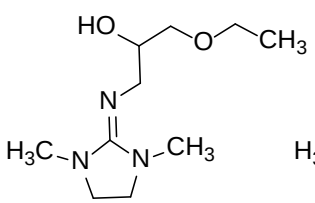
Candidates Identified from reduced model.



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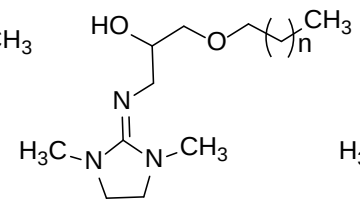
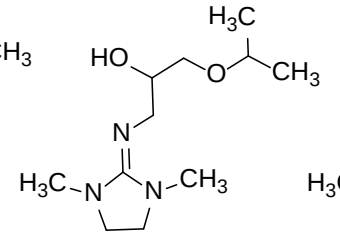


n = 1, 2

94,139



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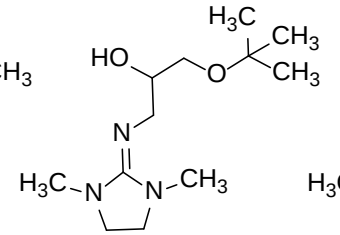

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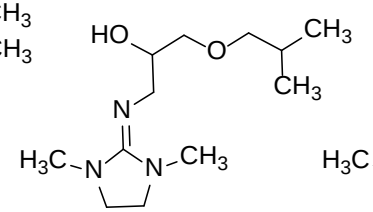

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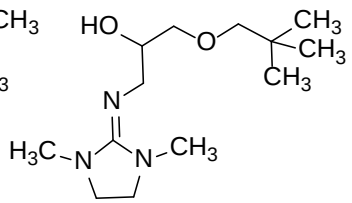

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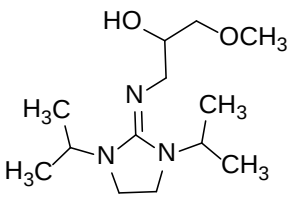

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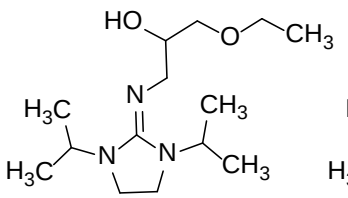

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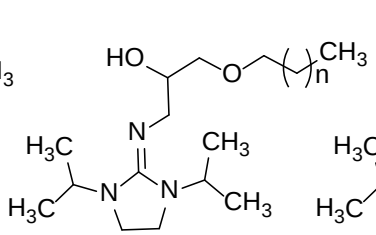

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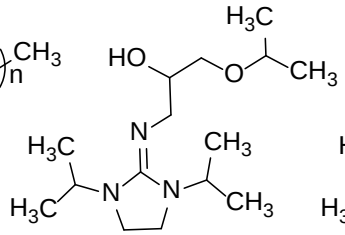
n/a, 14



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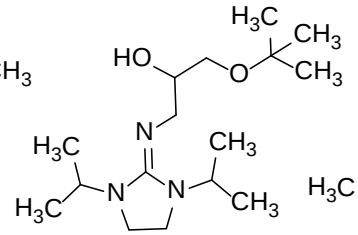

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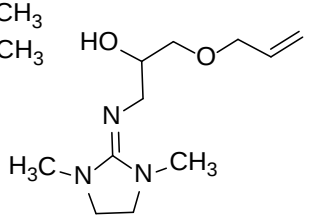
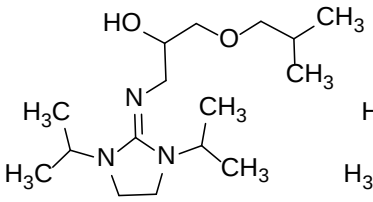


n/a



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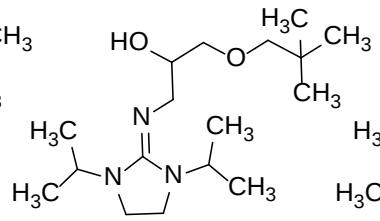
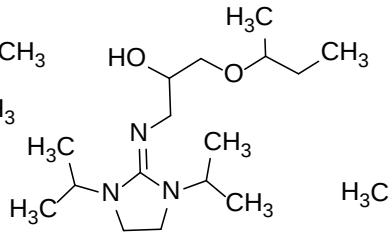


n/a



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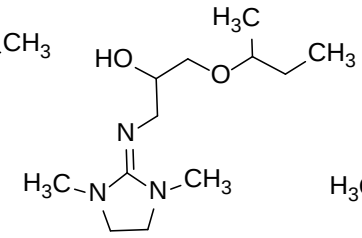

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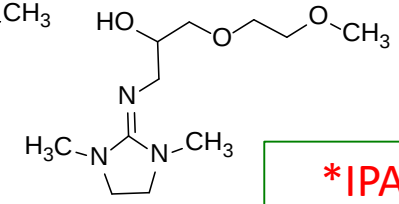

198

*IPADM-2-BOL = 150 cP

High P_{int} Favors Neutral Alkylcarbonic Acid

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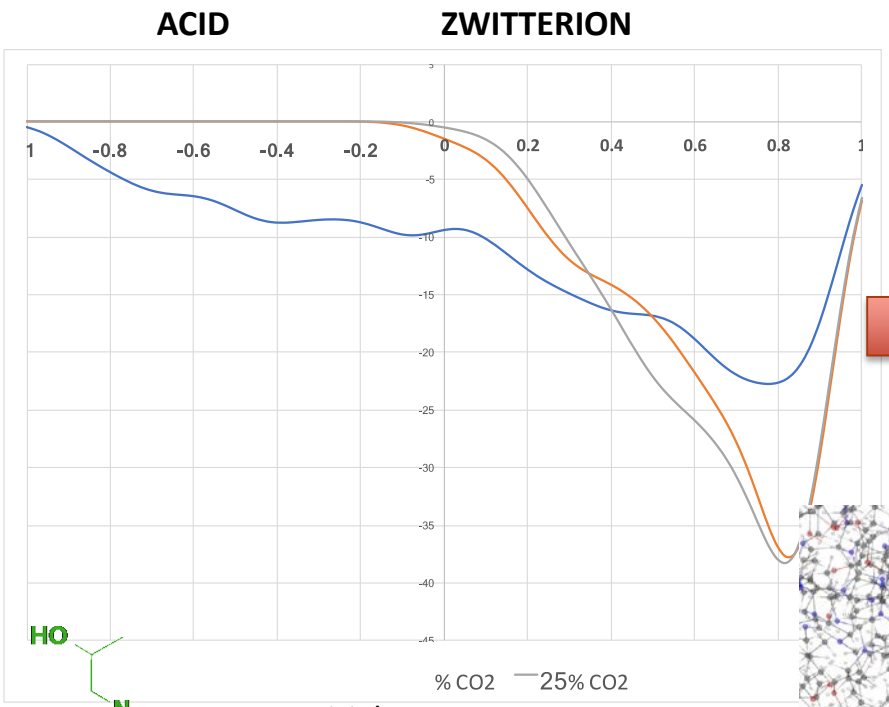
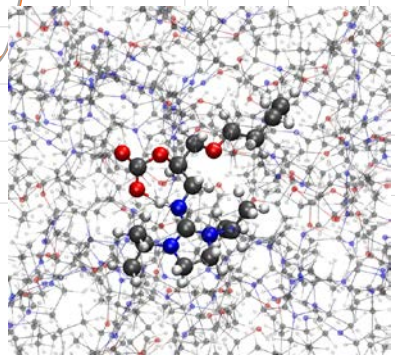
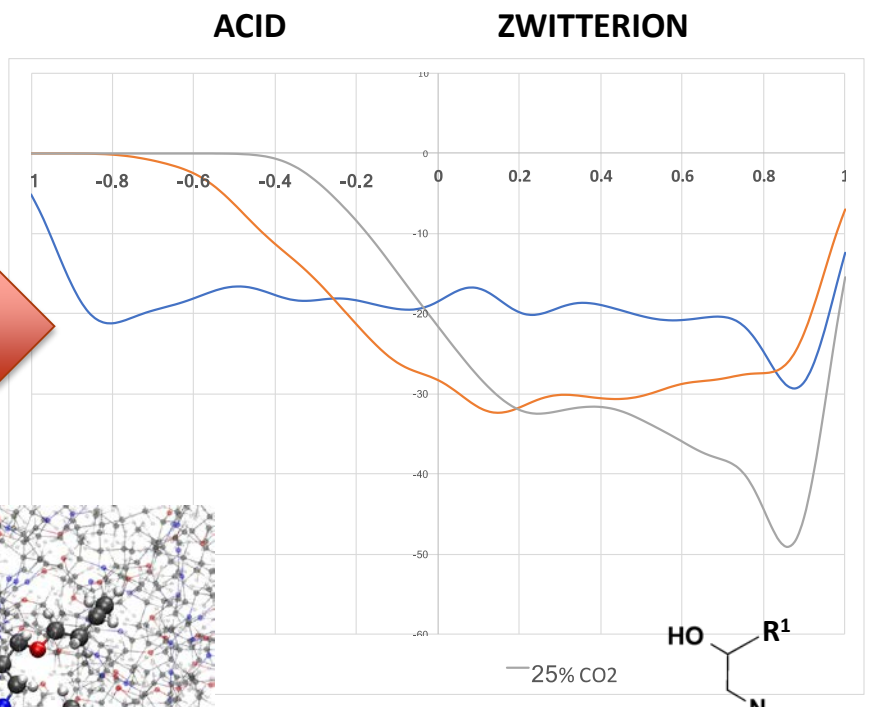
Internal H-bonding begins to favor neutral forms of capture, reducing the concentration of ions in solution.



Initial





After 10 ps

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Predicted Solvent Structure of Final Derivatives

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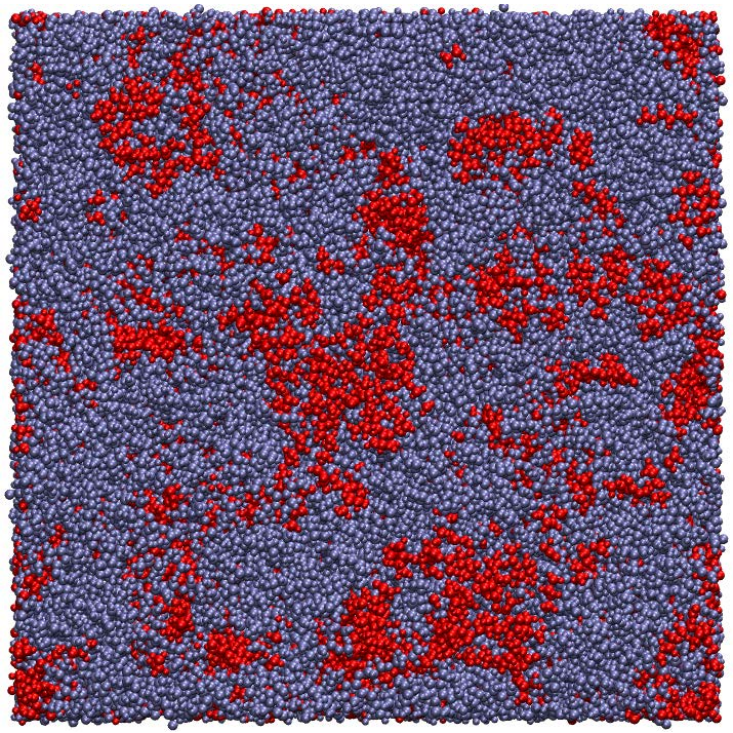
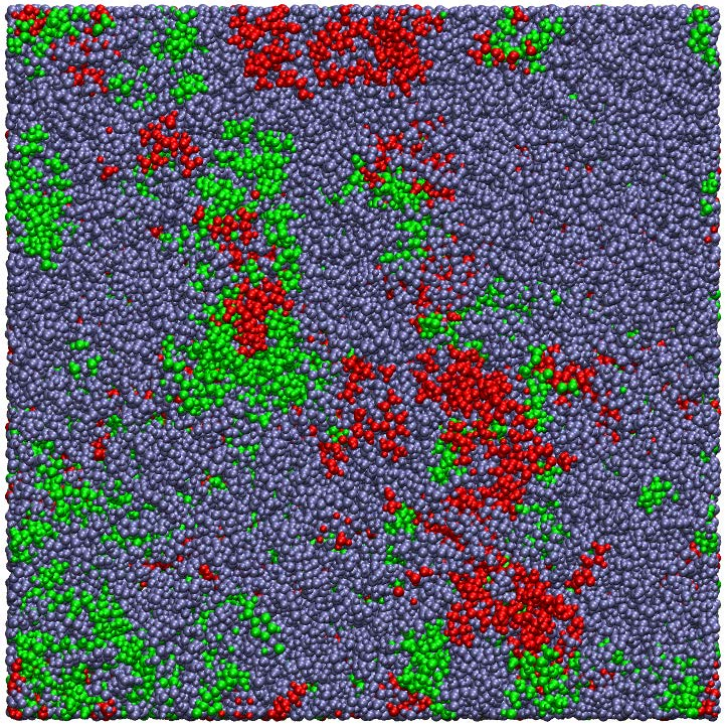
Solvents retain heterogeneous structure with reduced ionicity, still allowing for PSAR.



25% CO_2 loading, all Zwitterion



25% CO_2 loading, 1:1 acid:Zwitterion

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High P_{int} and Neutral Capture Combined

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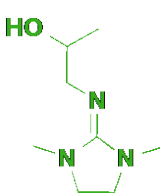
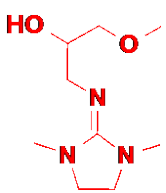
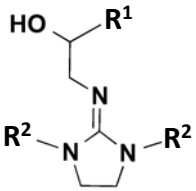
New derivatives are 98% lower in viscosity while retaining all other properties







IPADM-2-BOL @ 40 mol% CO_2
MEIPADM-2-BOL @ 35 mol% CO_2
BEIPADIPA-2-BOL @ 42 mol% CO_2

CO_2BOL Generations

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High P_{int} and Neutral Capture Combined

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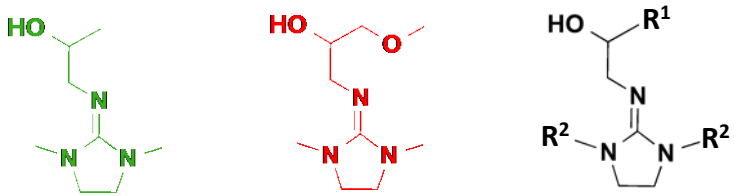
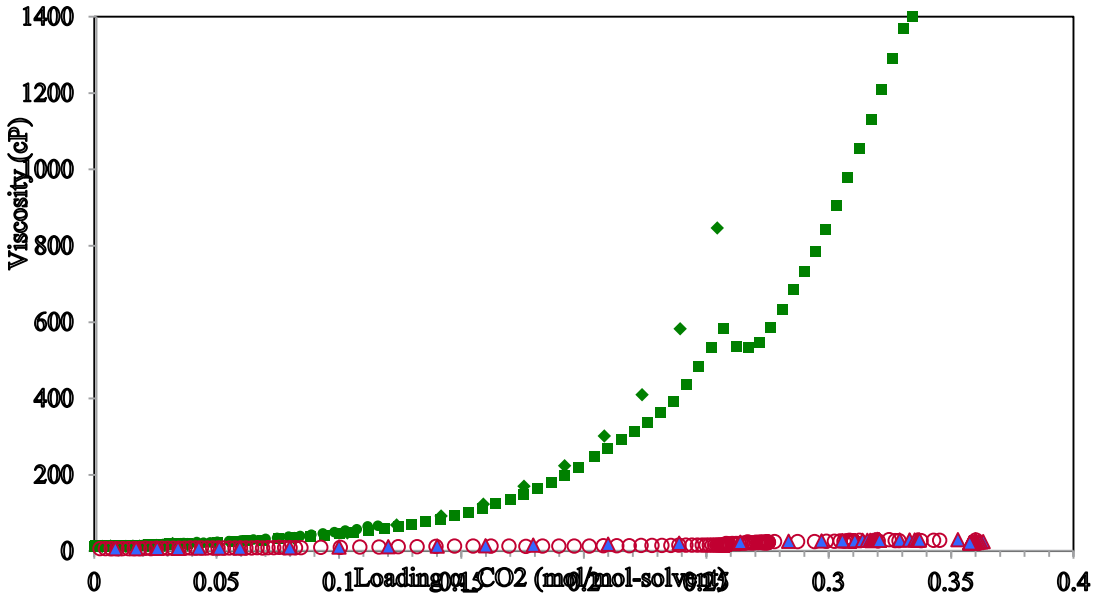
New derivatives are 98% lower in viscosity while retaining all other properties



IPADM-2-BOL @ 40 mol% CO_2
MEIPADM-2-BOL @ 35 mol% CO_2
BEIPADIPA-2-BOL @ 42 mol% CO_2



CO_2BOL Generations

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Research Highlights - Testing

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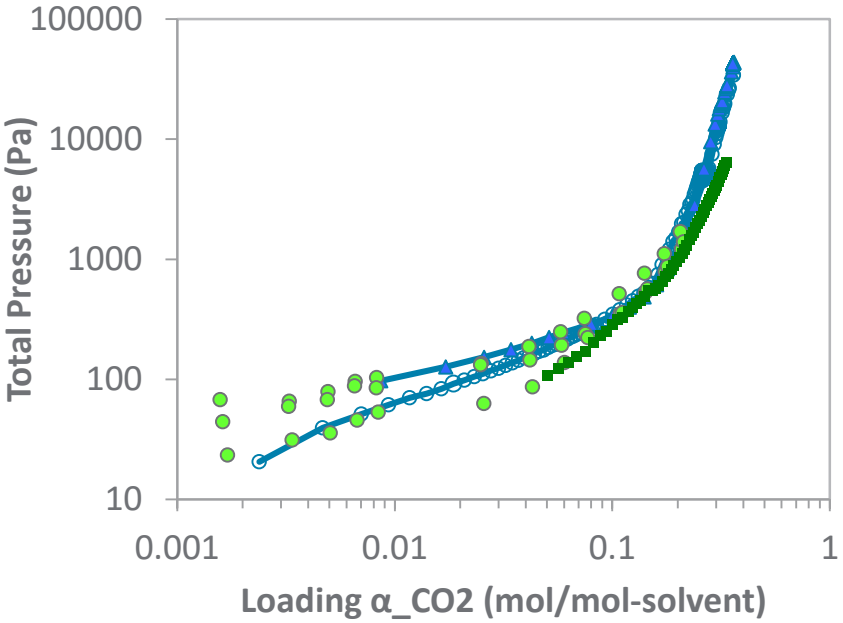
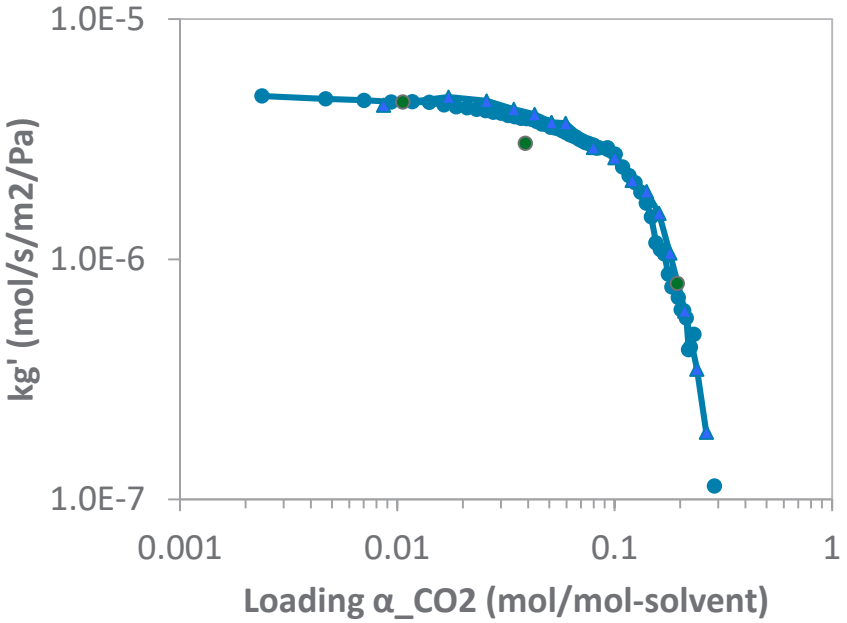
PVT testing shows physical and thermodynamic properties are retained.





- Comparable P* at 40 ˚C to IPADM-2-BOL at 40 ˚C
- Comparable mass transfer of CO_2 (*kg'*) to IPADM-2-BOL at 40 ˚C

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Synthesis of Optimal CO_2BOL Derivatives

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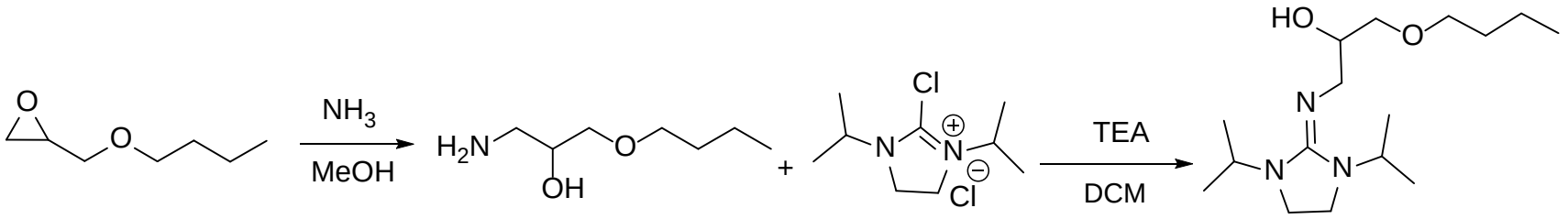
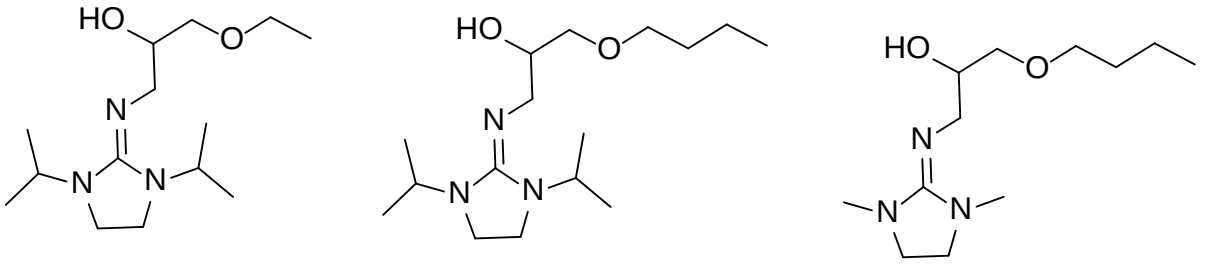
Synthesis of 4 candidate final derivatives identified from reduced model predictions.

Current synthetic route for CO_2BOL derivatives:



1 **2** **3** **1-BEIPADIP-2-BOL**

CO_2 capture capacity of selected substrates:



	1-EEIPADIP-2-BOL	**1-BEIPADIP-2-BOL**	**1-BEIPADM-2-BOL**
CO_2 uptake capacity:	4.45 wt%	6.5 wt%	8.2 wt%

Carbodiimide Route-Alternative Synthesis

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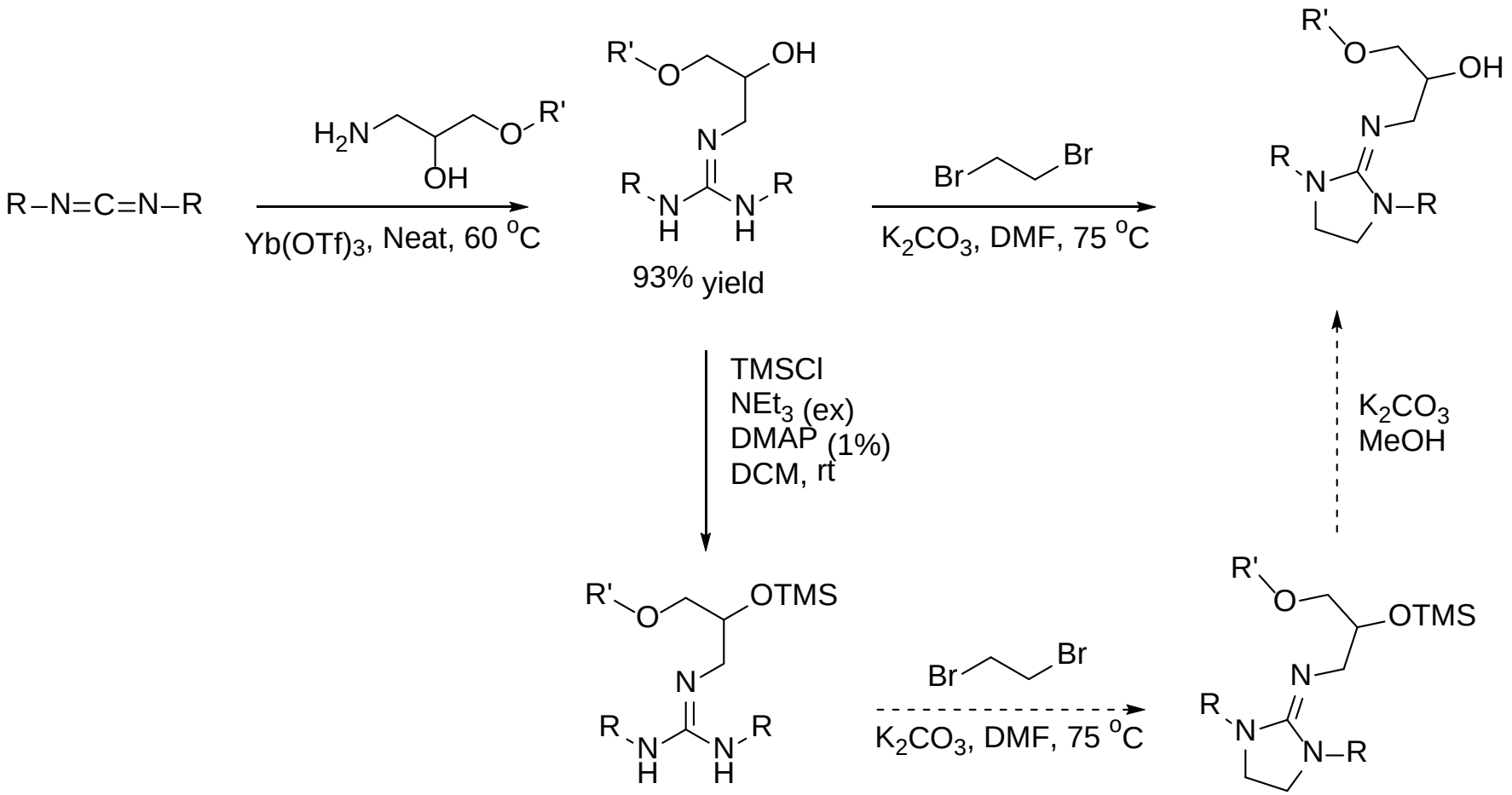
Projected to meet $10/kg cost target in Milestone 8.



CO_2BOL Solvent Class

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Conclusions:

- Viscosity increases have been removed
- Other material properties retained
- Suggested spawn-off into DOCCSS with collaborative efforts with Fluor and CCSI2 and LLNL

Project Team & Acknowledgements

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Dr. Phillip Koech

Dr. Vanda Glezakou
Dr. Roger Rousseau

Dr. Feng Zheng

Solvent Design
Retrosynthetic-analysis
Synthesis & Scaleup

Computational Modeling
Physical property projections

Materials Testing & Analysis

Process Modeling
Performance Projections

Dr. Deepika Malhotra

Dr. David Cantu

Greg Whyatt
Charles Freeman

Andy Zwoster

Mark Bearden

FLUOR®

Dr. Paul M. Mathias
Dr. Satish Reddy

GE Global Research

Dr. Robert Perry
Tiffany Westendorf
Benjamin Wood

Lawrence Livermore National Laboratory

Dr. Josh Stohlaroff,
Dr. John Vericella

EPRI ELECTRIC POWER RESEARCH INSTITUTE

Abhoyjit Bhown