# Hydrogen Storage in Novel Organic Clathrates

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*This presentation does not contain any proprietary or confidential information*

Project ID #
STP53

# Overview

University of Missouri-Columbia

Pacific Northwest National Laboratory

## Timeline

- Project start date: FY05
- Project end date: FY07
- Percent complete: New Project

## Budget

- Expected Total Project Funding

Phase I - 1 year

-DOE Share: 347,791

Phase II - 1 year:

-DOE Share: 352,791

- DOE Funding for FY05/07: 700,582

## Barriers

•Weight and volume

•Hydrogen capacity and reversibility

## Targets

Gravimetric capacity: >6%

Volumetric capacity: >0.045 kg $H_2$/L

Min/Max delivery temp: -30/85°C

## Partners

University of Missouri-Columbia; Synthesis, characterization and final project.

Pacific Northwest National Laboratory; Characterization, modeling and final project.

# KEY PERSONNEL

| | | |
|---|---|---|
| Dr. Jerry Atwood | PI | University of Missouri |
| Dr. B. Peter McGrail | Co-PI | PNNL |
| Dr. Liem X. Dang | Co-Inv | PNNL |
| Dr. L. Rene Corrales | Co-Inv | PNNL |

# OBJECTIVES

- To develop and demonstrate hydrogen storage in and release from clathrates and related organic compounds

- Synthesize organic compounds which contain void space in the solid state structure

- Demonstrate absorption and retention of hydrogen in such solid state compounds under mild conditions

- Use principles of crystal engineering to modify crystal structures so as to meet or exceed the DOE storage goals

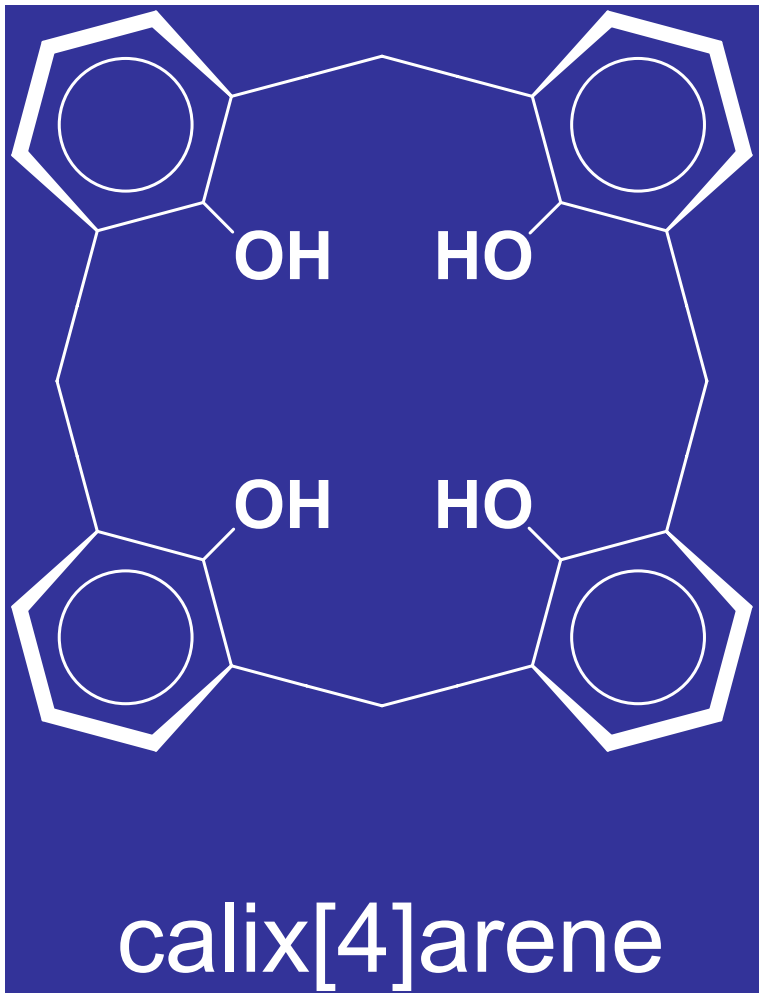
# Advantages and Benefits

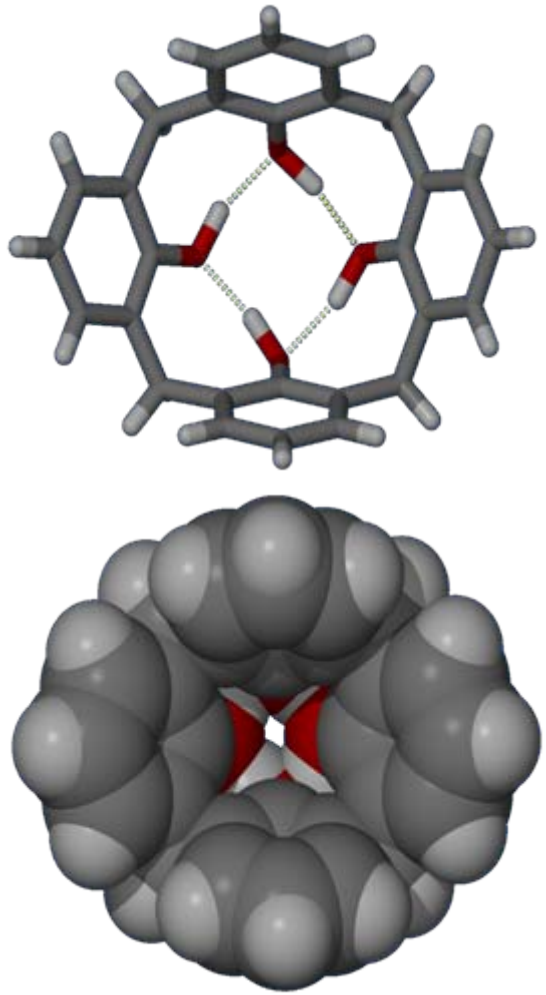
| Feature of Technical Concept | Benefit |
|---|---|
| No ionic or covalent bond breaking or chemical reaction products | Storage and release cycling without degradation of the host or loss of efficiency |
| Gas release with small temperature change | Low energy requirements for hydrogen release |
| High-pressure tank not required for storage | Lower vehicle weight and improved safety |

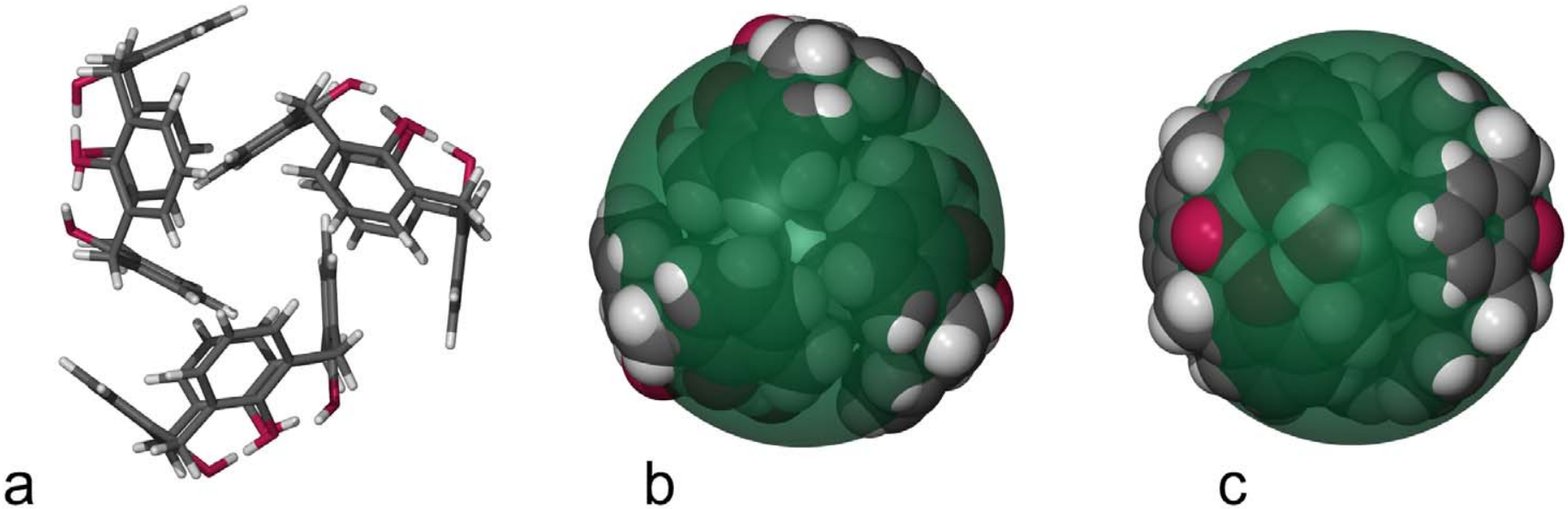
# Solving Technical Problems and Mitigation Risks

| Risk | Mitigation |
| --- | --- |
| Clathrate absorbs $H_2$ only at a low percentage | Chemical modification of clathrate |
| Clathrate still absorbs $H_2$ only at a low percentage | Synthesize a new type of clathrate |
| Key X-ray structure cannot be obtained | Perform X-ray structure of related compound and use X-ray powder data to assure key structure |

# *Calix[4]arene is useful for gas, hydrogen sorption work*

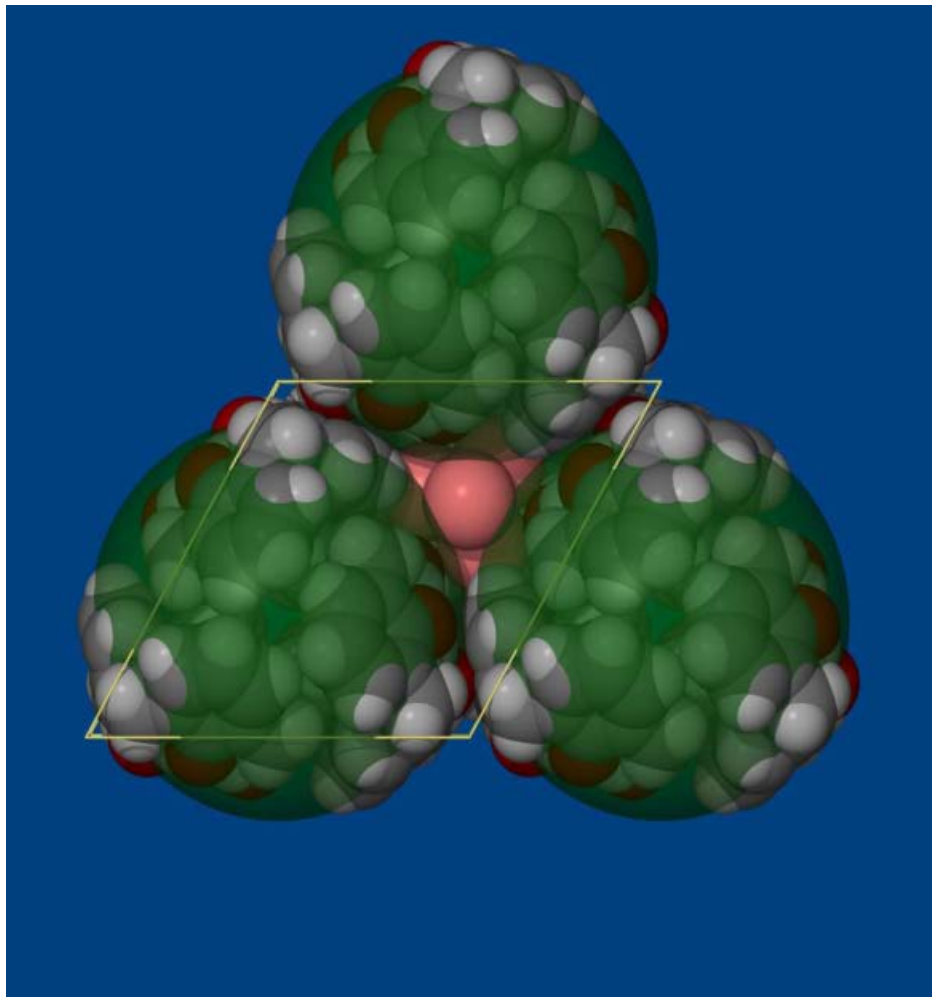


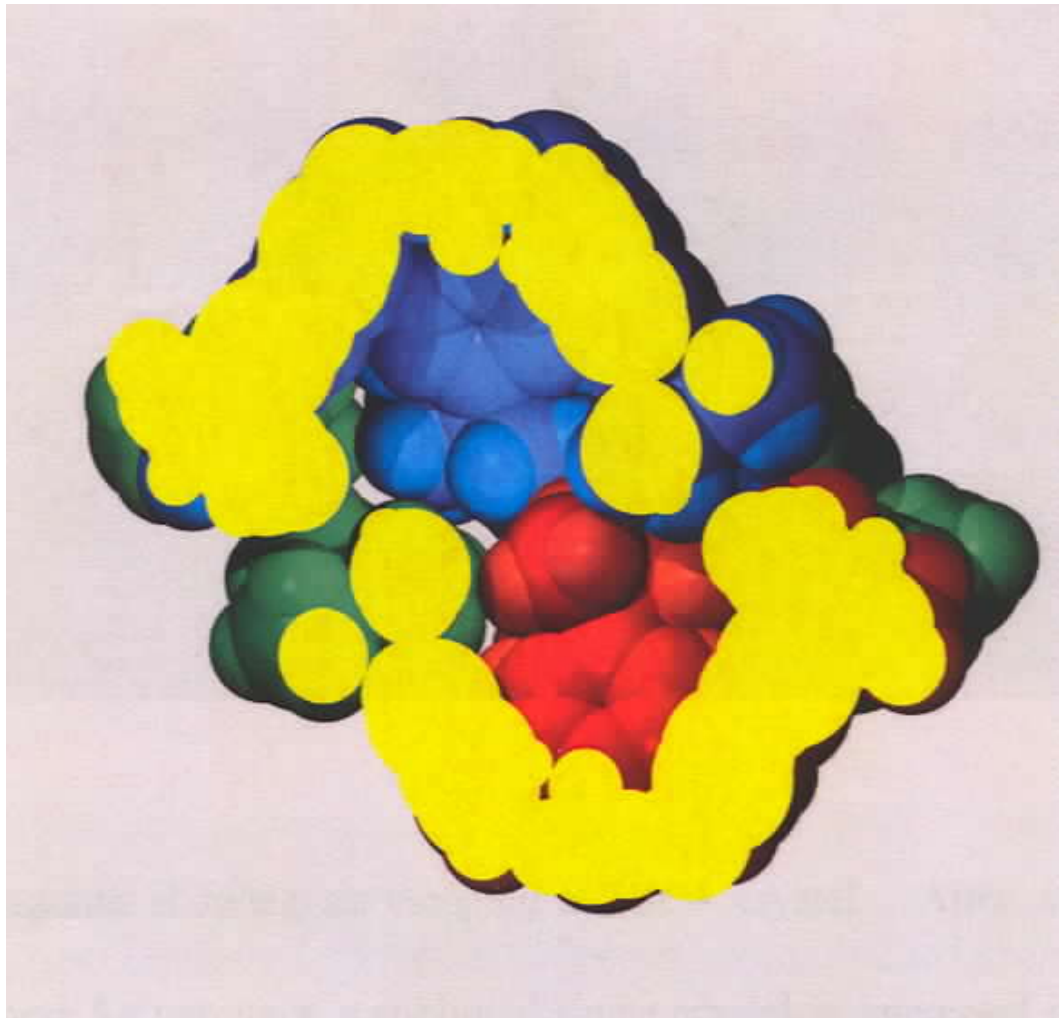



*Trimer of calix[4]arenes forms spherical assembly held together by non-covalent bonds.*

*Hexagonal close-packed arrangement of spheres creates lattice with void space for housing hydrogen molecules.*

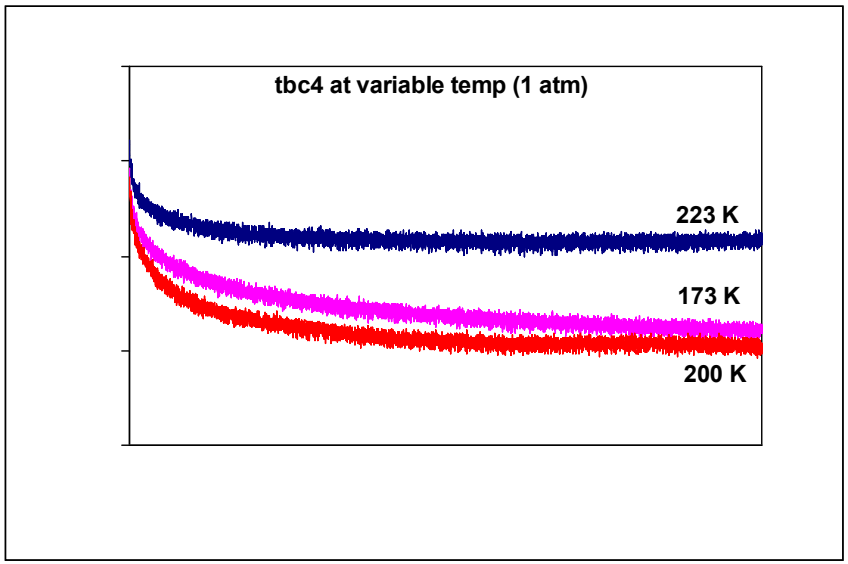


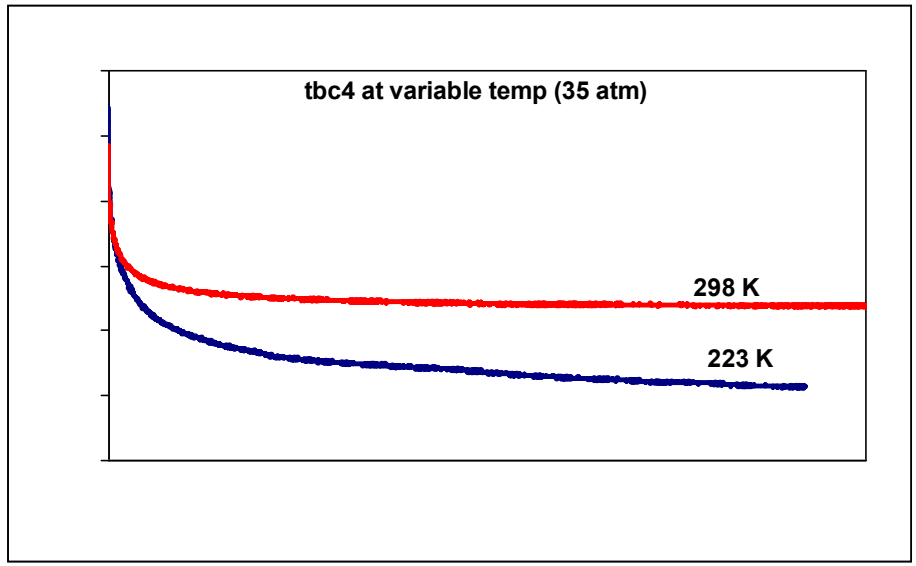
*Section of crystal structure of (tbc4) p-tert-butyl-calix[4]arene displaying enclosed cavity.*



# $H_2$ Sorption by Non-Porous Crystals

*Proof of concept: ca. 0.5% $H_2$ by wt*

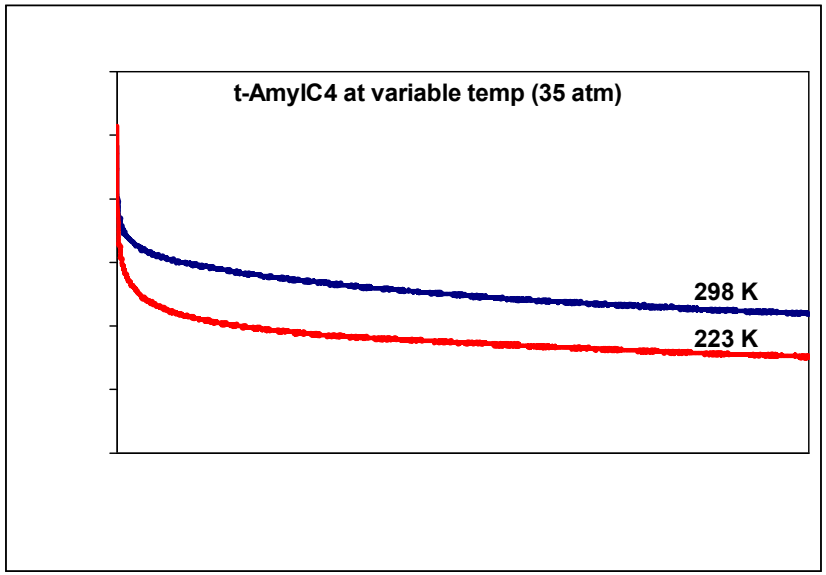


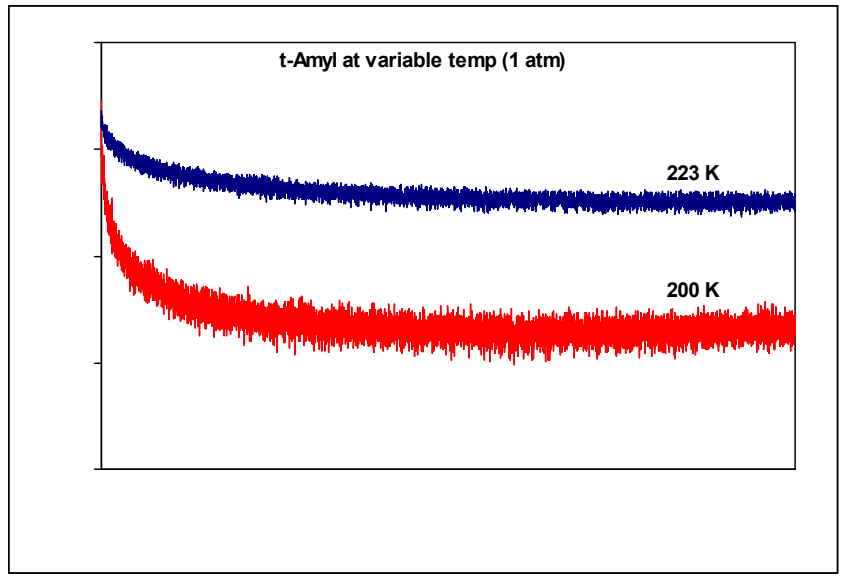




***HYDROGEN SORPTION DATA, preliminary***

# $H_2$ Sorption by Non-Porous Crystals



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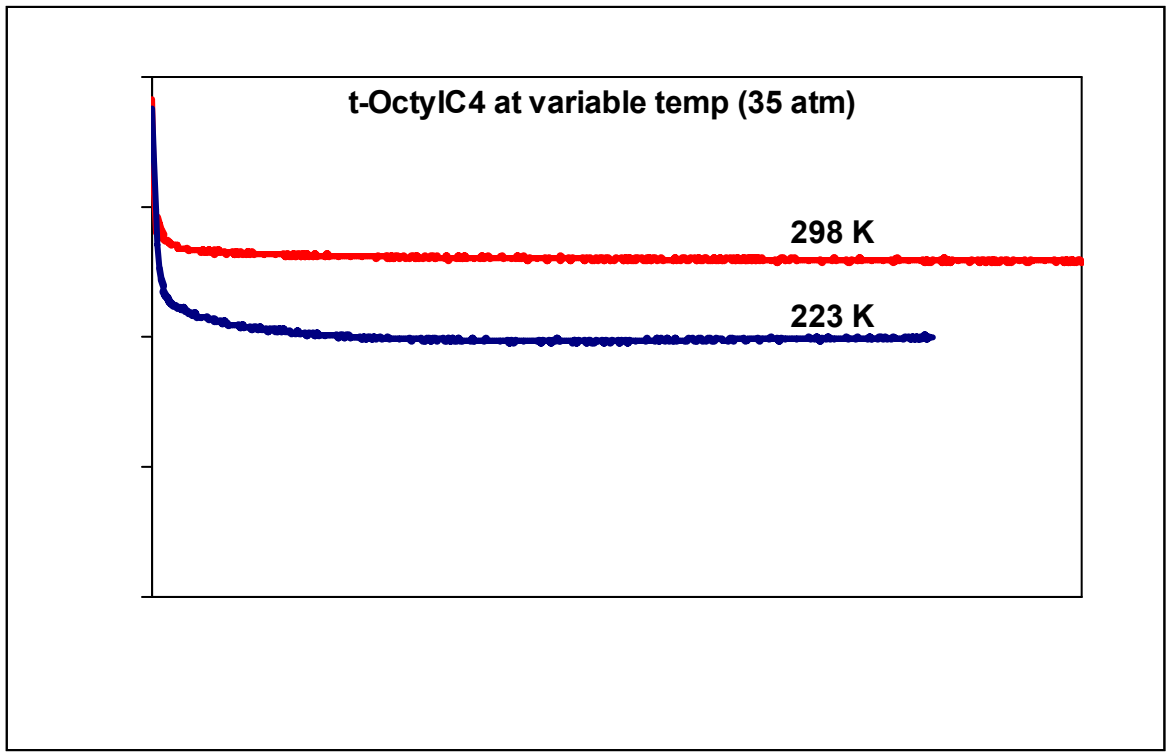


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# Summary of Program Plans

University of Missouri-Columbia

Pacific Northwest National Laboratory