Hydrogen Storage in Novel Organic Clathrates

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This presentation does not contain any proprietary or confidential information

Project ID #
STP53

Overview

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

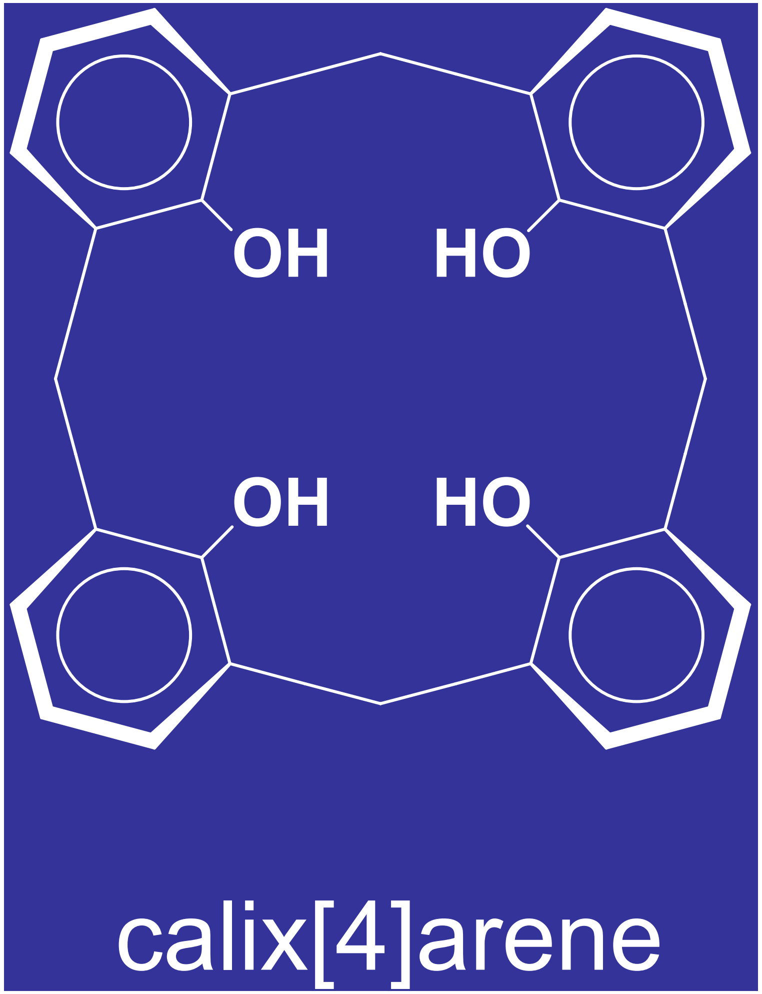
Advantages and Benefits

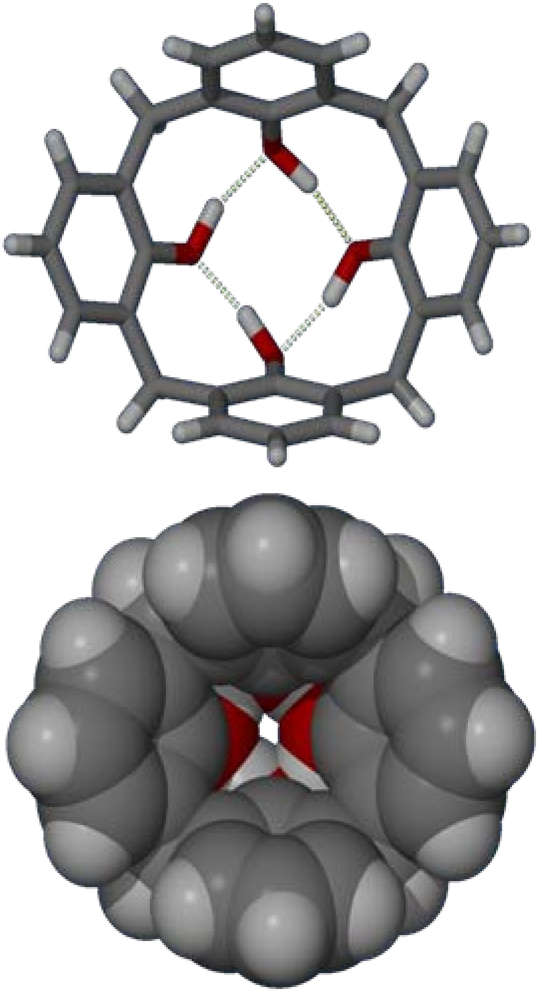
Feature of Technical Concept	Benefit
No ionic or covalent bond breaking or chemical reaction products	Storage and release cycling without degradation of the host or loss of efficiency
Gas release with small temperature change	Low energy requirements for hydrogen release
High-pressure tank not required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

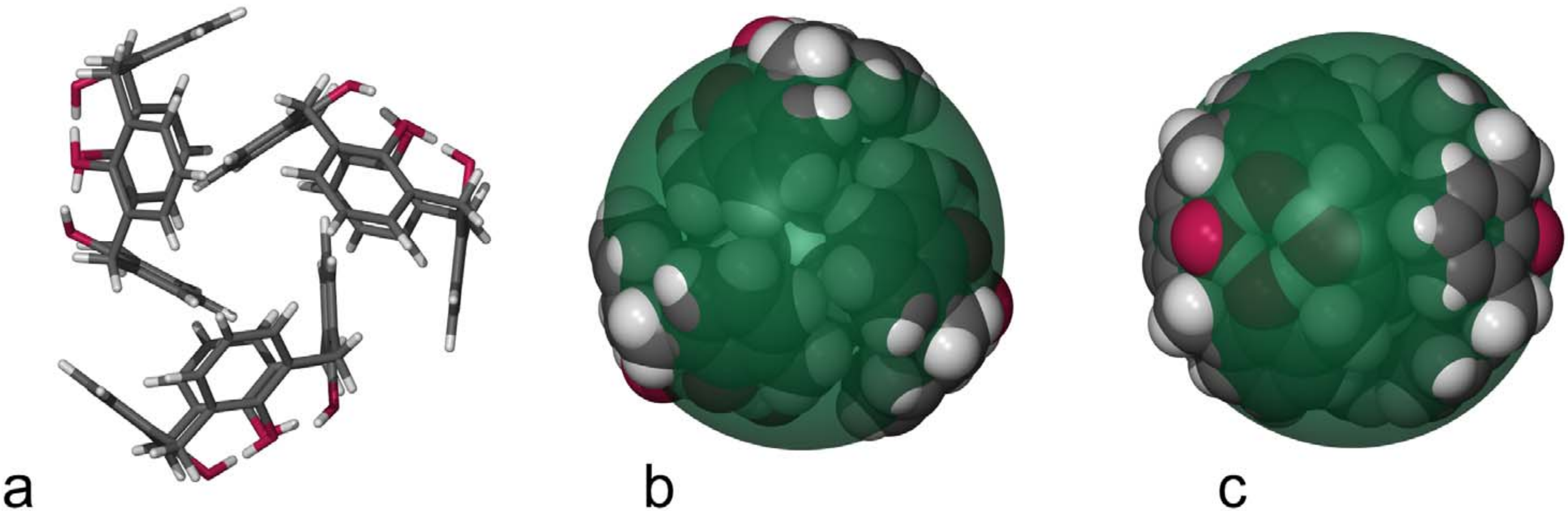
Solving Technical Problems and Mitigation Risks

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

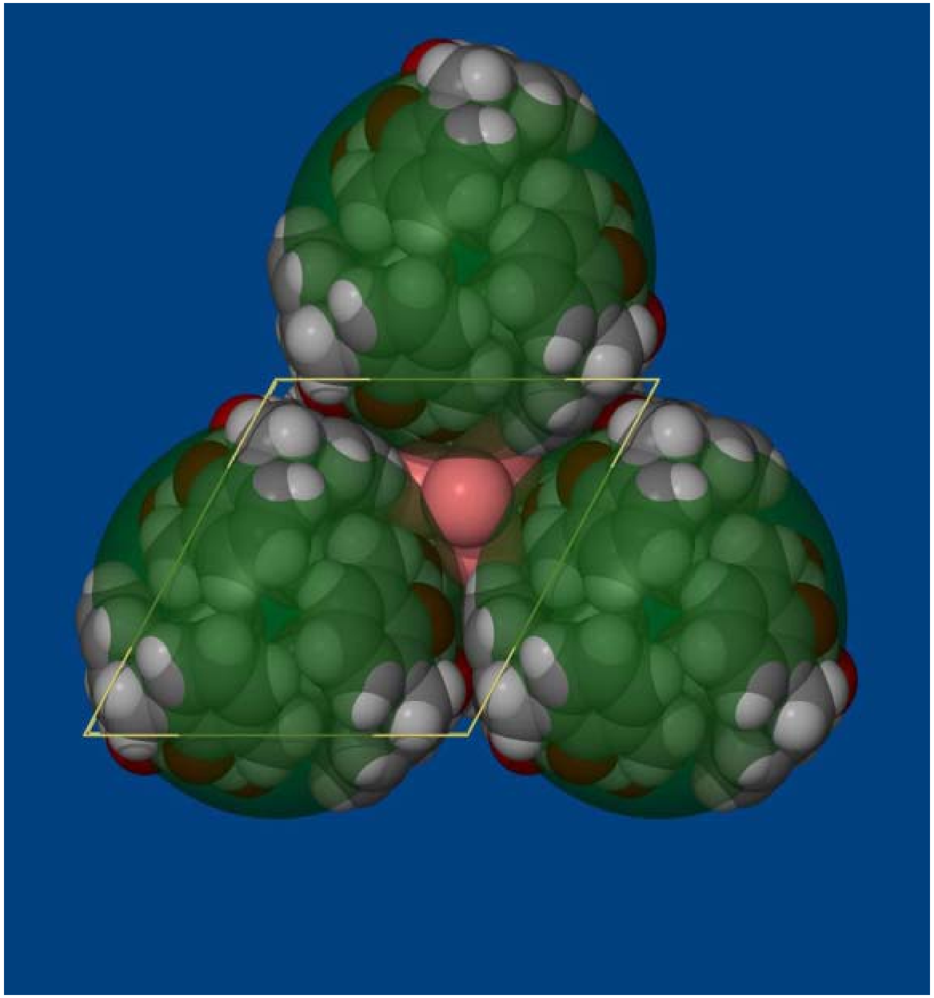




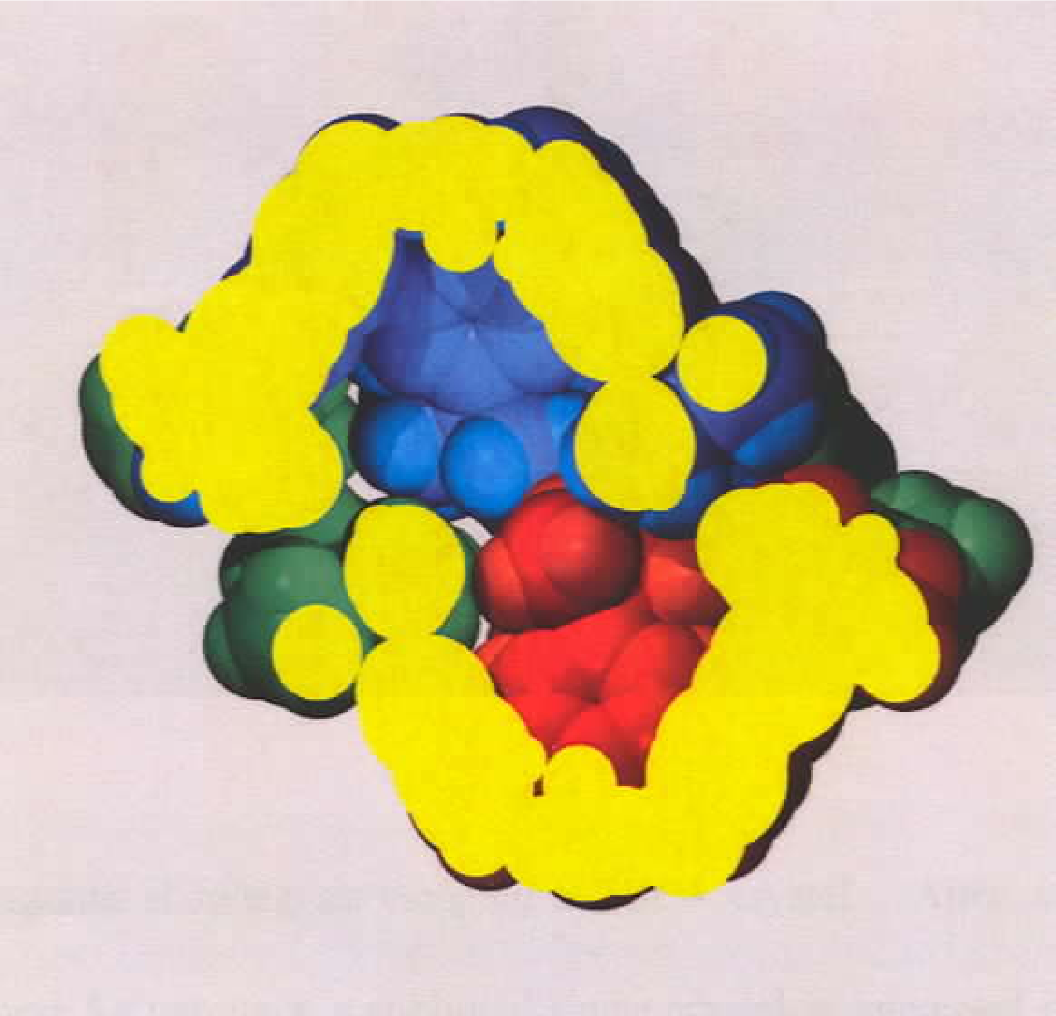


Trimer of calix[4]arenes forms spherical assembly held together by non-covalent bonds.

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

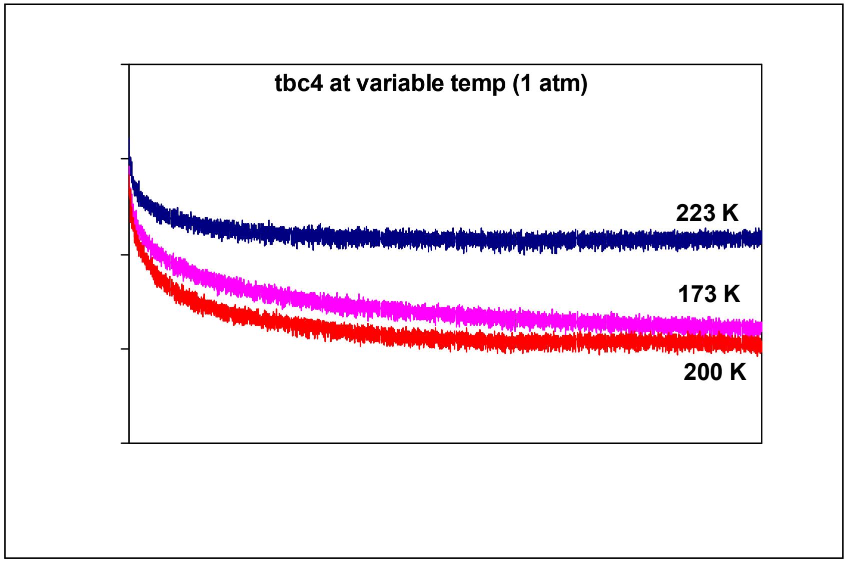


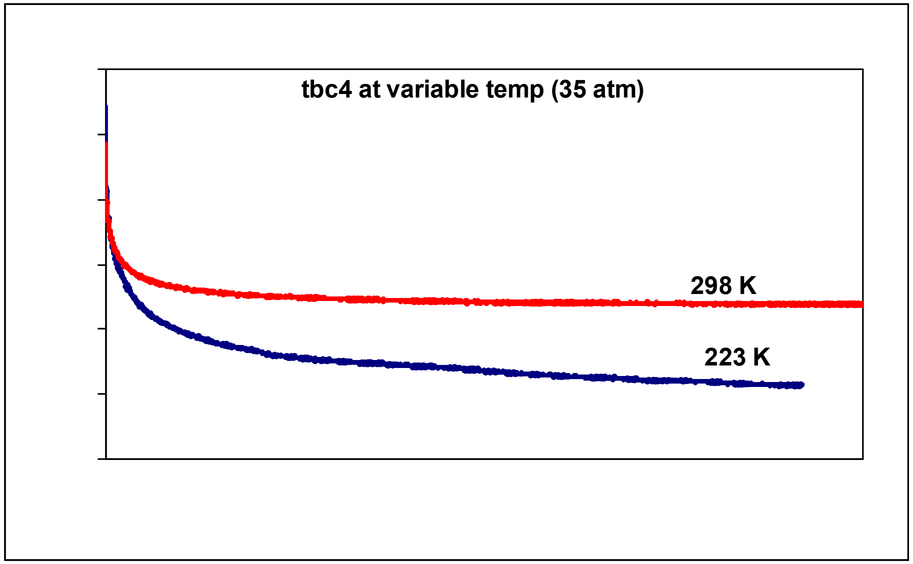
Section of crystal structure of (tbc4) p-tert-butyl-calix[4]arene displaying enclosed cavity.



H_2 Sorption by Non-Porous Crystals

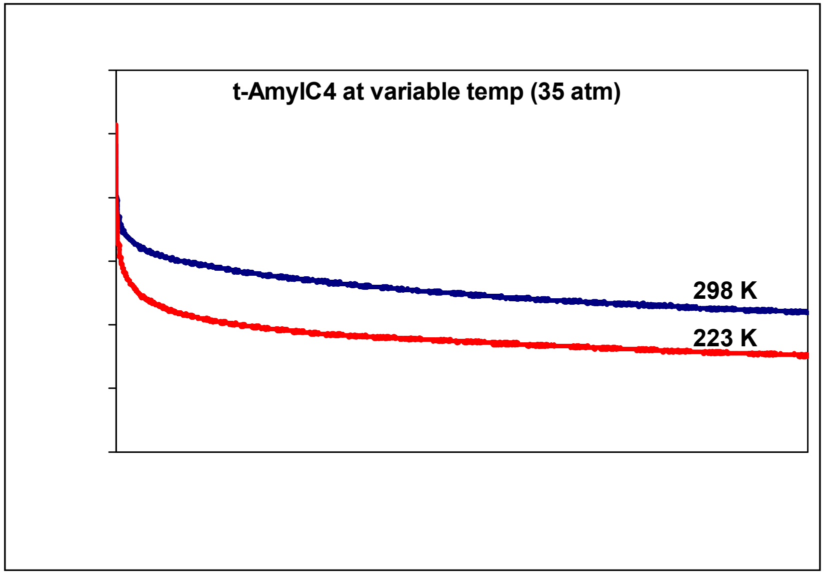
Proof of concept: ca. 0.5% H_2 by wt

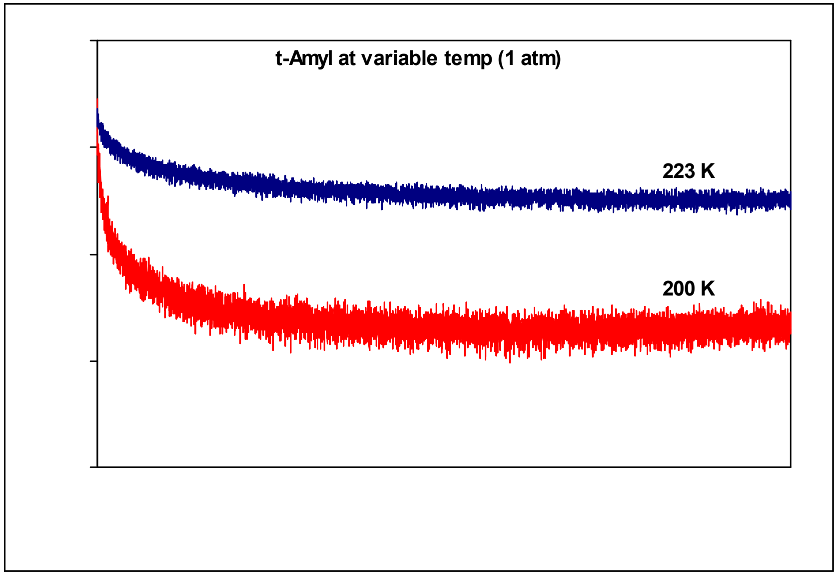




HYDROGEN SORPTION DATA,
preliminary

H_2 Sorption by Non-Porous Crystals





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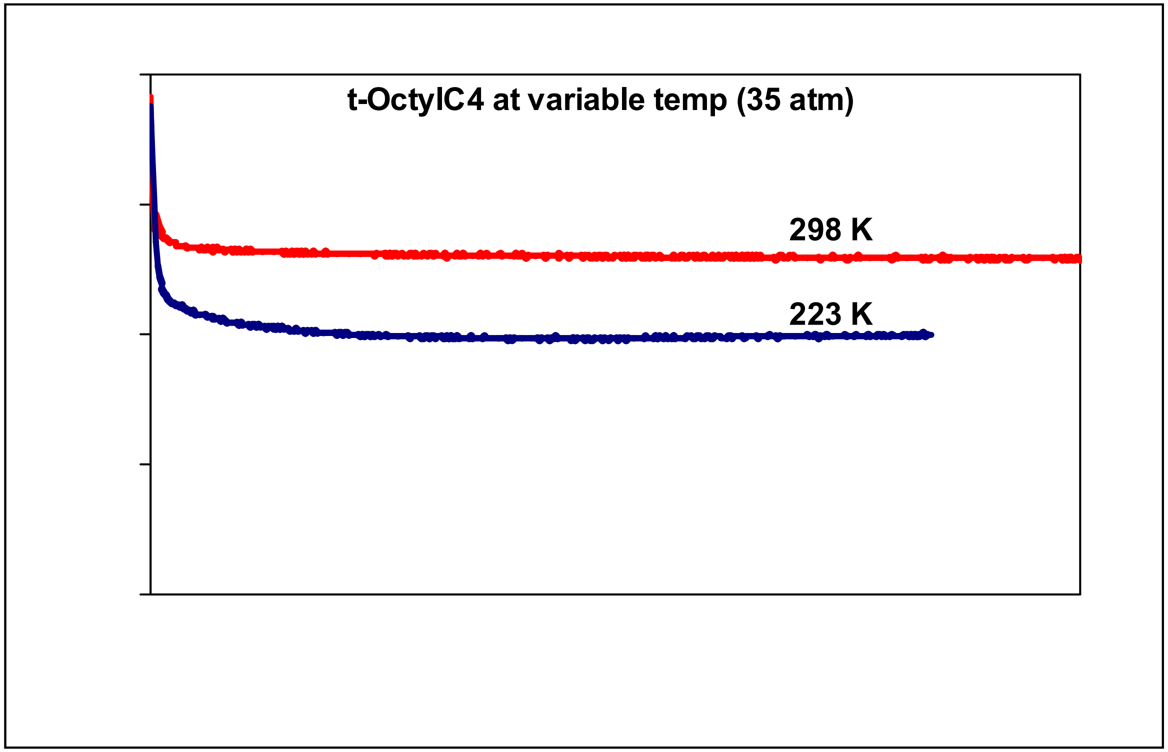

HYDROGEN SORPTION DATA, preliminary

University of Missouri-Columbia

Pacific Northwest National Laboratory

Summary of Program Plans