Hydrogen Storage in Molecular Compounds

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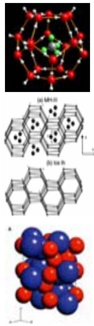
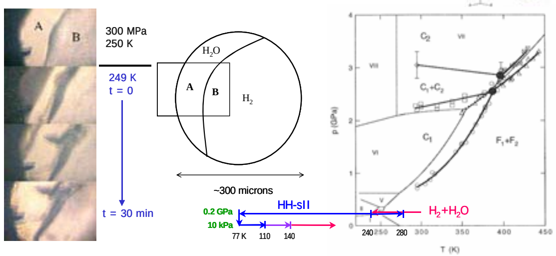
Molecular Compounds

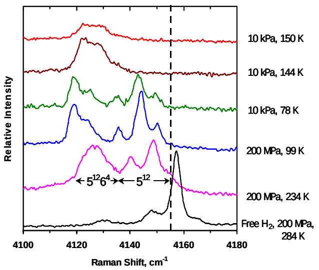
- Clathrates
  - Crystalline structures based on a hydrogen-bonded water framework ('*host*' lattice) with cavities which contain '*guest*' molecules
- Filled Ice
  - Hydrates with structures related to known ice phase
- van der Waals Compounds
  - Stoichiometric crystals of mixtures of atoms and molecules held together by weak van der Waals forces



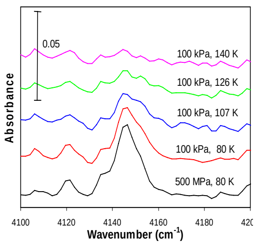
H_2-H_2O System



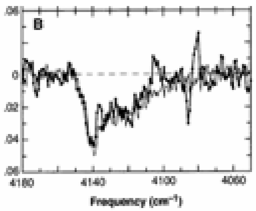
Raman and FTIR Spectroscopy



- HH-sII in small, icy bodies?



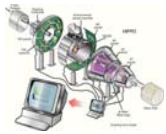
W. Mao *et al*, *Science* 2002

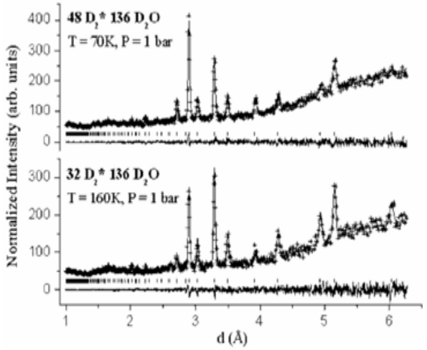


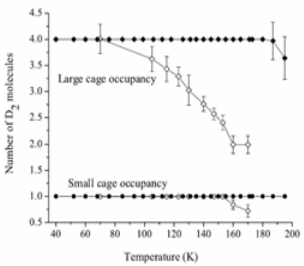
Spectra from WL5, protostar in the ρ Ophiuchus cloud complex
Sandford *et al*, *Science* 1993

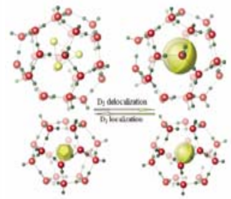
Neutron Study

- Neutrons scatter by interacting with the nucleus of an atom rather than the electron cloud, so, unlike x-rays and electrons, the scattering power (cross-section) of an atom is independent of its atomic number. So:
  - it is easier to sense light atoms, such as hydrogen, in the presence of heavier ones.
  - the nuclear dependence of scattering allows isotopes of an element to have substantially different scattering lengths. Isotopic substitution can be used to label different parts of the sample.
- But, the neutron fluxes are much lower than synchrotron x-ray sources necessitating large samples.
- Neutron interaction with the nucleus of an atom is weak, making them a highly penetrating probe. This feature allows the use of complex sample environments (e.g. Al pressure cells) that would be opaque to x-rays.



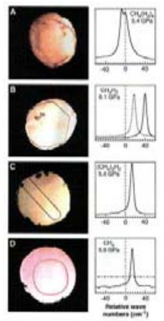


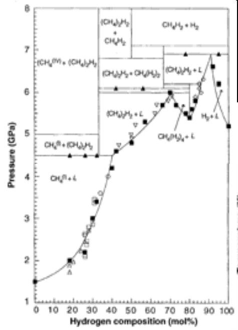


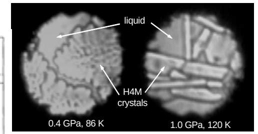


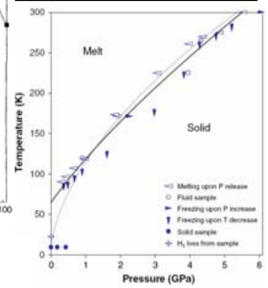
Lokshin *et al*, *PRL* 2004

H_2-CH_4 System









Somayazulu *et al*, *Science* 1996

W. Mao *et al*, *CPL* 2005

Hydrogen Storage

		H_2 wt.%	kWh/kg	kWh/L
HH-sII	$H_2(H_2O)_2$	3.5 - 5.3	1.2 - 1.8	1.0 - 1.5
HH-C2	$H_2(H_2O)$	11.2	3.7	3.5
HM4	$(H_2)_4(CH_4)$	33.4	11.1	~10
DOE target	2005	4.5	1.5	1.2
DOE target	2010	6	2	1.5
DOE target	2015	9	3	2.7

W. Mao *et al*, *PNAS* 2004

Future Work

- H4M holds the largest amount of hydrogen of any compound. How does it do this? We need to solve its crystal structure and hydrogen dynamics using neutron diffraction
- Can we add other molecules to stabilize the hydrogen clathrate structure while the additional molecules are also a useful fuel? Dual fuels and ternary systems
- Can we use more ionic, hydrogen-bonded molecules (such as ammonia borane) to form clathrate-like cages to hold hydrogen above room temperature?

Acknowledgements

This work has benefited from the use of the Lujan Neutron Scattering Center at LANSCE, which is funded by the Department of Energy's Office of Basic Energy Sciences. Los Alamos National Laboratory is operated by the University of California under DOE Contract W-7405-ENG-36."