Hydrogen Storage in Molecular Compounds

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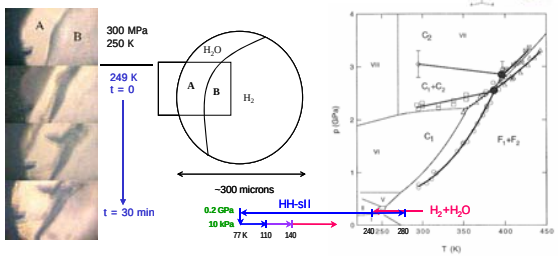
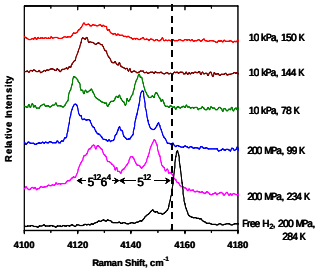
Molecular Compounds

- 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

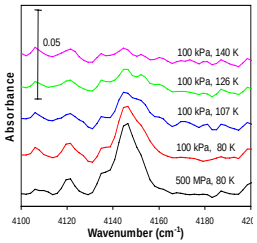
H_2-H_2O System



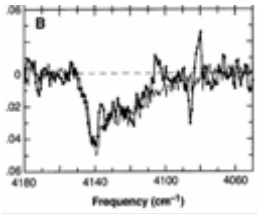
Raman and FTIR Spectroscopy



• HH-sII in small, icy bodies?



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

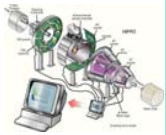


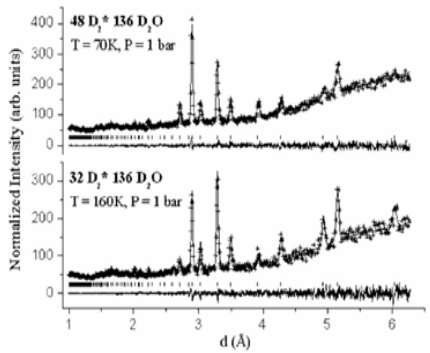
Spectra from WL5, protostar in the ρ Ophiuchus cloud complex

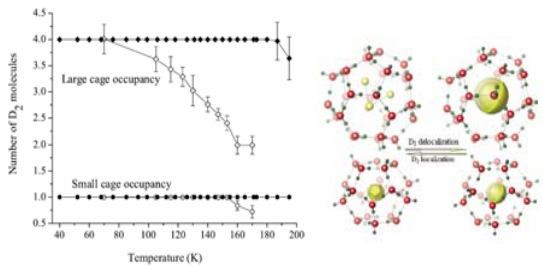
Sandford *et al*, *Science* 1993

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.

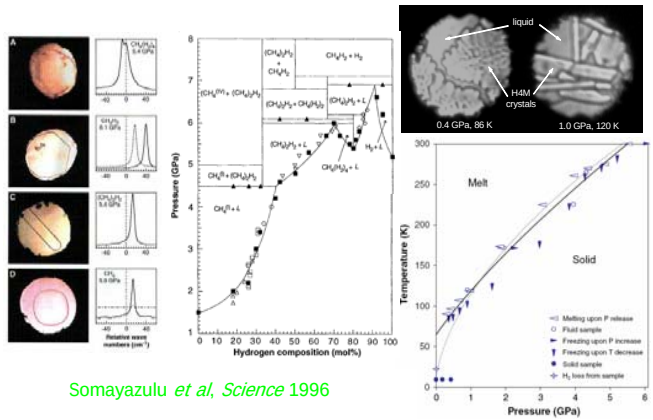






Lokshin *et al*, *PRL* 2004

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

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