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POSITRONS, QUANTUM CRYSTALS, AND NANOPARTICLES (OH MY!) – QUANTUM MECHANICS IN ACTION AT THE USAF (BRIEFING CHARTS)

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BRIEFING CHARTS

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Positrons, Quantum Crystals, and Nanoparticles (Oh My!) - Quantum Mechanics in action at the USAF

C. Michael Lindsay
Energetic Materials Branch
Air Force Research Laboratory

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Predicting Future Technologies

- “Nothing is less predictable than the development of an active scientific field.”
- Charles Francis Richter (1980)
- “Trying to predict the future is like trying to drive down a country road at night with no lights while looking out the back window.”
- Peter Drucker





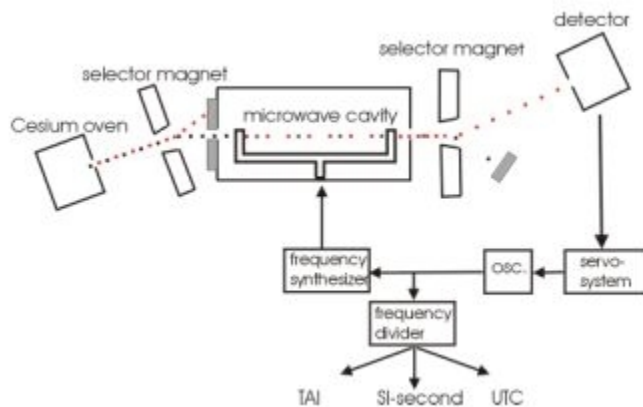
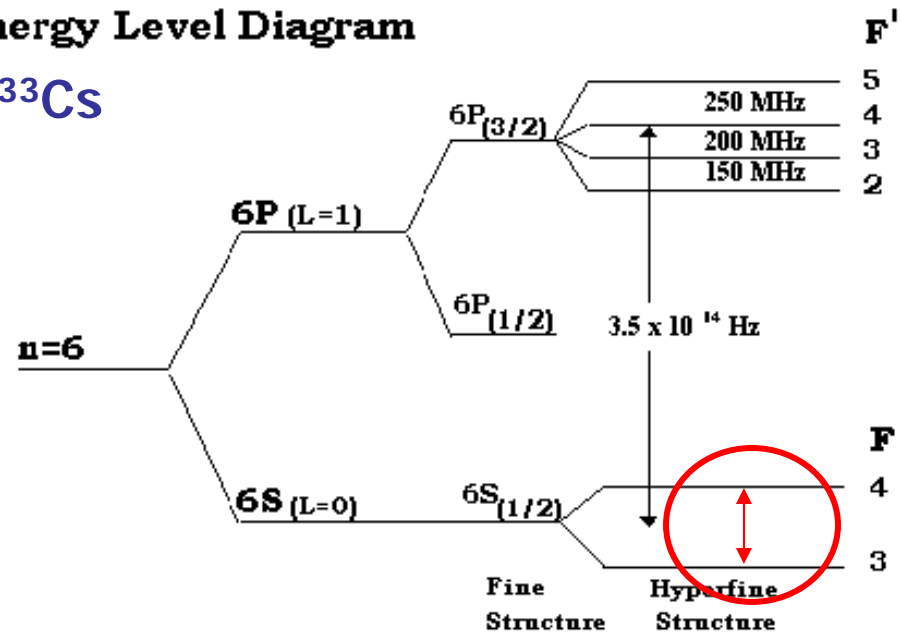
Case 1: Quantum Mechanics of Atoms (1937)



Isidor Isaac Rabi

Energy Level Diagram

^{133}Cs



The first method for accurately measuring hyperfine frequencies by molecular beam resonance was developed by I.I. Rabi and his associates in 1937 at Columbia University

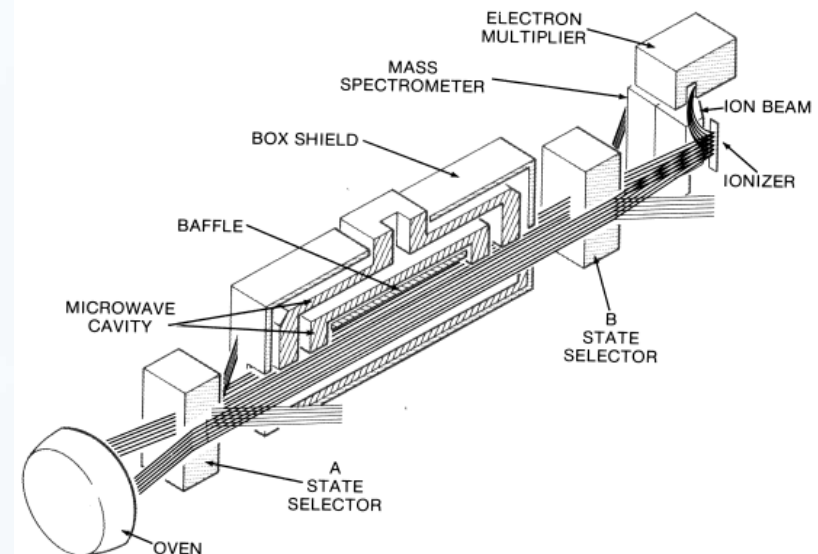
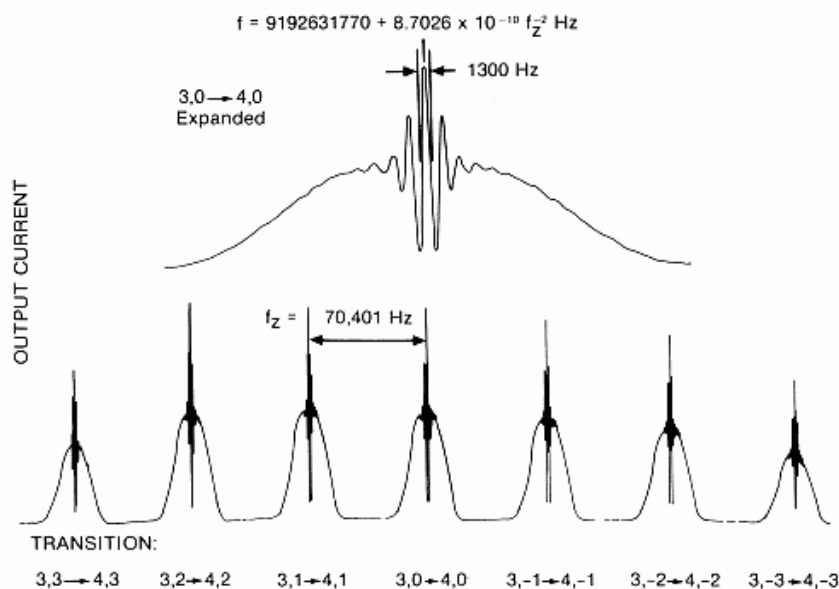
Phys. Rev. 55, 1176 - 1181 (1939)





Hyperfine structure of Cesium-133

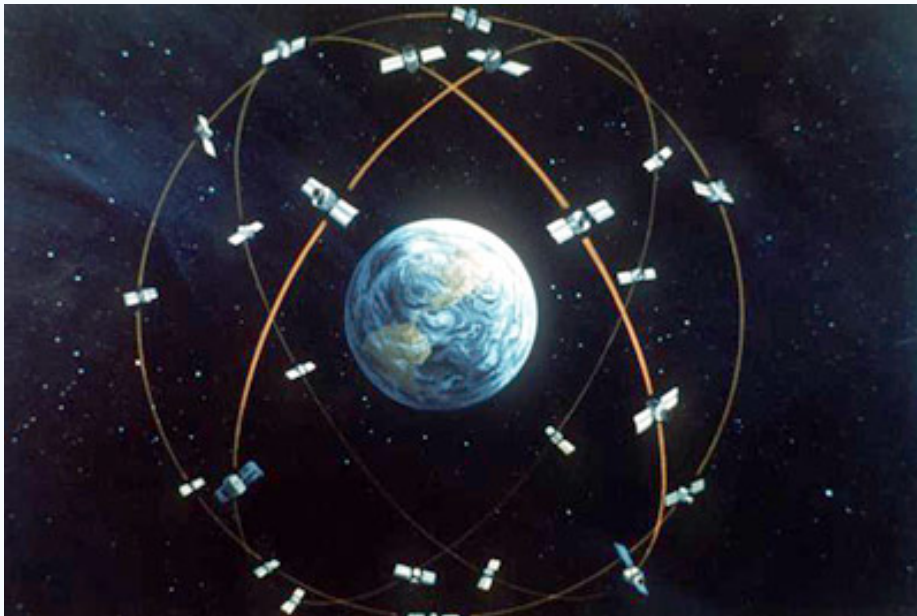
- 9.192 631 770 GHz (Cs-133 Hyperfine Beat)



Precision of ~ 1 part in 10^{12} !



Enabling Technology - GPS!



- 20,000 km - 300,000 km per second
- Four satellites required to pinpoint 3-D location
- Each of the 24 GPS satellites holds four atomic clocks, which every day get an accurate time transfusion from the Air Force, which "borrows" time from the United States Naval Observatory.
- Requires 1 part in 10^{12} temporal precision in order to predict position within 1 meter

(I. I. Rabi won the Nobel Prize in Physics 1944

N.F. Ramsey won the Nobel Prize in Physics 1989)



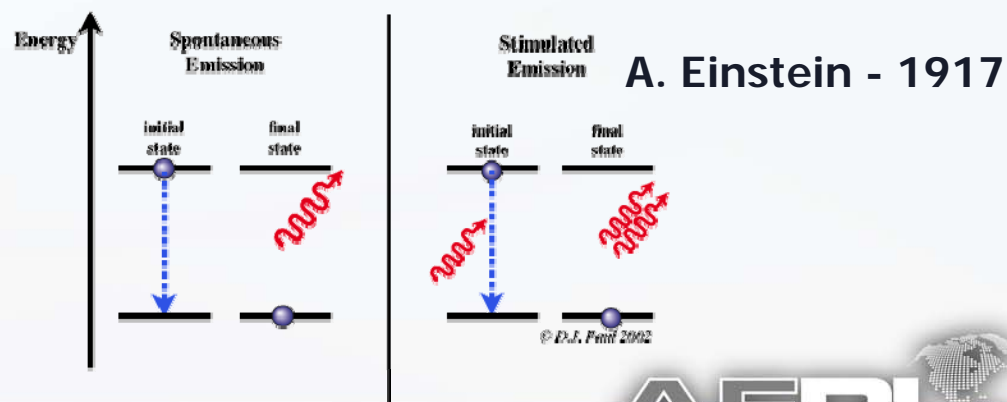
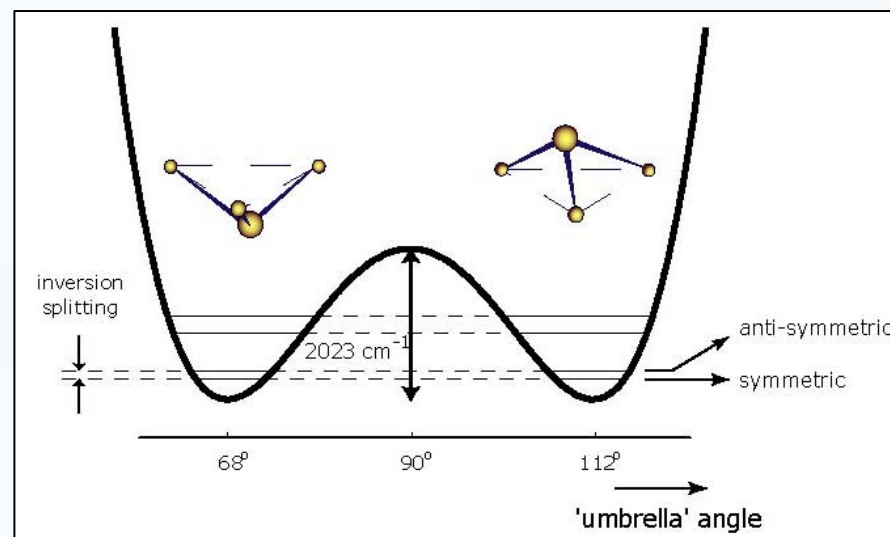


Case 2: Quantum Mechanics of Molecules (1953)



Charles Townes

- Research stimulated by DoD's attempts at 1 ¼ cm RADAR





The Ammonia MASER



Scanned at the American
Institute of Physics

Description: L-R: C.H. Townes, J. P. Gordon, and T. C. Wang. Wang stands next to the first ammonia-beam maser. The second ammonia-beam maser is in front center with side removed so that internal structure can be seen. Columbia University.

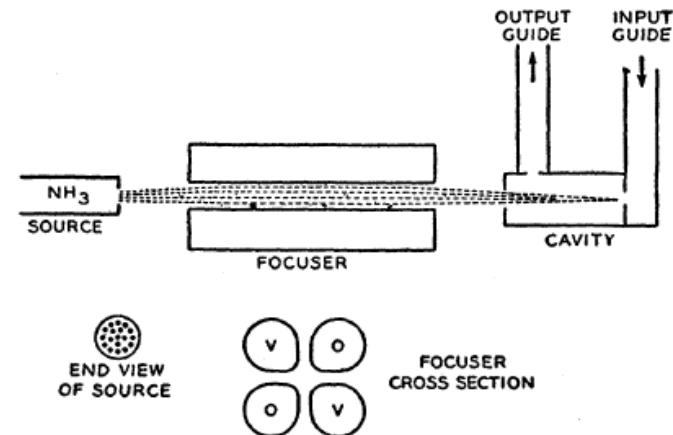


FIG. 1. Simplified diagram of the essential parts of the maser.

Gordon, Zeiger, and Townes, *Nature* **318** 162 (1985)

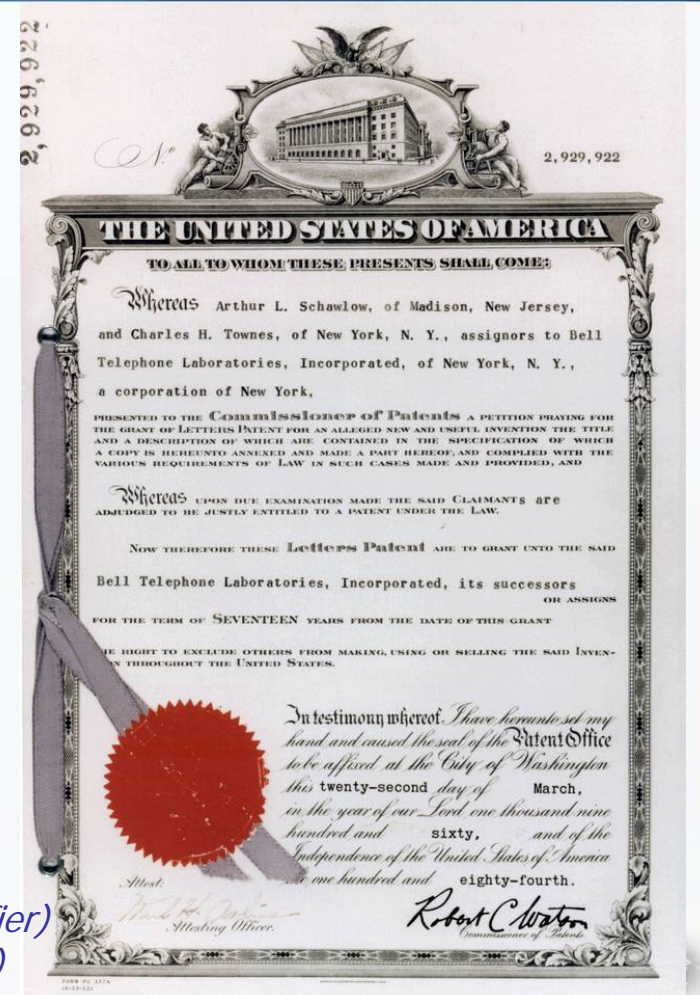




Extend MASER technique to IR and Visible

- Schawlow (Bell Labs) and Townes (consulting with Bell) realized that extending infrared or visible would be an even more powerful tool for spectroscopy.
- In 1957-58 they worked out the details on extending the MASER to the visible and applied for a patent. They were awarded a patent in 1960 and that same year Theodore Maiman (Hughes Aircraft Company) built a pulsed Ruby Laser.

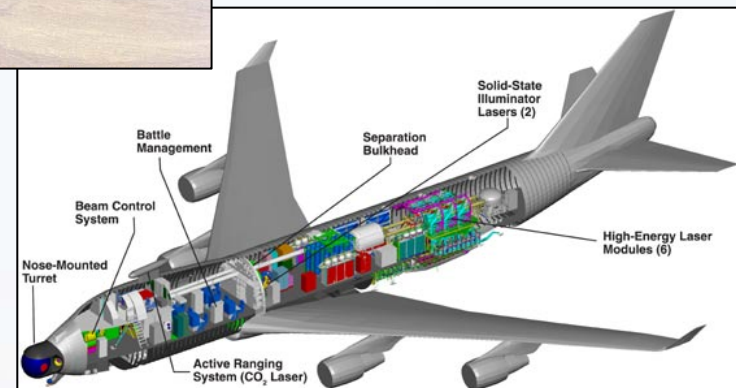
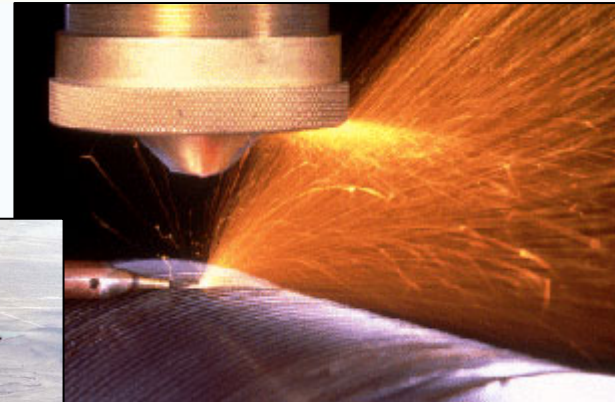
*Charlie Townes – Nobel Prize in Physics – 1964 (Maser/laser amplifier)
Arthur Schawlow – Nobel Prize in Physics – 1981 (develop. of laser)*

**AFRL**



Military Applications of Lasers

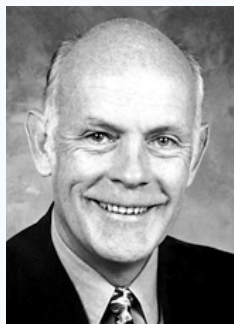
- Laser guided munitions
- Laser machining
- Laser sights
- Airborne laser
- Laser ranging
- ...



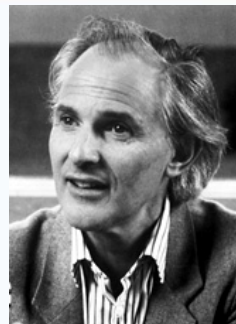
AFRL



Case 3: Unidentified Spectra in Interstellar Clouds

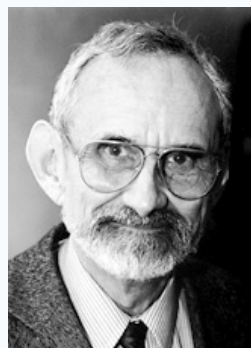
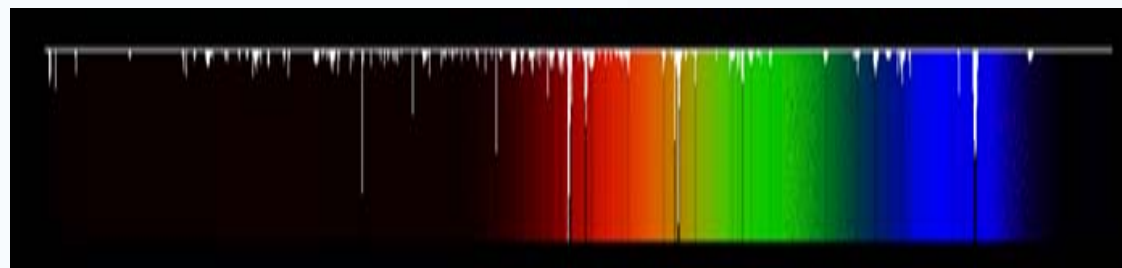


Richard Smalley



Harry Kroto

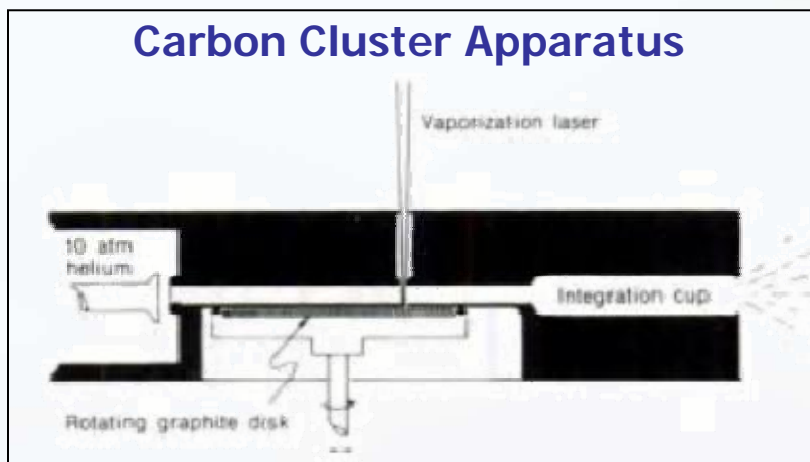
Diffuse Interstellar Bands



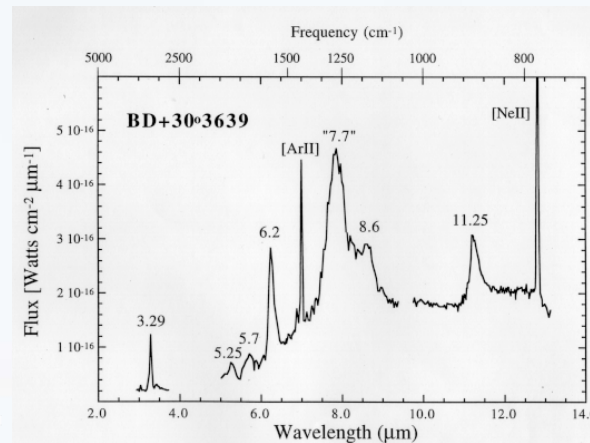
Robert Curl

Proposed that carbon clusters were a source of interstellar spectral features

Carbon Cluster Apparatus



Unidentified Infrared Bands





C₆₀: Buckminsterfullerene

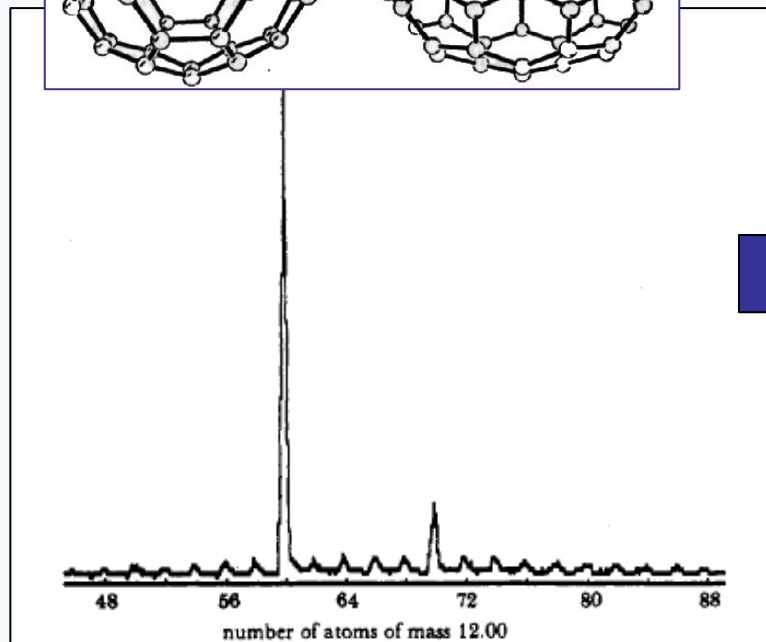
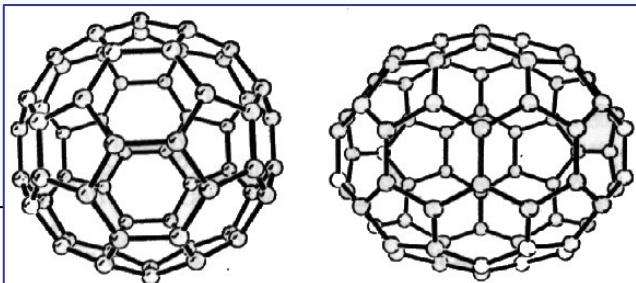
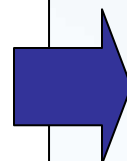
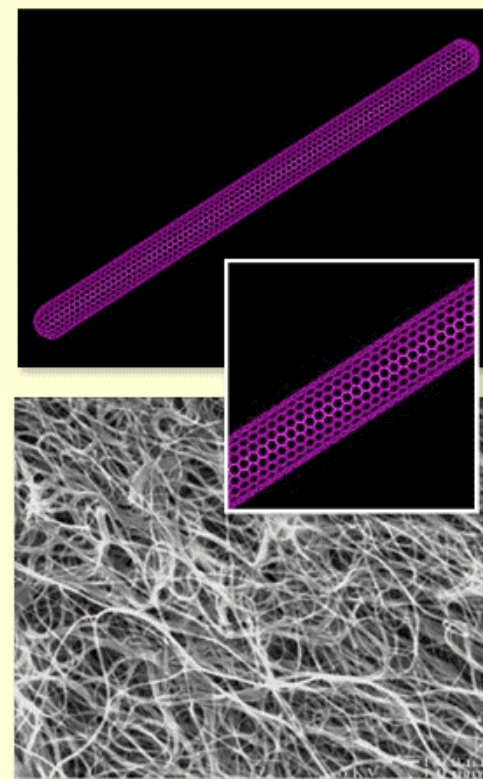


Figure 6. Time-of-flight mass spectrum carbon clusters produced by laser vaporization of graphite under the optimum conditions for observation of a dominant C₆₀ cluster signal.³ Note also the prominence of C₇₀.



MOLECULAR PERFECTION: THE FULLERENE IDEAL

1. The strongest fiber that will be ever made
2. Electrical Conductivity of Copper or Silicon
3. Thermal Conductivity of Diamond
4. The Chemistry of Carbon
5. The size and perfection of DNA

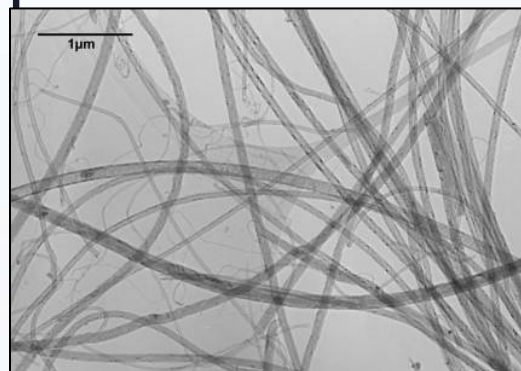
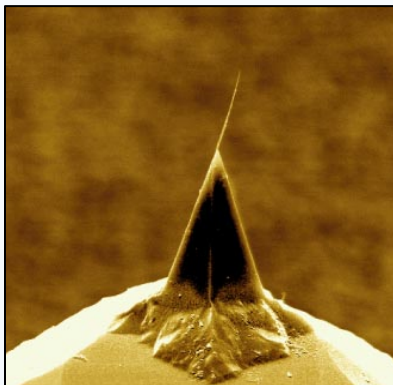
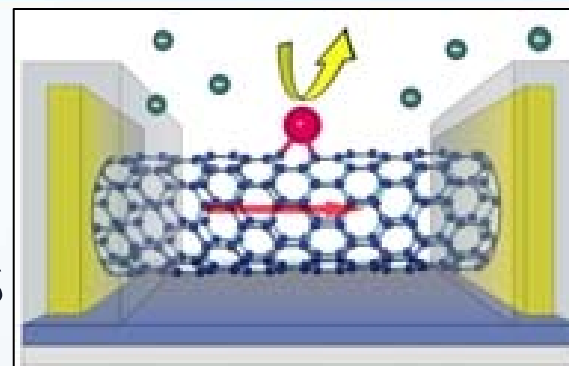


Kroto, *et al.* Nature 318 162-163 (1985)



(Near-Future) Applications of Carbon Nanotubes

- Fuel storage (H_2 , CH_4 , etc...)
- Structural composite materials
- Ultra-high conductivity electronics
- Ultra efficient field induced electron emitters
- Conductive plastics





More Serendipitous Discoveries...

Chemistry

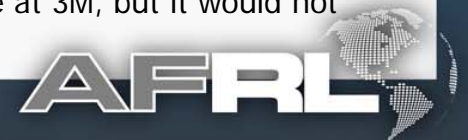
- **Polyethylene** by Hans von Pechmann, who prepared it by accident in 1898 while heating diazomethane
- **Teflon**, by Roy J. Plunkett, who was trying to develop a new gas for refrigeration and got a slick substance instead, which was used first for lubrication of machine parts
- **Cyanoacrylate** glue (a.k.a. Superglue) was accidentally twice discovered by Dr. Harry Coover, first when he was developing a clear plastic for gunsights and later, when he was trying to develop a heat-resistant polymer for jet canopies.
- **Aspartame** (a.k.a. NutraSweet) was also accidentally ingested by G.D. Searle chemist James Schlatter, who was trying to develop a test for an anti-ulcer drug.

Physics

- **Radioactivity**, by Henri Becquerel. While trying to investigate phosphorescent materials using photographic plates, he stumbled upon uranium.
- **X rays**, by Wilhelm Roentgen. Interested in investigating cathodic ray tubes, he noted that some fluorescent papers in his lab were illuminated at a distance
- **Electromagnetism**, by Hans Christian Oersted. While he was setting up his materials for a lecture, he noticed a compass needle deflecting from magnetic north when the electric current from the battery he was using was switched on and off.
- The **thermoelectric effect** was discovered accidentally by Estonian physicist Thomas Seebeck, in 1821, who found that a voltage developed between the two ends of a metal bar when it was submitted to a difference of temperature.

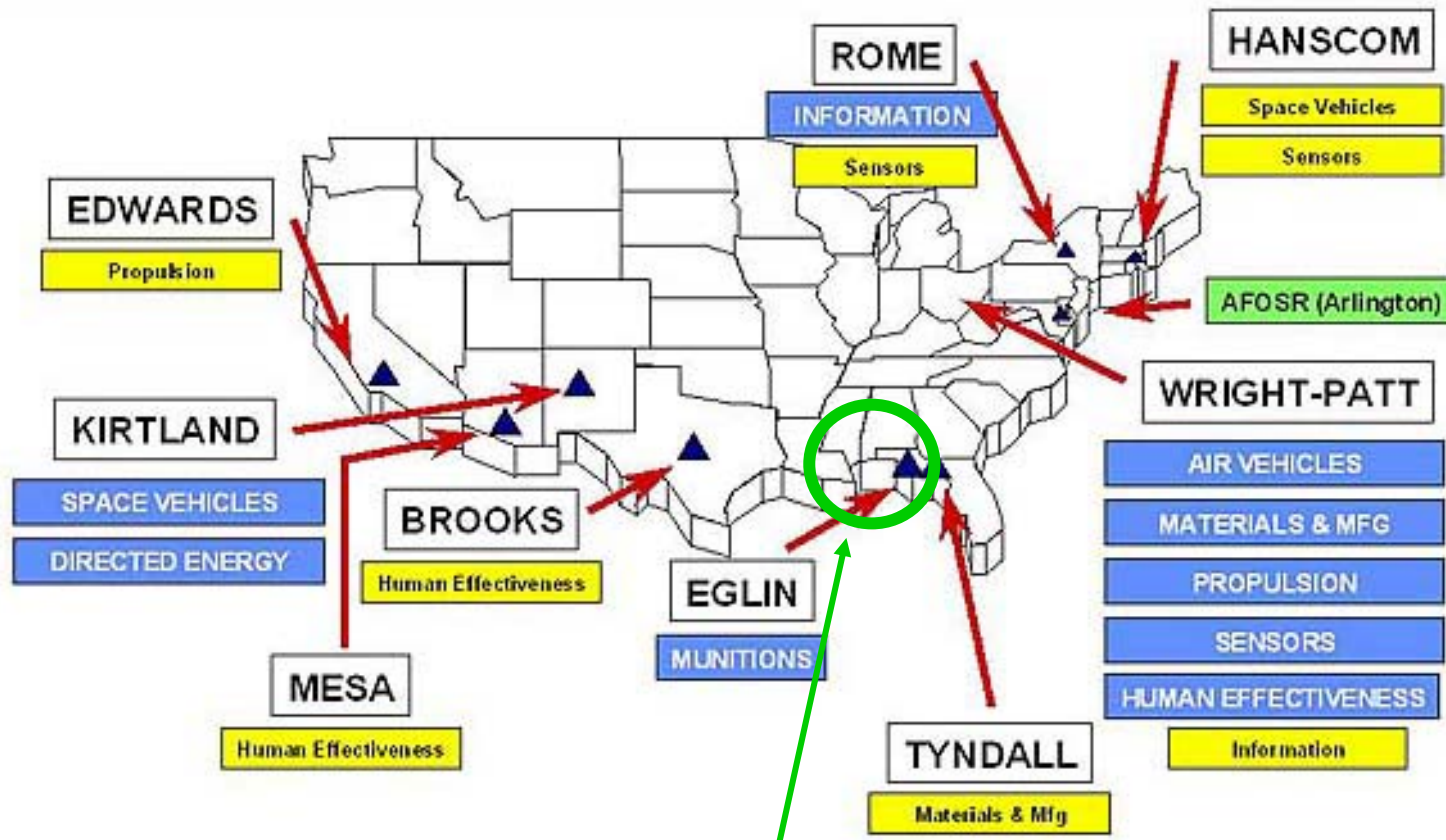
Technology

- Discovery of the principle behind **inkjet printers** by a Canon engineer. After putting his hot soldering iron by accident on his pen, ink was ejected from the pen's point a few moments later.
- The **microwave oven** was invented by Percy Spencer while testing a magnetron for radar sets at Raytheon, he noticed that a peanut candy bar in his pocket had melted when exposed to radar waves.
- **Post-it Notes** by Spencer Silver and Arthur Fry. They tried to develop a new glue at 3M, but it would not dry. So they devised a new use for it.





Air Force Research Laboratory



- Eglin AFB / Munitions Directorate/ Energetic Materials Branch





AFRL/RWMER – LASEM Lab

Laboratory for **A**ppplied **S**pectroscopy of **E**nergetic **M**aterials

New Basic and Applied
Research Team at Eglin
AFB (~ 4 years old)

Team Members (but
expanding)

- PI's (Physical Chemists)
- NRC Post docs
(Materials and Physical chemists)
- Military Officers (A-Chemist, P-Chemist and a Physicist)
- Technicians
- **(3-4 Open Postdoc Positions)**





AFRL/RWMER – LASEM Lab

Laboratory for **A**ppplied **S**pectroscopy of **E**nergetic **M**aterials

Research Areas

- Explosives
- Reactive composite materials
- Thermite and inter-metallic materials
- Energetic thin films
- Cryogenic matrices
- Energetic core-shell nanoparticles
- Positron/plasma/positronium storage

Diagnostics

- Vis, FIR, MIR, NIR spectroscopy
- γ -ray spectroscopy
- Positron spectroscopy
- Matrix isolation spectroscopy
- TOF/QMS – mass spectrometry
- XRF/XRD
- SEM, optical microscopy
- Radiographic imaging





Cryogenic Matrices – Basic Research Interests

- Ultra-low temperature chemistry – synthesize systems under different conditions than ambient
- Energy dissipation – stabilize pre-reactive systems
- Quantum Condensed Phases – unusual properties
 - Powerful annealing behavior
 - Unprecedentedly sharp transitions
 - Superfluidity
 - liquid helium, solid parahydrogen
- New regime for exploration – many surprises





Introduction - Antimatter Giggle Factor



One vision of bulk antimatter storage in the 23rd century.

Star Trek
Episode # 47
“Obsession”
(Paramount,
1967).

Skepticism of near-term practical energy storage is justified.

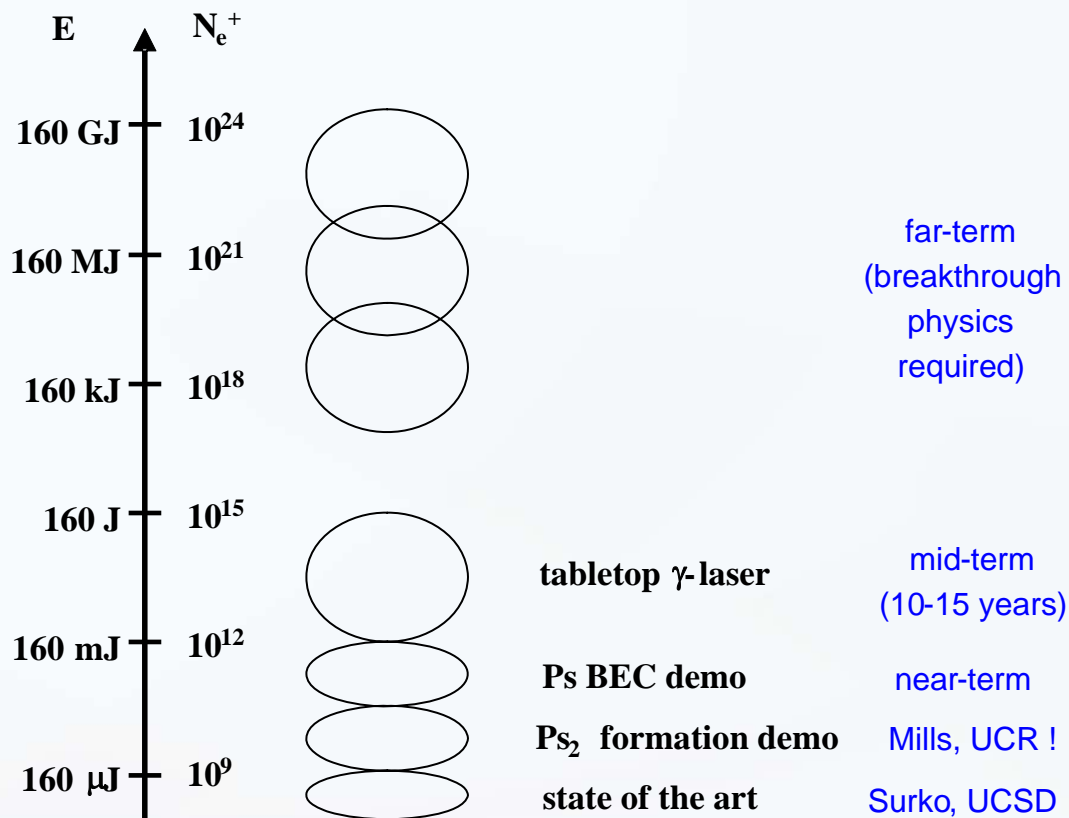




Introduction - Reality Check

Annihilation energy:
 $E = 2 N_{e^+} m_e c^2$

Brillouin (B ~ 1 T) and
Space Charge (V ~ 100 kV) →
limits on
bare e^+ storage in ~ 1 m³



e^+ = positron; Ps = positronium (e^+/e^- bound pair);

PEC = Positron Energy Conversion Project; BEC = BoseEinstein Condensation





Introduction - Positron Moderation

Generic positron production scheme:

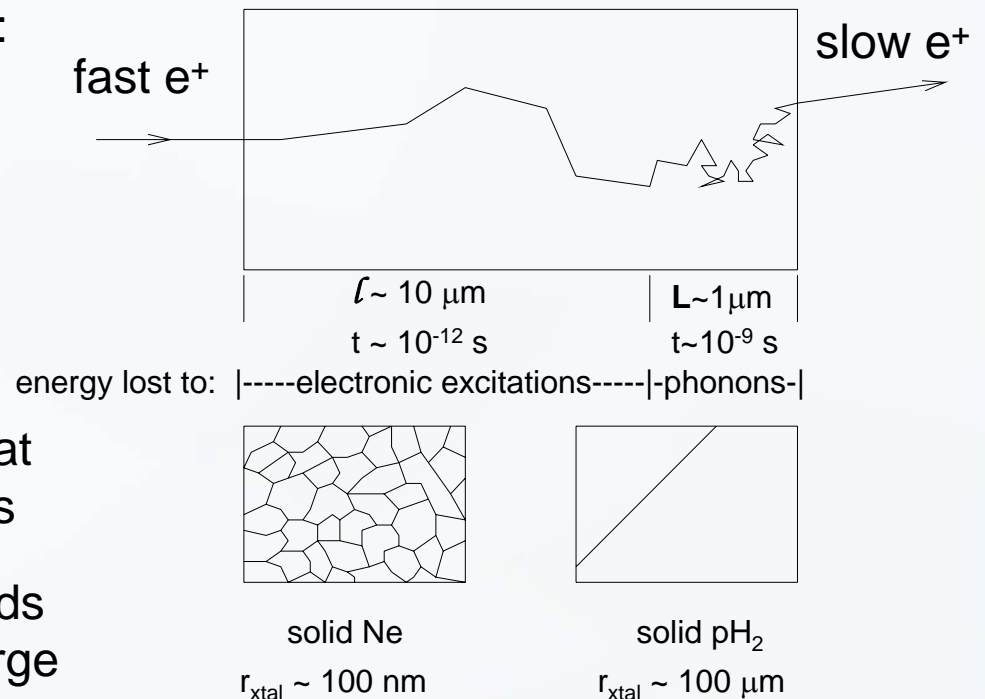
- (1) nascent fast e^+ ($E \sim 100$ keV)
- (2) **moderation** ($E \sim 1$ eV)
- (3) e^+ and/or Ps trapping

Solid Ne is best known moderator
 $\varepsilon \approx 0.5$ %; so 99.5 % are wasted

Slow e^+ scatter, trap, and annihilate at defects \Rightarrow lost to moderation process

High quality parahydrogen (pH_2) solids should permit slow positrons to emerge from deeper within moderator

Moderation efficiency increases as L / ℓ



[E.M. Gullikson and A.P. Mills, Jr.,
Phys. Rev. Lett. **57**, 376 (1986)]

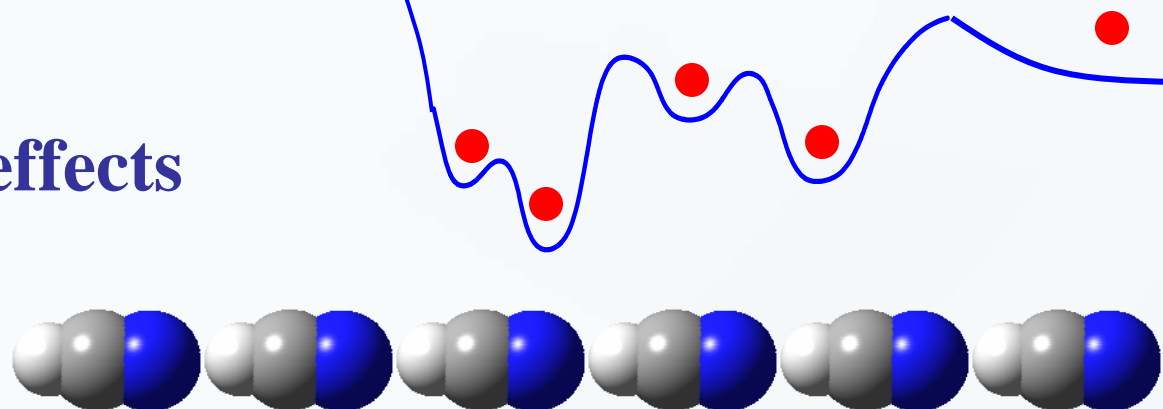




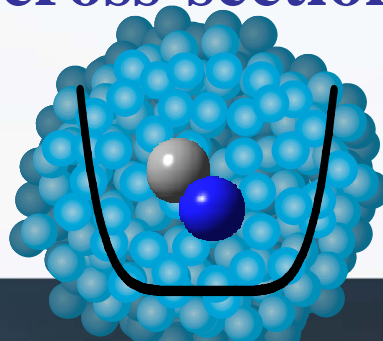
Ultra-low Temperature Chemistry

- Reactions occur in a dissipative environment

- Steric effects



- Large “reaction” cross-sections



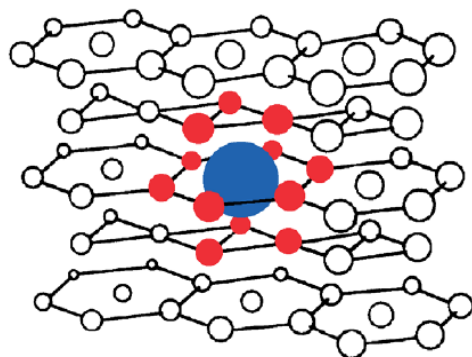


About solid parahydrogen

Solid parahydrogen features:

- Weak intermolecular interactions
- Slow relaxation timescales
- Quantum crystal: self-annealing via tunneling
- Homogeneous environment
- Large intermolecular distance, 3.78 Å

Methane in solid $p\text{-H}_2$



- $p\text{-H}_2$
- nearest neighbor $p\text{-H}_2$
- methane

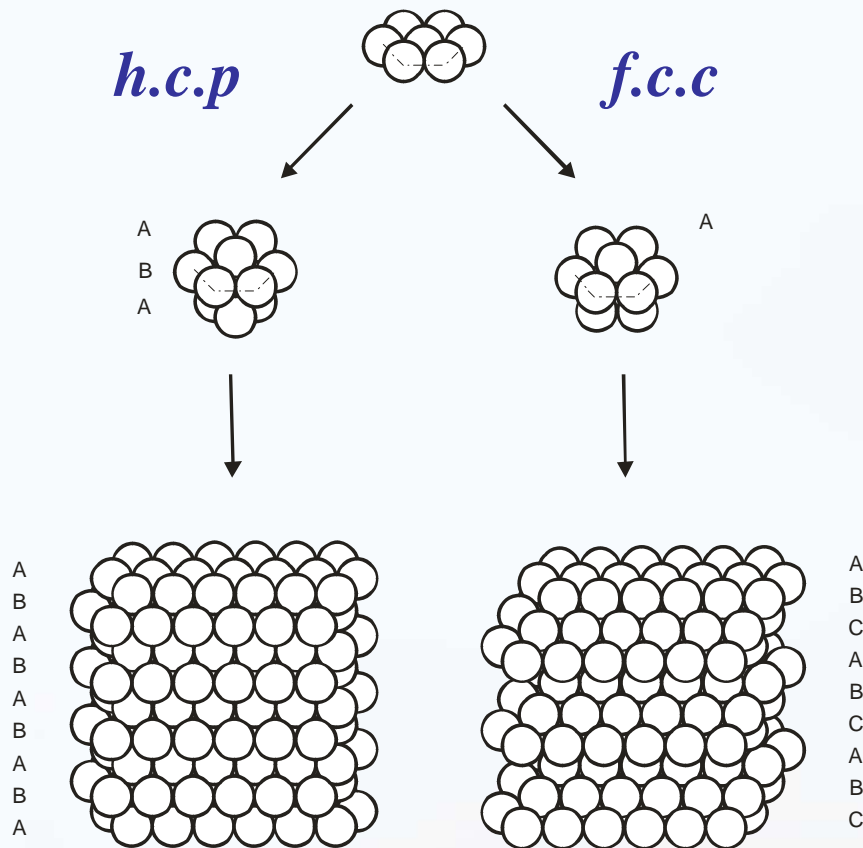
Parahydrogen as a matrix:

- Very small matrix shifts, predictable (-0.5 %)
- Nearly free rotation for small molecules
- High impurity mobility
- Narrow spectral linewidths (<100 MHz possible)
- Dopants induce infrared activity in matrix





Close packing crystal structure



- Symmetry: *h.c.p.* – D_{3h} ; *f.c.c.* – O_h
- Reduced symmetry in *h.c.p.* provides directionality to the crystal and thus enables polarization sensitive measurements to be performed.
- Relative stability of *f.c.c.* and *h.c.p.* structures depends on many-body long-range interactions.
- Most stable structure in rare gas solids (RGS) is *f.c.c.* *

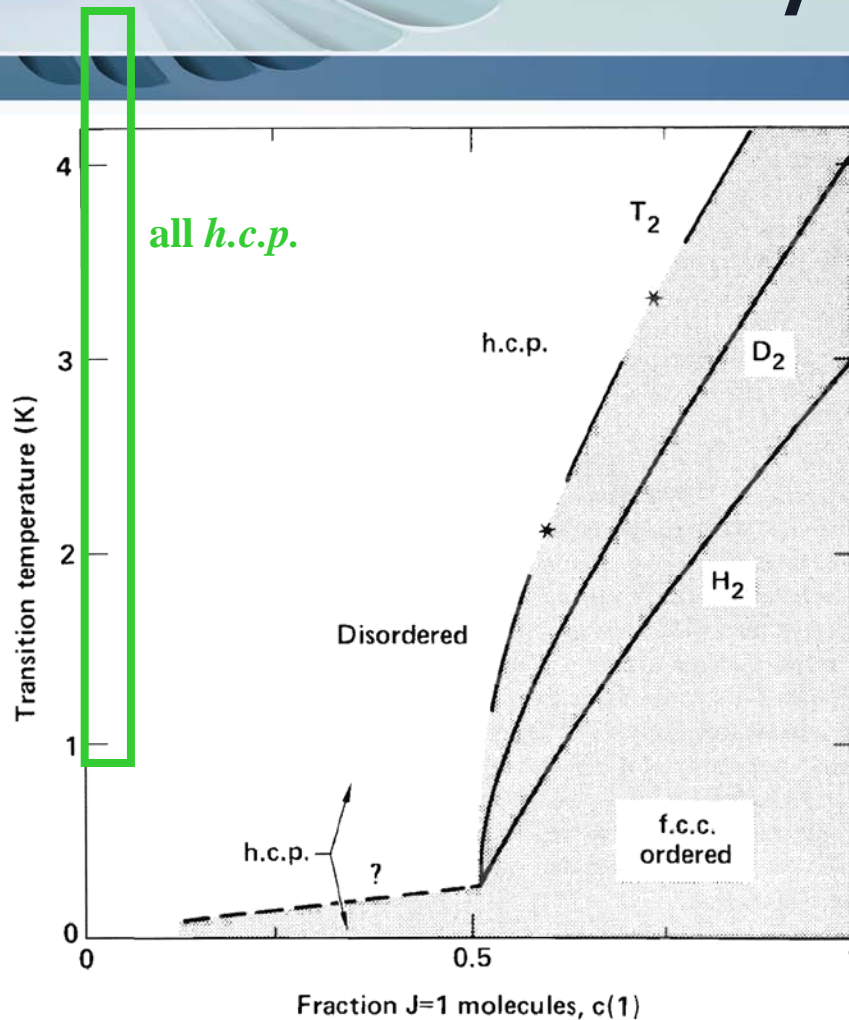
* Excluding solid helium

Adapted from P. C. Souers, *Hydrogen Properties for Fusion Energy*, (1986)





f.c.c versus *h.c.p.*



P. C. Souers, *Hydrogen Properties for Fusion Energy*, (1986).

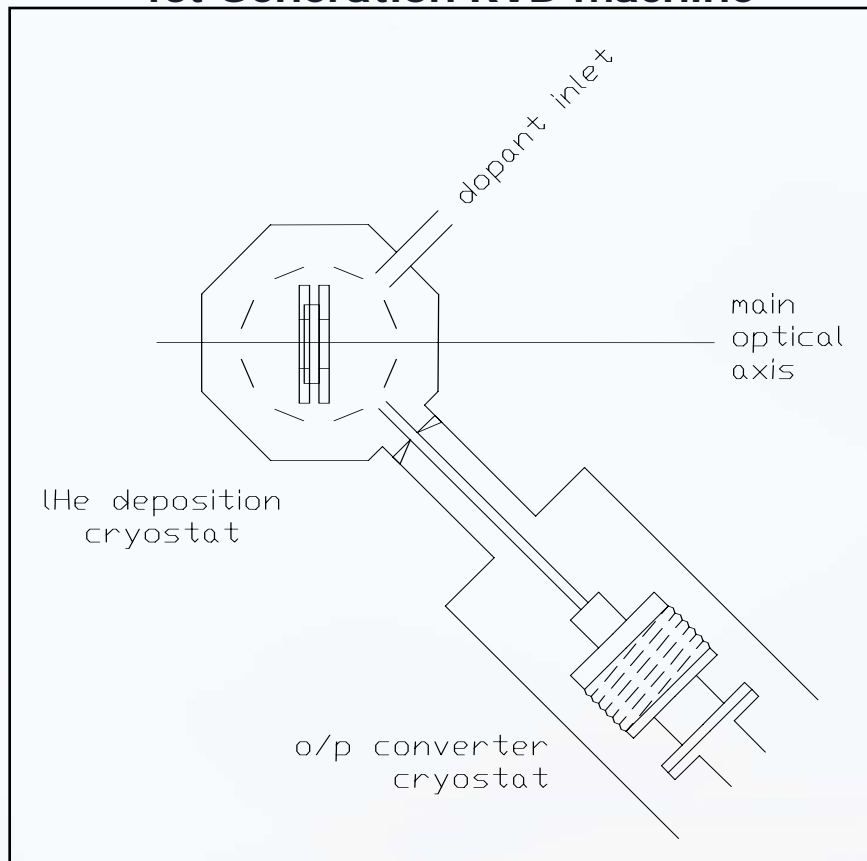
J. Van Kranendonk, *Solid Hydrogen*, (1983).

- Unlike RGS, solid parahydrogen ($J=0$) has *h.c.p.* as the lowest energy crystal structure.
- *h.c.p.* more stable than *f.c.c.* by ~ 1 mK per molecule.
- Solid parahydrogen synthesized by rapid vapor deposition at low temperature produces a mixture of *f.c.c.* and *h.c.p.* phases. Nearly exclusive *h.c.p.* structure produced upon annealing above ~ 4.5 K.



Rapid Vapor Deposition

1st Generation RVD machine



- Original machine built at Edwards AFB in 1995.
- Optical path normal to substrate.
- Rotating molecules:
 $\Delta m = 0$ transitions suppressed relative to $\Delta m = \pm 1$

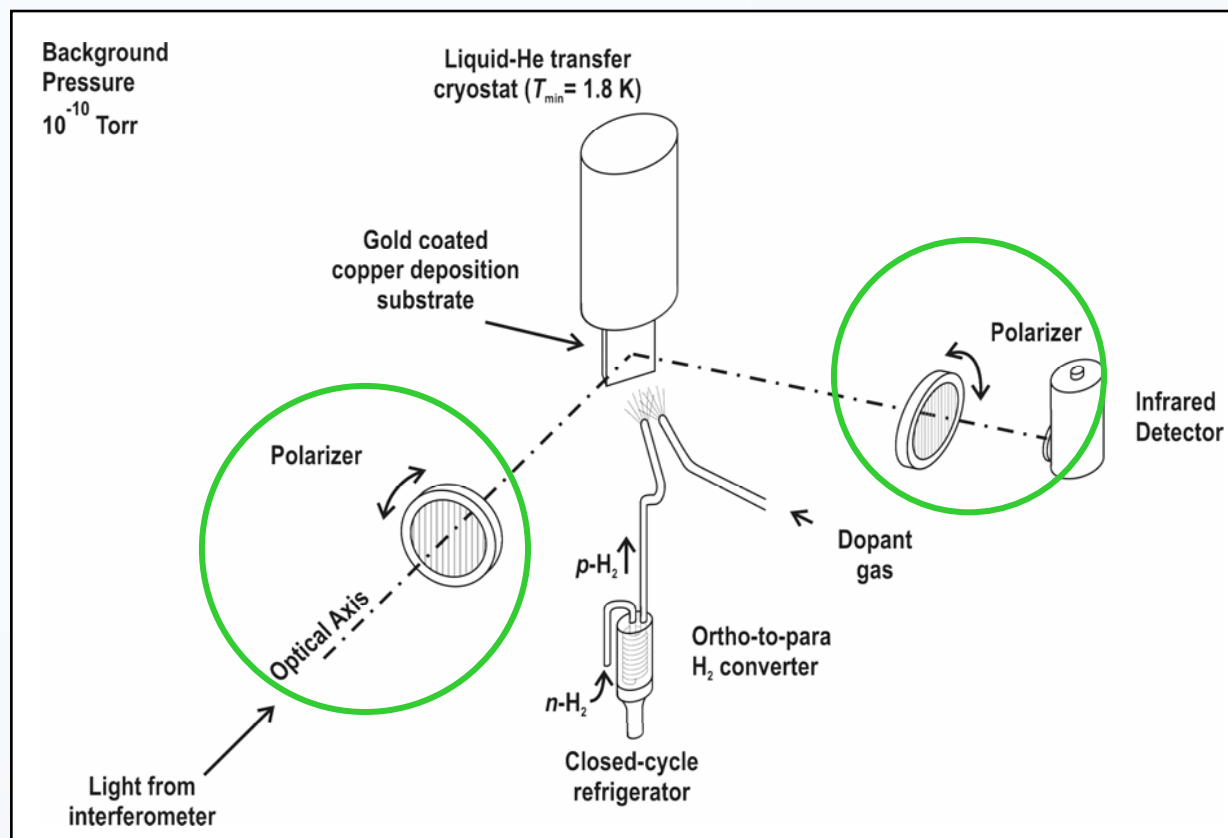
M.E. Fajardo and S. Tam, *J. Chem. Phys.* **108**, 4237 (1998).
S. Tam and M.E. Fajardo, *Rev. Sci. Instrum.* **70**, 1926 (1999).



Eglin AFB Rapid Vapor Deposition Instrument

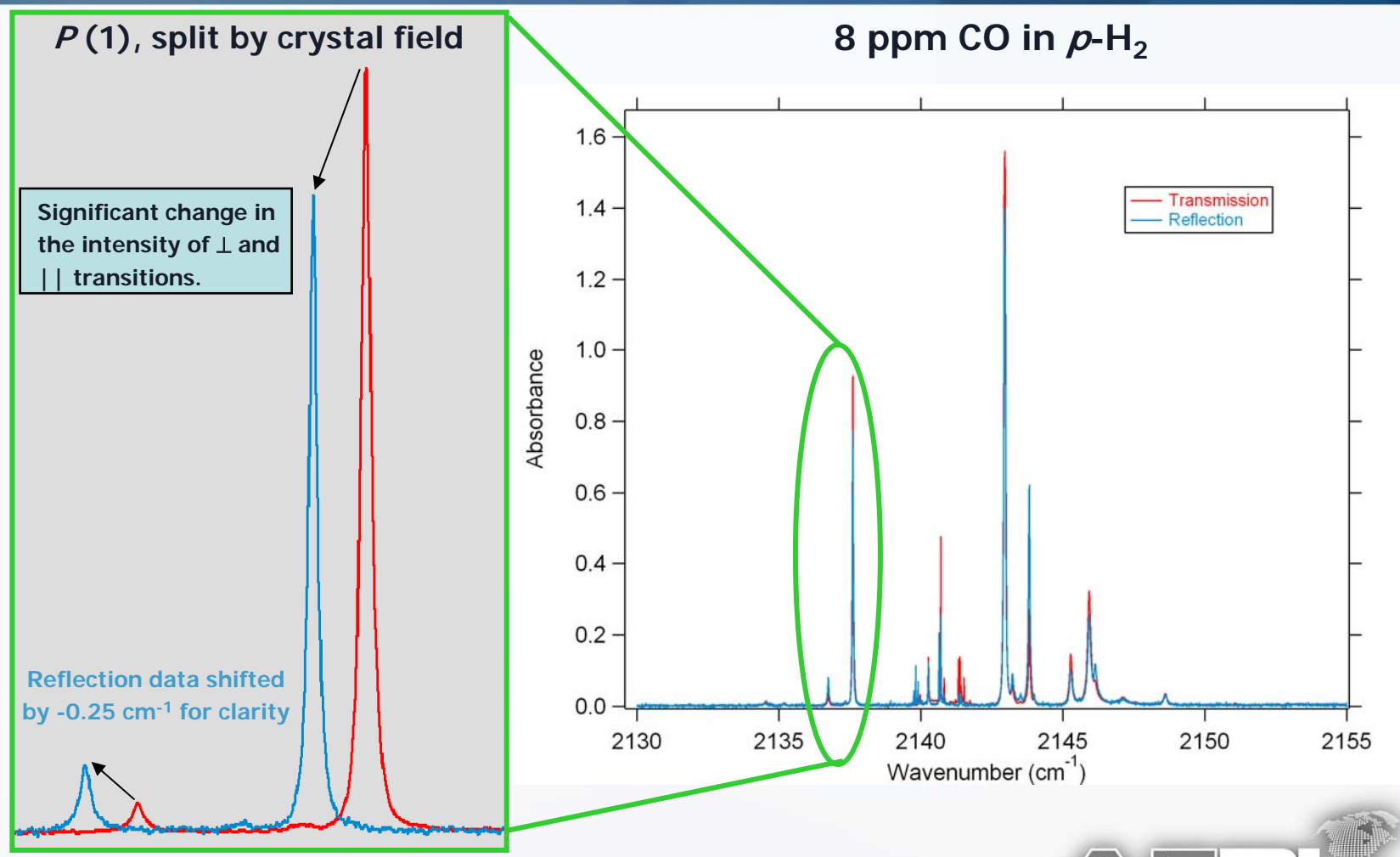
2nd Generation RVD machine

- Reflection based set-up (FTIR).
- $[o\text{-H}_2] < 100$ ppm.
- $p\text{-H}_2$ deposition rate ~ 150 mmol/hr \rightarrow 2-3 mm/hr thickness.
- Deposition at 2.3 K. Sample annealed at 4.3 K for 15-30 min.





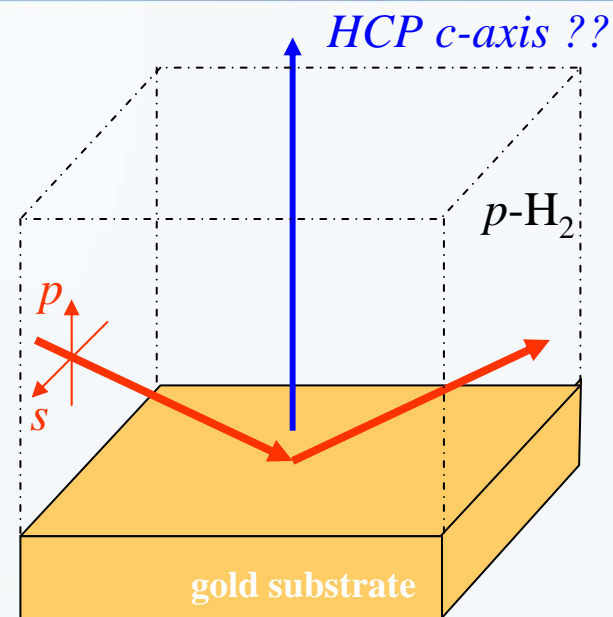
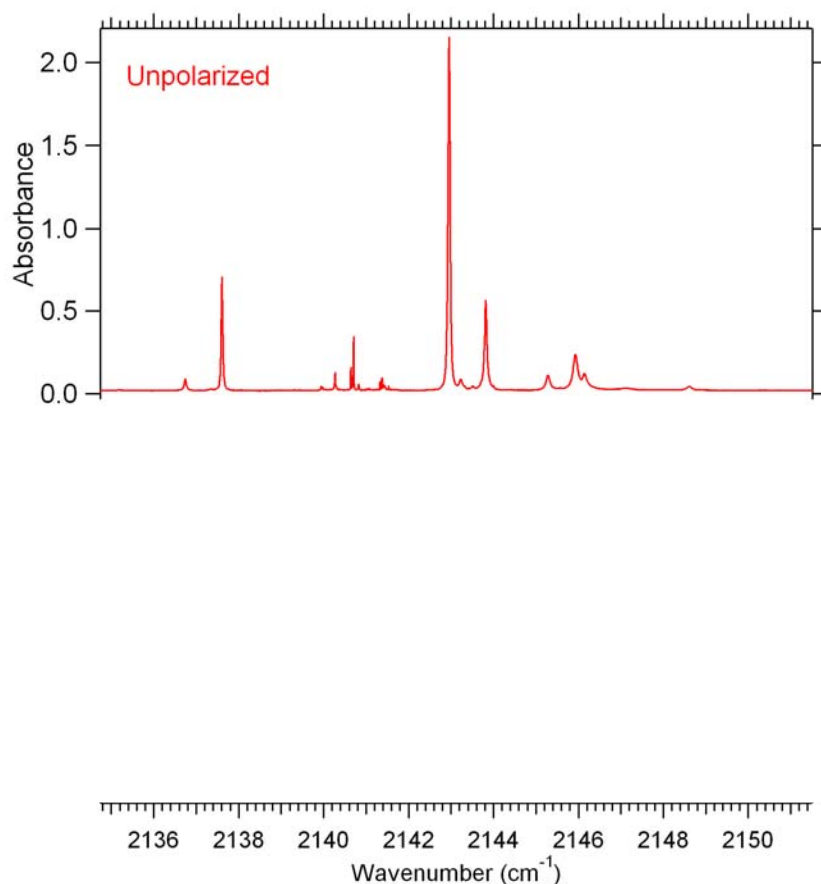
Optical Geometry: Reflection Versus Transmission





Polarization Spectroscopy

8 ppm CO in *p*-H₂



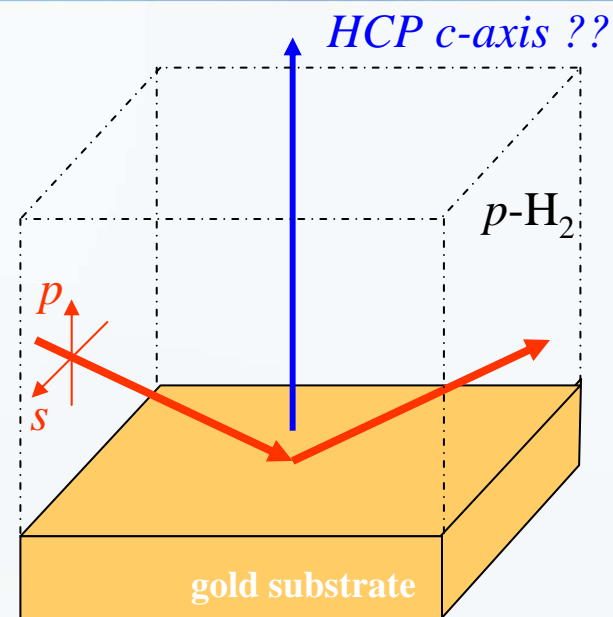
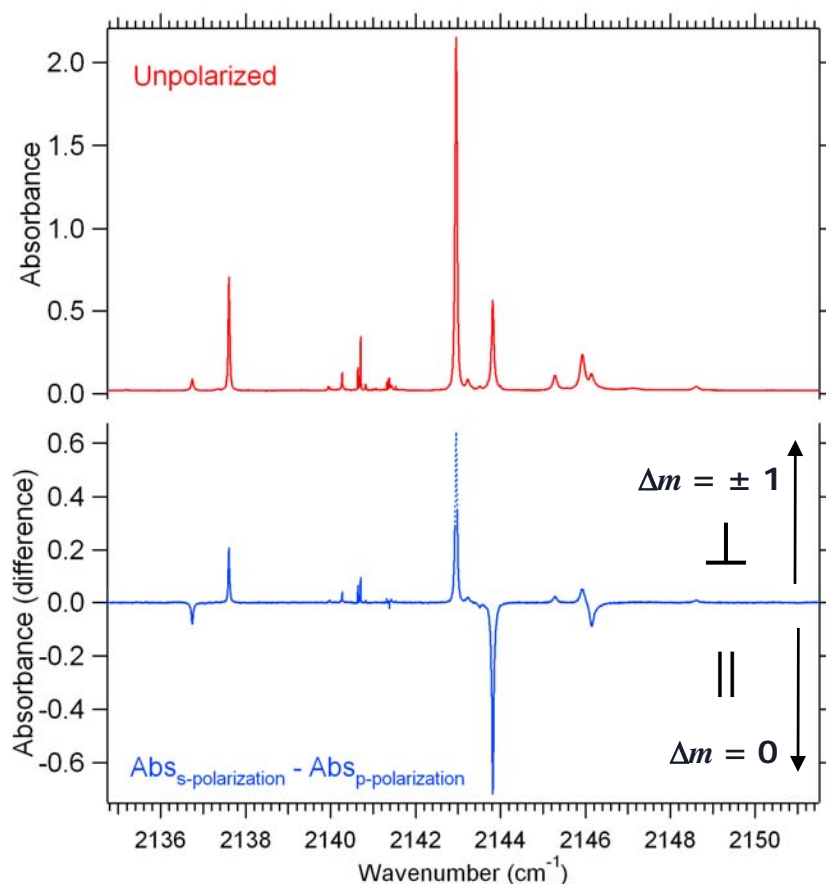
Polarization analysis provides:

- An assignment of the perpendicular and parallel components to the crystal field perturbed rotational structure (*i.e.* Δm)
- $Abs_{s-pol} - Abs_{p-pol} = \frac{1}{2} \mu_{\perp}^2 - \frac{1}{2} \mu_{\parallel}^2$



Polarization Spectroscopy

8 ppm CO in p -H₂



Polarization analysis provides:

- An assignment of the perpendicular and parallel components to the crystal field perturbed rotational structure (*i.e.* Δm)
- $Abs_{s-pol} - Abs_{p-pol} = \frac{1}{2} \mu_{\perp}^2 - \frac{1}{2} \mu_{\parallel}^2$



Rotation of “Large” Molecules in Solid Parahydrogen





Rotation in the Solid Matrices

- Rare gas matrices and traditional molecular matrices:
 - Small hydrides: HX, H₂O, NH₂, NH₃, CH₃, CH₄
 - *Perhaps* ClF, CN (ESR and IR spectra conflict)
- Solid parahydrogen:
 - Very low angular anisotropy, and weak intermolecular interactions
 - Small hydrides: HX, H₂O, NH₃, CH₃, CH₄
 - “*Large*” molecules: N₂, O₂, CO, NO, HCN, ... *more?*

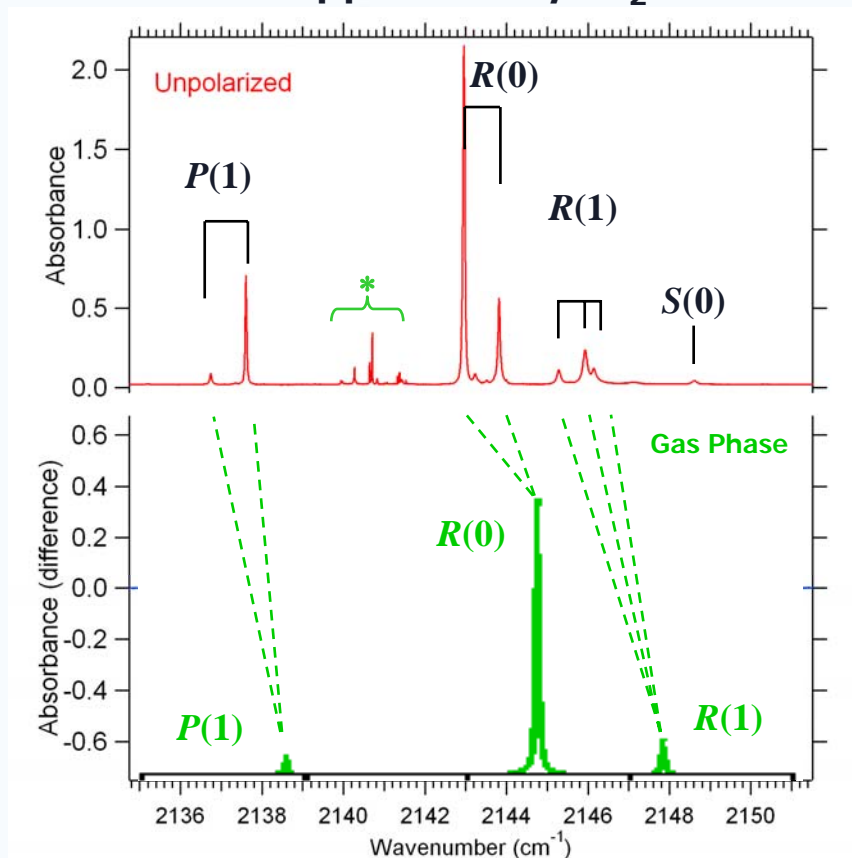
Narrow spectral lines widths and the ability to examine the rotation of larger molecules allows us to examine the impurity-matrix interactions with remarkable clarity





CO and HCN in parahydrogen

8 ppm CO in p -H₂

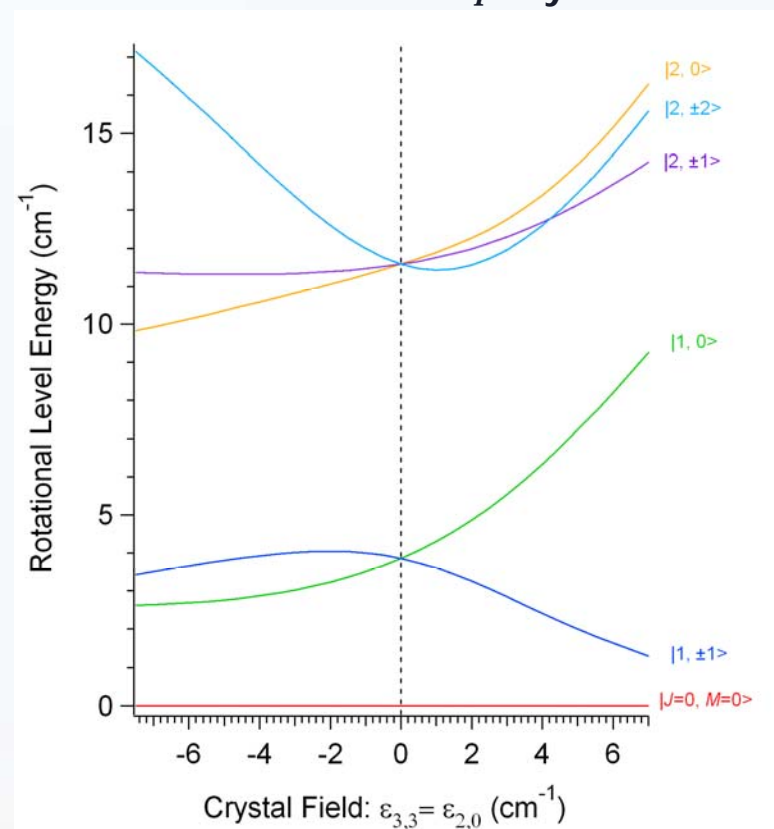


* o -H₂ clustering

Simulation uses theory of: Devonshire, Proc. Roy. Soc. London A 153, 601 (1936);
Bowers and Flygare, J. Chem. Phys., 44, 1389 (1966).

Simulation:

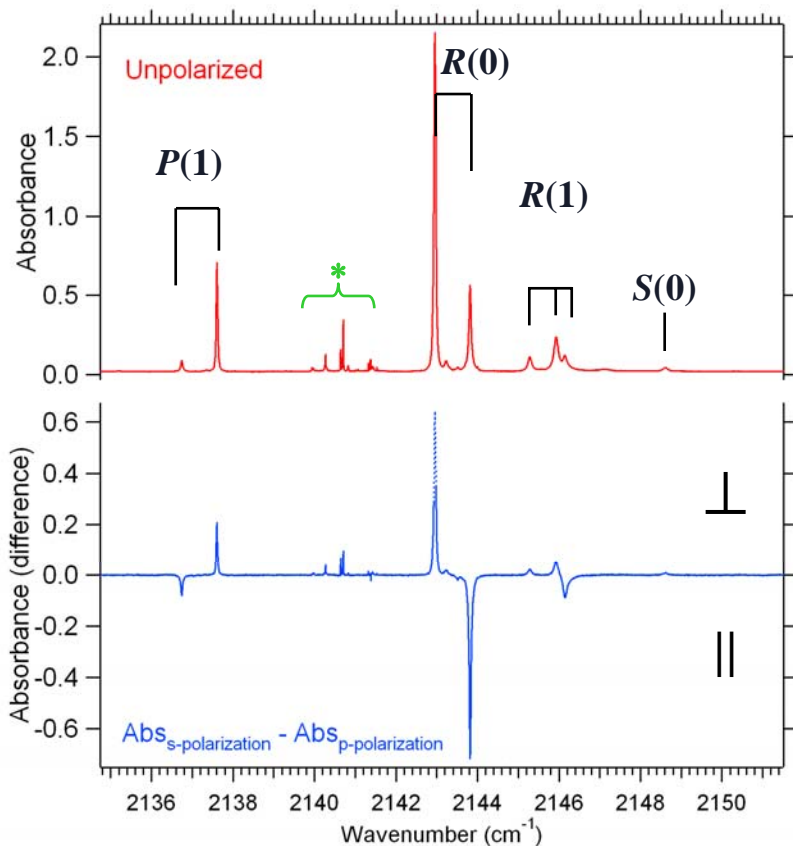
Linear molecule in $h.c.p$ crystal field



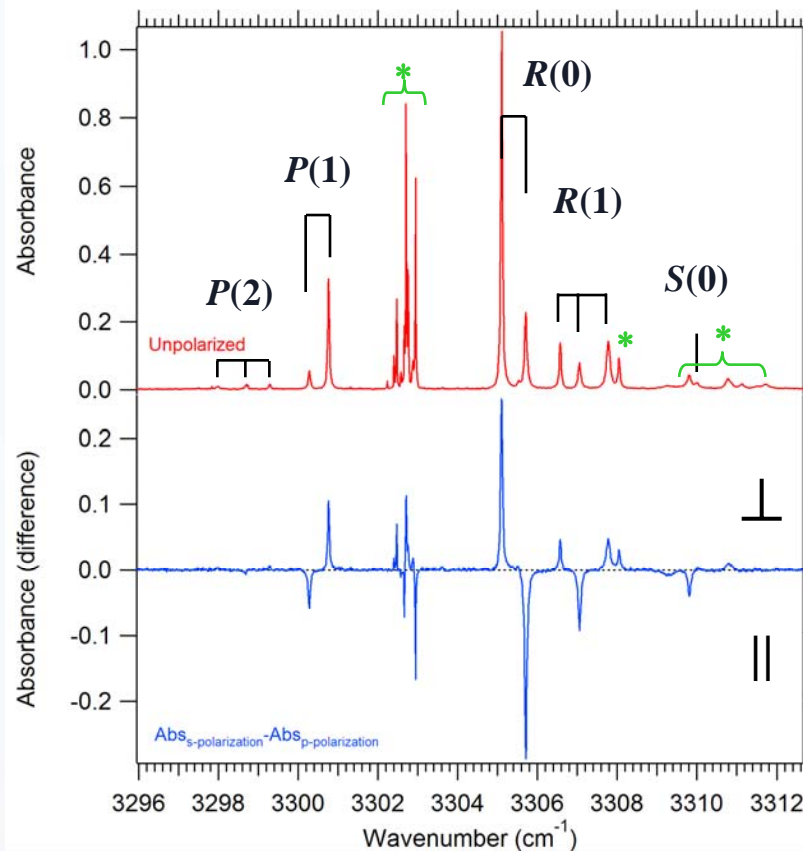


CO and HCN in parahydrogen

8 ppm CO in p -H₂



8 ppm HCN in p -H₂



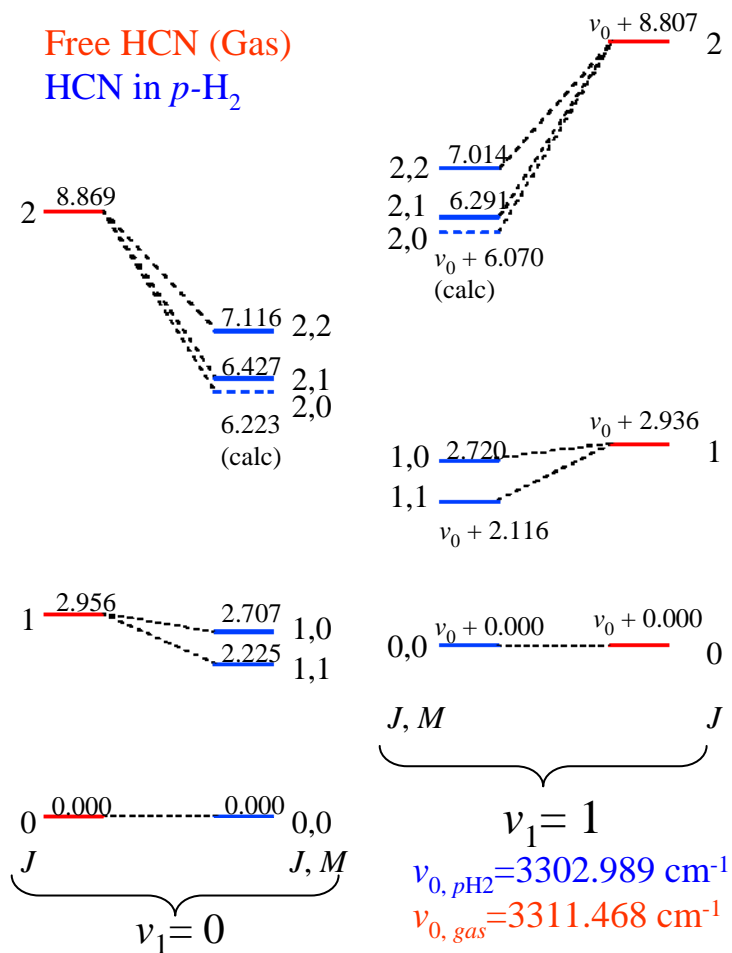
* o -H₂ clustering





Interpretation of the Rotational Fine Structure- HCN

Energy Level Diagram (cm⁻¹)



Crystal field theory (linear molecule in HCP lattice) *

$$H = H_{r,v} + V_{\text{cry}}$$

$$V_{\text{cry}} = \epsilon_2 C_{2,0}(\Omega_{\text{HCN}}) + \epsilon_3 [C_{3,-3}(\Omega_{\text{HCN}}) - C_{3,3}(\Omega_{\text{HCN}})]$$

$$\text{where } C_{l,m}(\Omega) = \left(\frac{4\pi}{2l+1} \right)^{1/2} Y_{l,m}(\Omega)$$

“Fitting” Results in cm⁻¹: (10 levels, 9 parameters)

	<i>p</i> -H ₂	Gas
<i>B</i>	1.475(5)	1.478
ΔB	-0.005(5)	-0.010
<i>D</i>	0.0675(5)	2.910 × 10 ⁻⁶
ΔD	0.0032(5)	0.025 × 10 ⁻⁶
<i>v</i> ₀	3302.989(5)	3311.4770
ϵ_2	-1.274(5)	-
$\Delta \epsilon_2$	-0.193(5)	-
ϵ_3	6.850(5)	-
$\Delta \epsilon_3$	0.767(5)	-

Identical!

× 20,000!

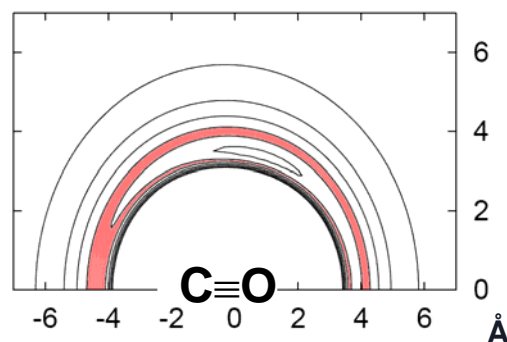
very large!

NOTE: Above perturbation does not converge for large *D*!
Treatment was modified to incorporate centrifugal distortion after crystal field calculation to avoid this problem.



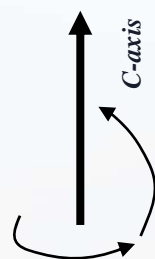
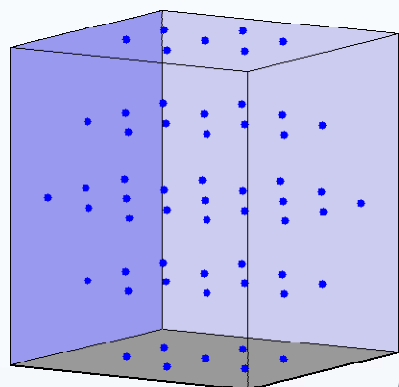
Prediction of Crystal Field Parameters: Truncation

H_2 -CO pair potential *



+

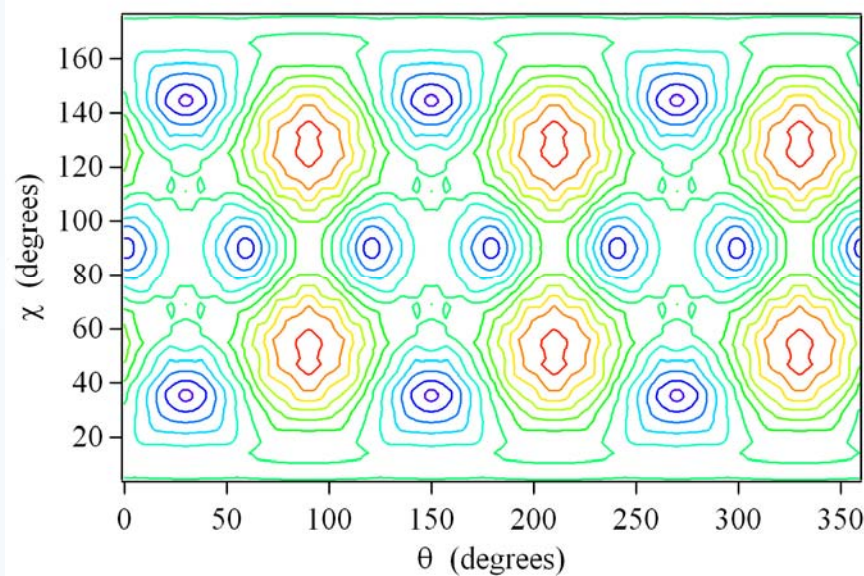
H_2 - *h.c.p.* lattice



θ (in-plane)

χ (out-of-plane)

Rotational PES for CO
in *h.c.p.* H_2 lattice (Rigid)

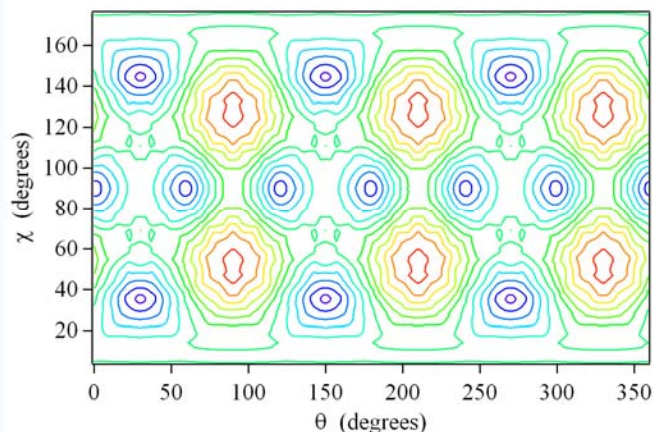


* SAPT/MC+BS, P. Jankowski and K. Szalwicz, *J. Chem. Phys.* **108**, 3554 (1998).

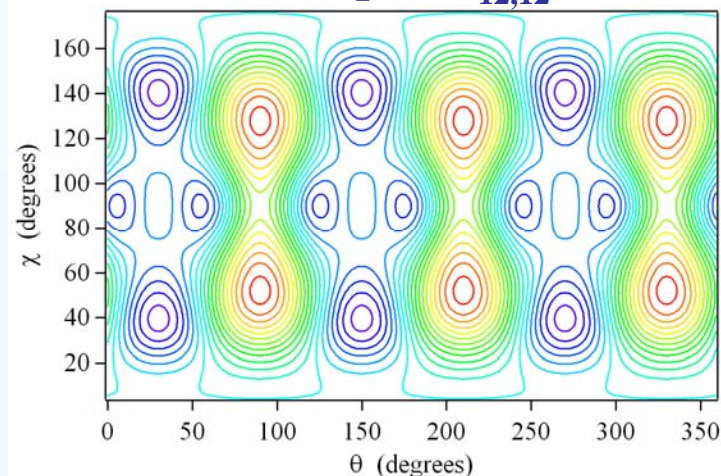


Prediction of Crystal Field Parameters: Truncation

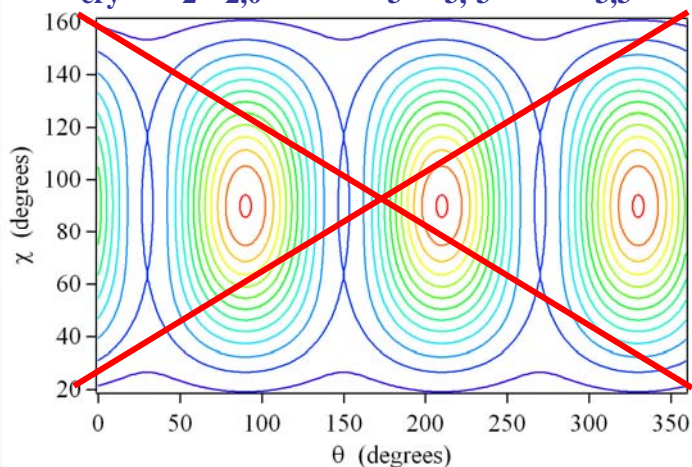
Rotational PES for CO



CFT -up to $C_{12,12}(\Omega)$



$$V_{\text{cry}} = \varepsilon_2 C_{2,0}(\Omega) + \varepsilon_3 [C_{3,-3}(\Omega) - C_{3,3}(\Omega)]$$



(2.52)*

ε (cm ⁻¹)	Term	ε (cm ⁻¹)	Term
1.39	$C_{3,3}(\Omega)$	0.07	$C_{9,3}(\Omega)$
1.23	$C_{5,3}(\Omega)$	0.04	$C_{12,6}(\Omega)$
0.74	$C_{4,0}(\Omega)$	0.04	$C_{8,0}(\Omega)$
-0.57	$C_{6,6}(\Omega)$	0.03	$C_{12,12}(\Omega)$
-0.43	$C_{6,0}(\Omega)$	0.03	$C_{12,0}(\Omega)$
0.35	$C_{7,3}(\Omega)$	-0.03	$C_{11,3}(\Omega)$
0.13	$C_{8,6}(\Omega)$	-0.03	$C_{2,0}(\Omega)$

(1.03)*

* Experimentally fitted values.



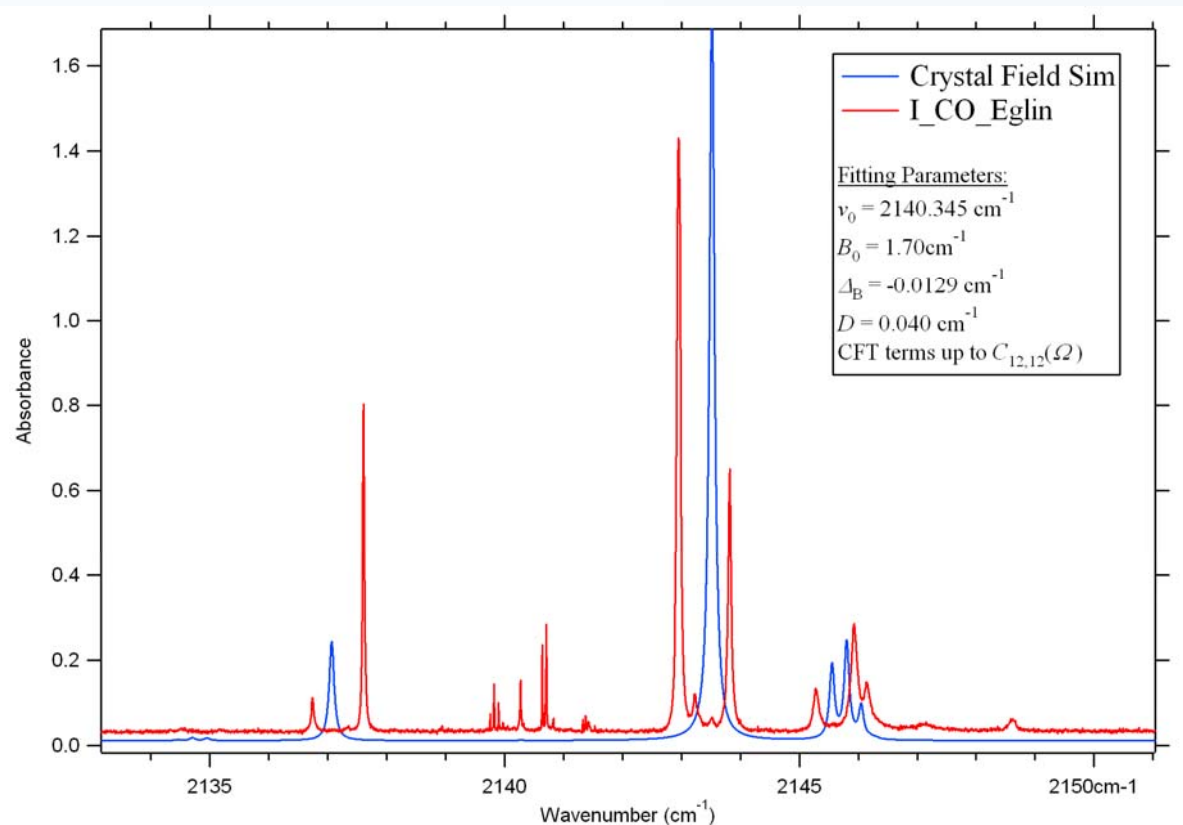


Estimation of Crystal Field Parameters: Simulated Spectrum for CO

- Underestimates crystal field splittings.
- $S(0)$ transition too weak.



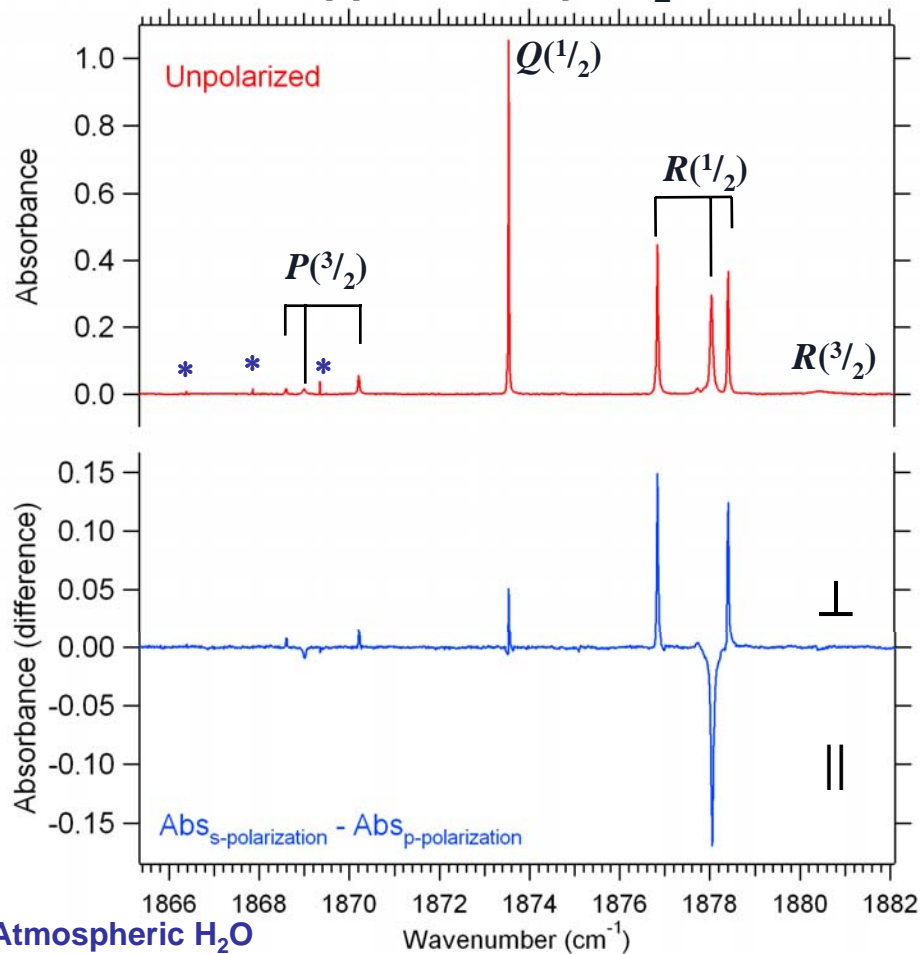
- Mixing underestimated
- First order perturbation insufficient?



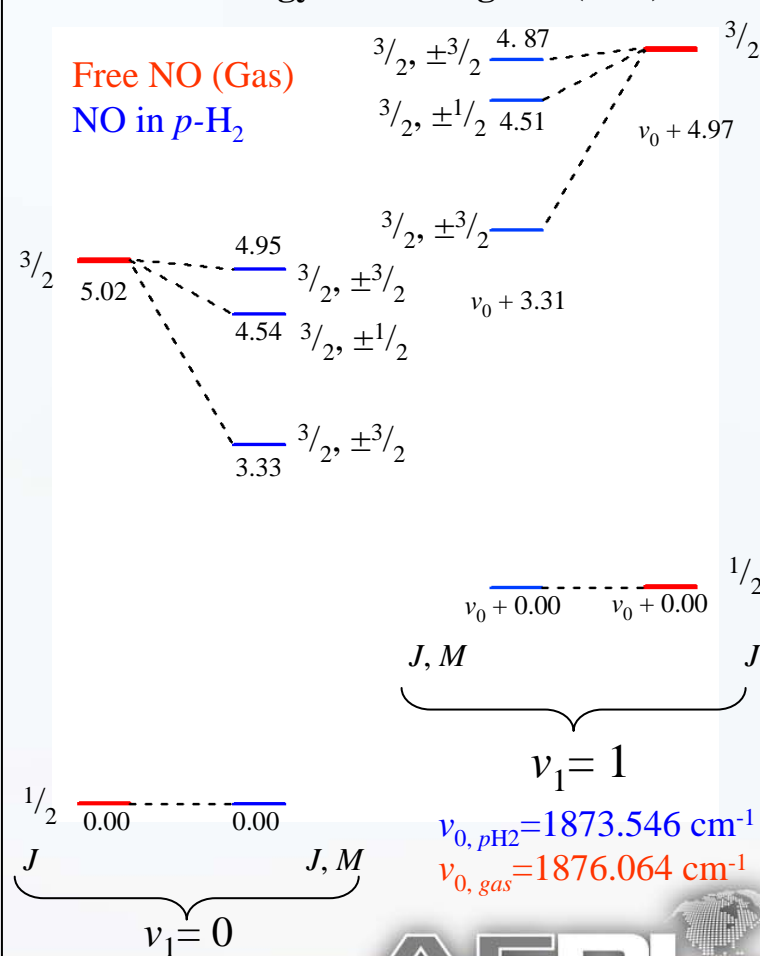


NO in Solid Parahydrogen

6 ppm NO in p -H₂

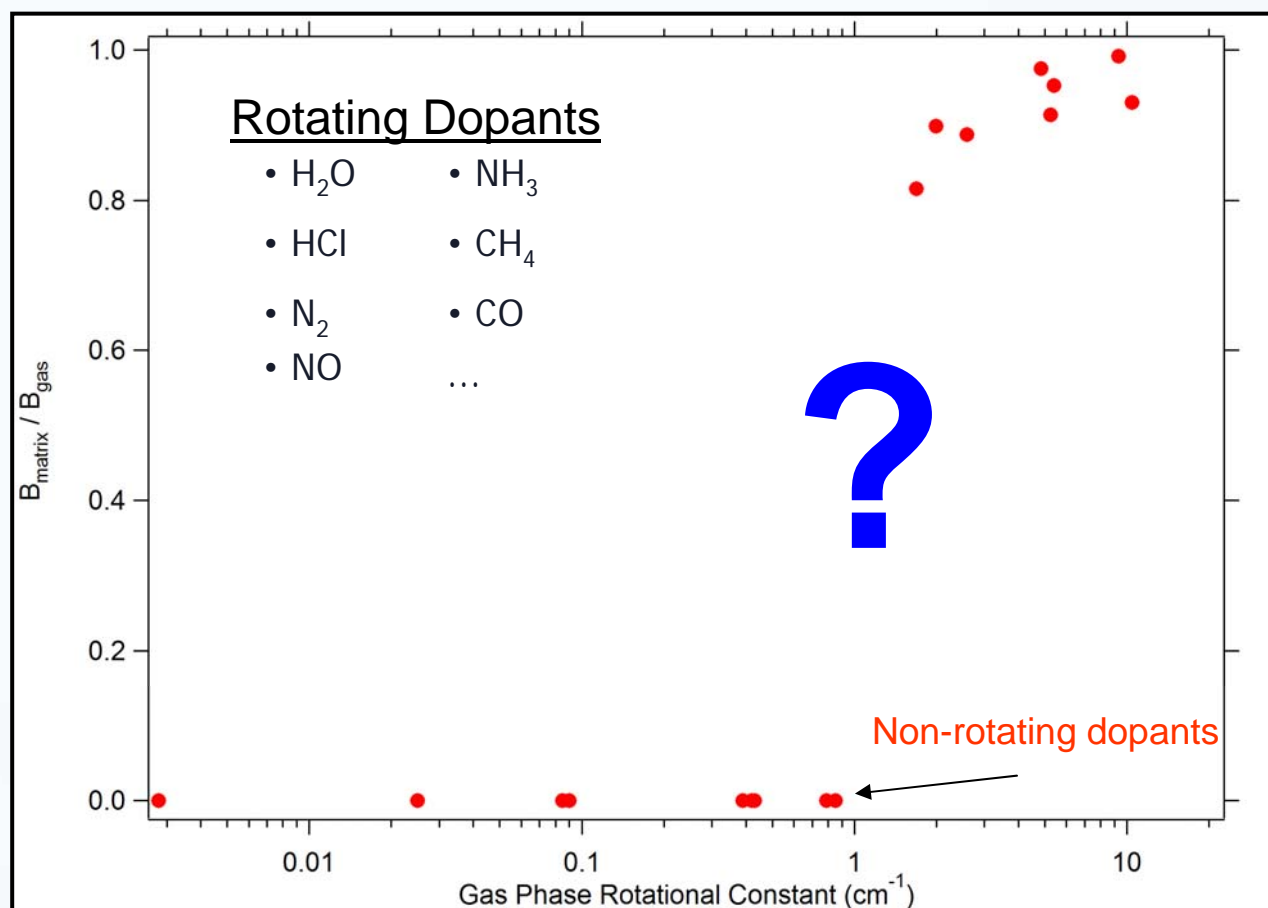


NO Energy Level Diagram (cm⁻¹)





Rotors Within Parahydrogen

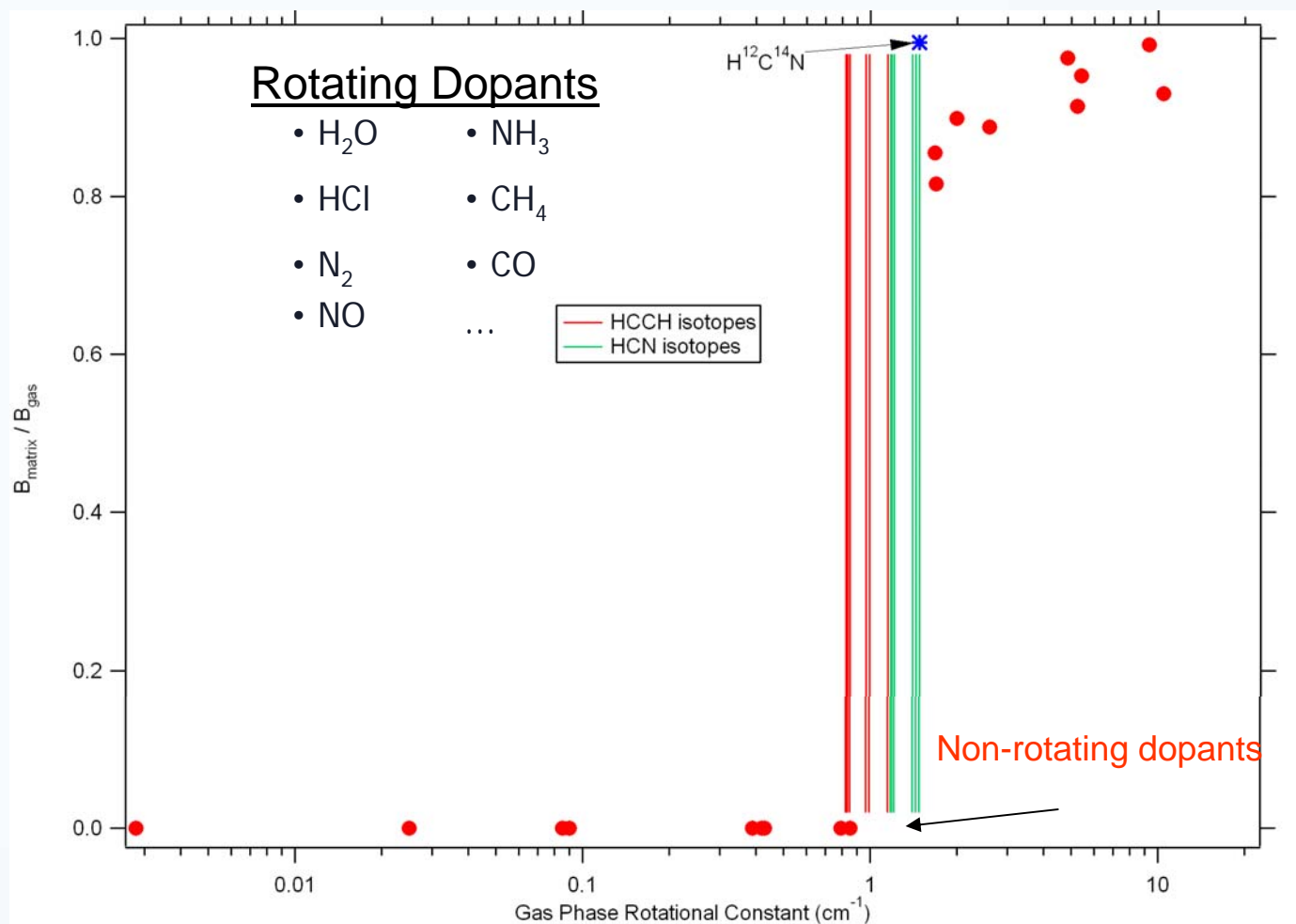


Data from the groups of M. E. Fajardo, Y.-P. Lee, and T. Momose (1995-2006).



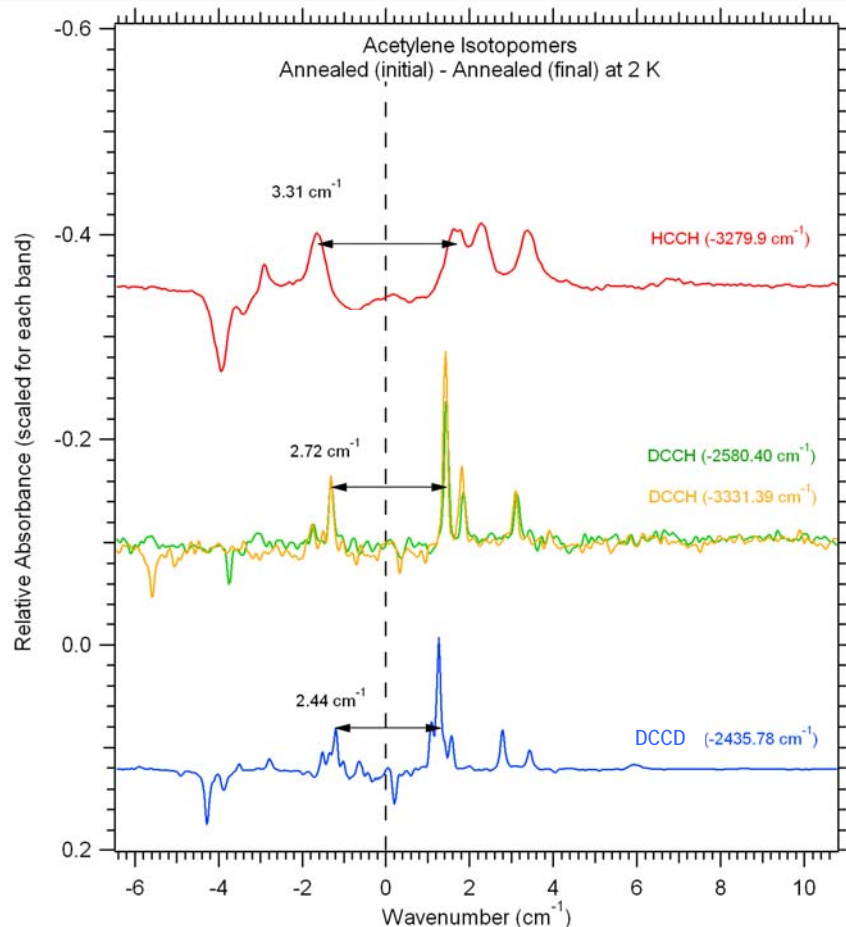


Rotors Within Parahydrogen





Preliminary C₂H₂ in parahydrogen



$E_{R(0)} - E_{P(1)} (4B)$				
	<u>Gas</u>		<u>pH₂</u>	
	Wavenumber	Relative	Wavenumber	Relative
HCCH	4.71 cm ⁻¹	1.00	3.35 cm ⁻¹	1
DCCH	3.97 cm ⁻¹	0.84	2.74 cm ⁻¹	0.82
DCCD	3.39 cm ⁻¹	0.72	2.47 cm ⁻¹	0.74

- Acetylene IR spectrum 'ages'... timescale of 30 minutes. Aging appears to be acetylene-acetylene clustering.
- "Rotational spectrum" disappears fairly quickly (but not with annealing!)

Y.P. Lee and collaborators *Chem. Phys. Lett.* **435** 247-251 (2007) – no rotation at 'high' [o-H₂]

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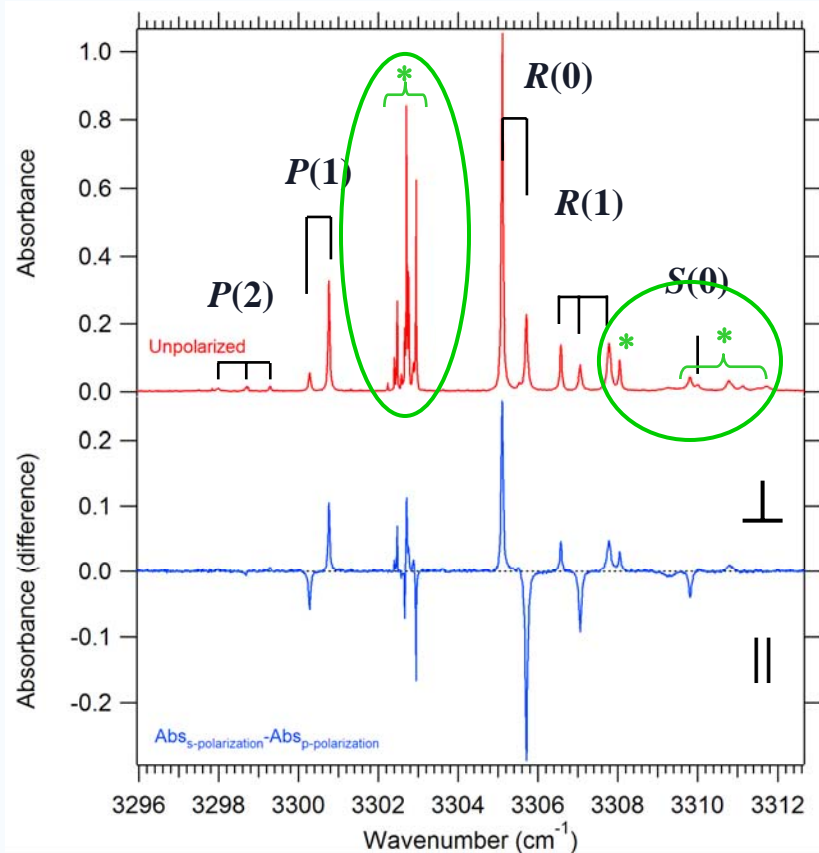
Dopant Cluster Formation in Solid Parahydrogen



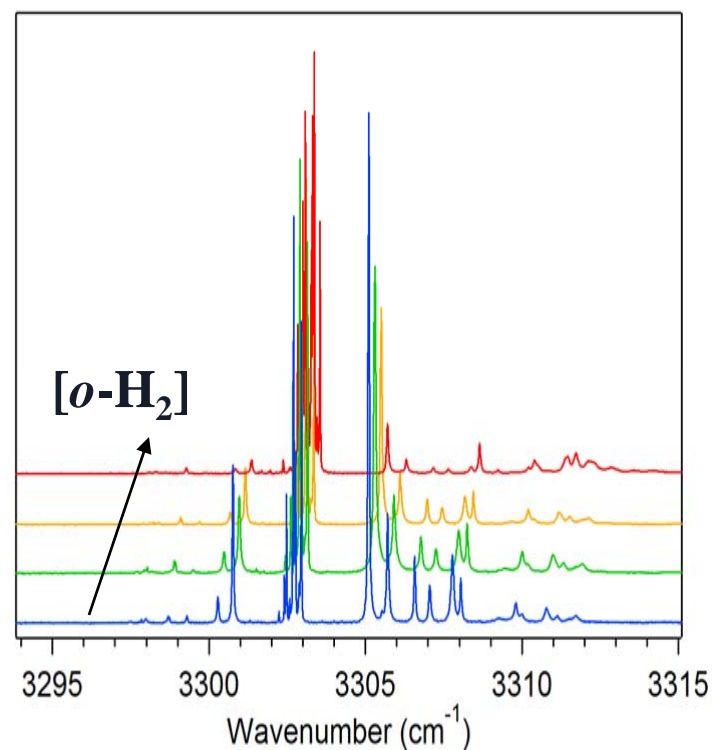


$o\text{-H}_2$ – HCN Clustering

8 ppm HCN in $p\text{-H}_2$

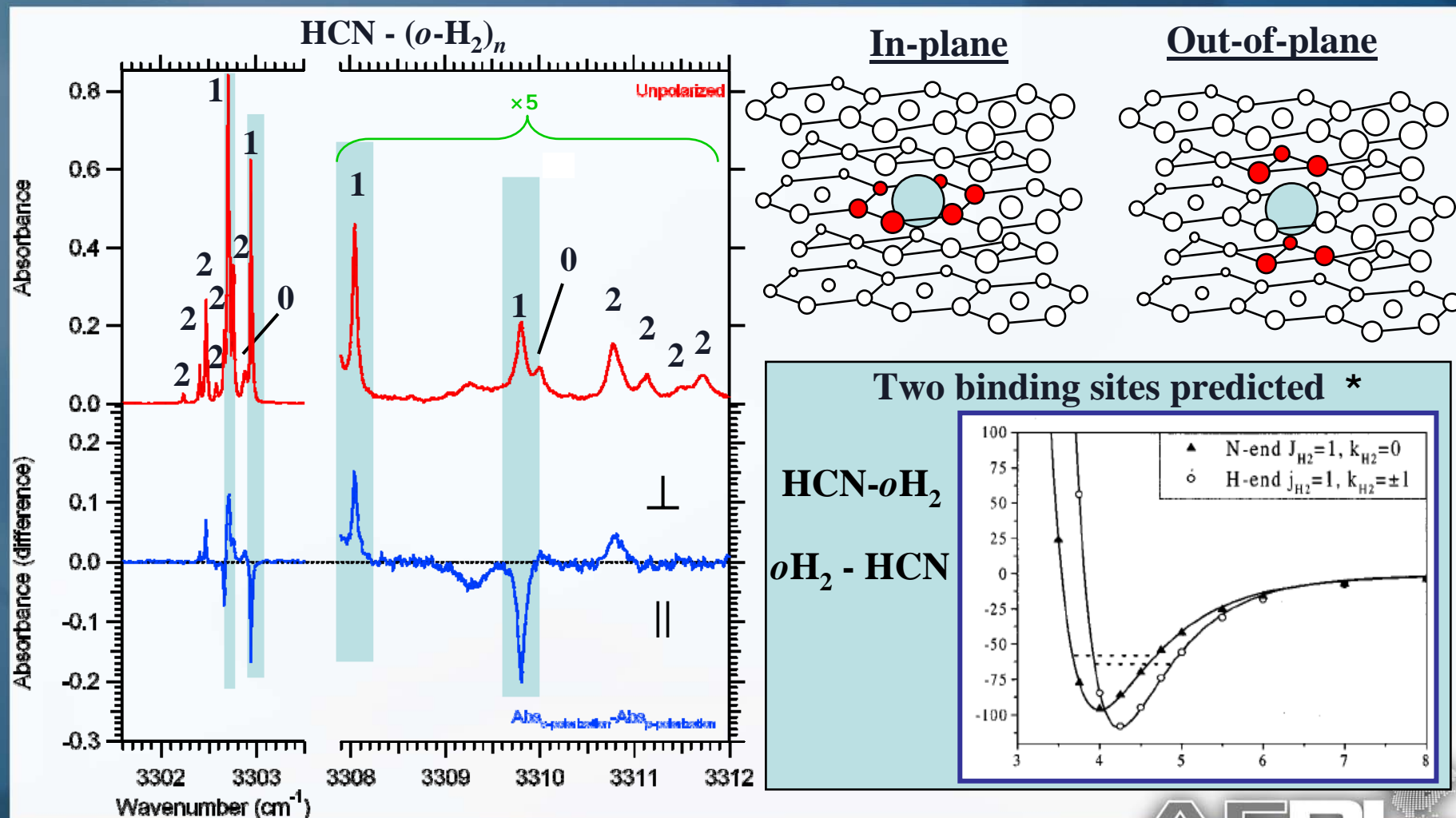


Orthohydrogen Dependence





$o\text{-H}_2$ - HCN Clustering

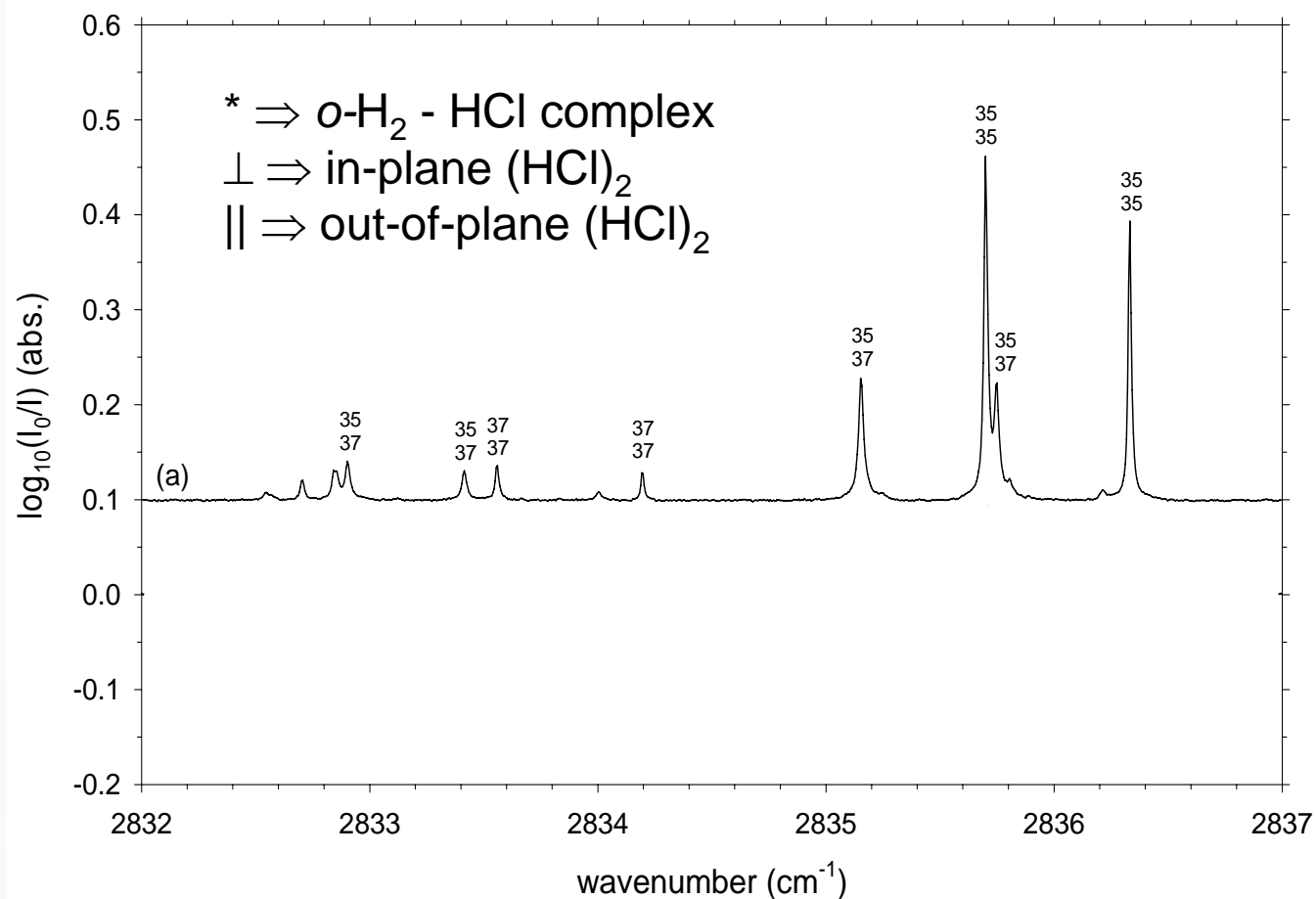


* Moore, Ishiguro, and Miller, *JCP* **115**, 5144 (2001)

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HCl dimer

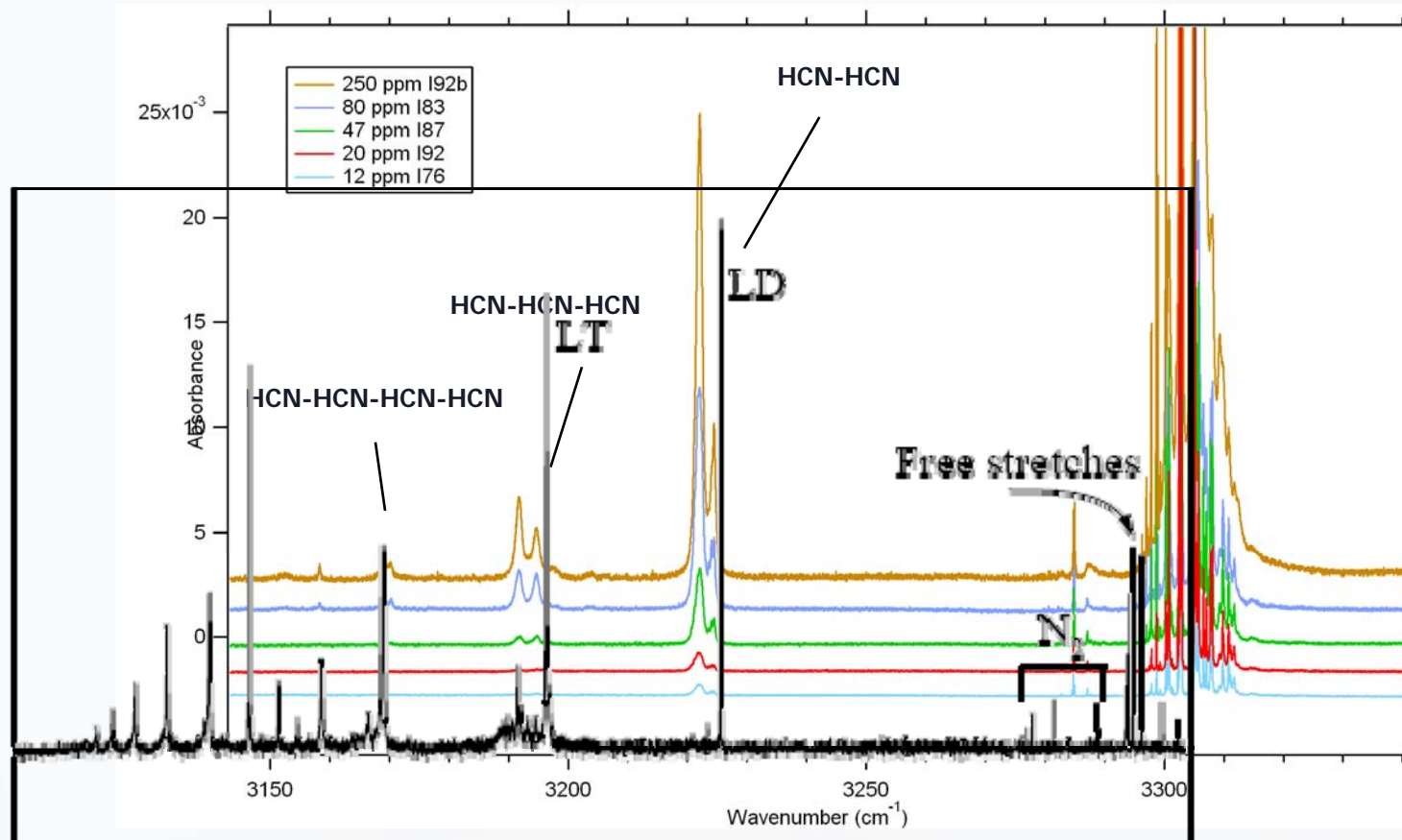


See Mario Fajardo's Poster for more details





HCN Clustering in $p\text{-H}_2(\text{s})$ – linear assembly in the solid state?



Preliminary data, work in progress





Crystallite Orientation and the Annealing Behavior of Doped Solid Parahydrogen

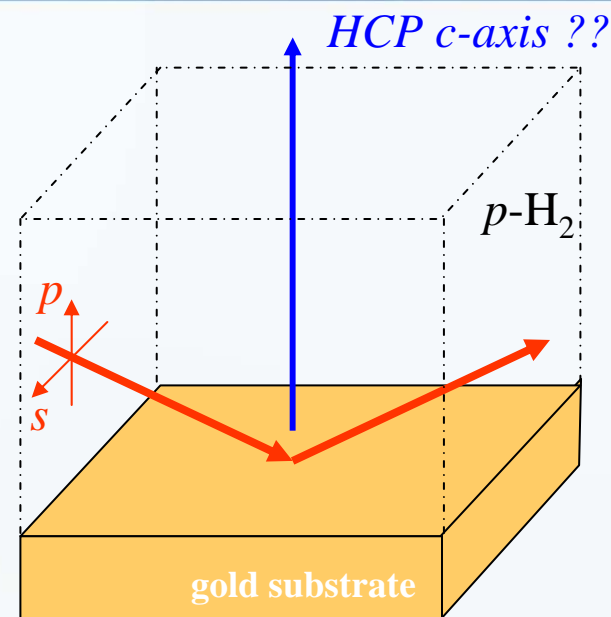




Orientation of Crystal Axis

- Lab frame versus crystal frame of reference.
- 's' – 'p' polarization provides moment relative to surface normal.
- Spectral fine structure sensitive to the local crystallite orientation.

Correlation between crystal axis and surface normal?



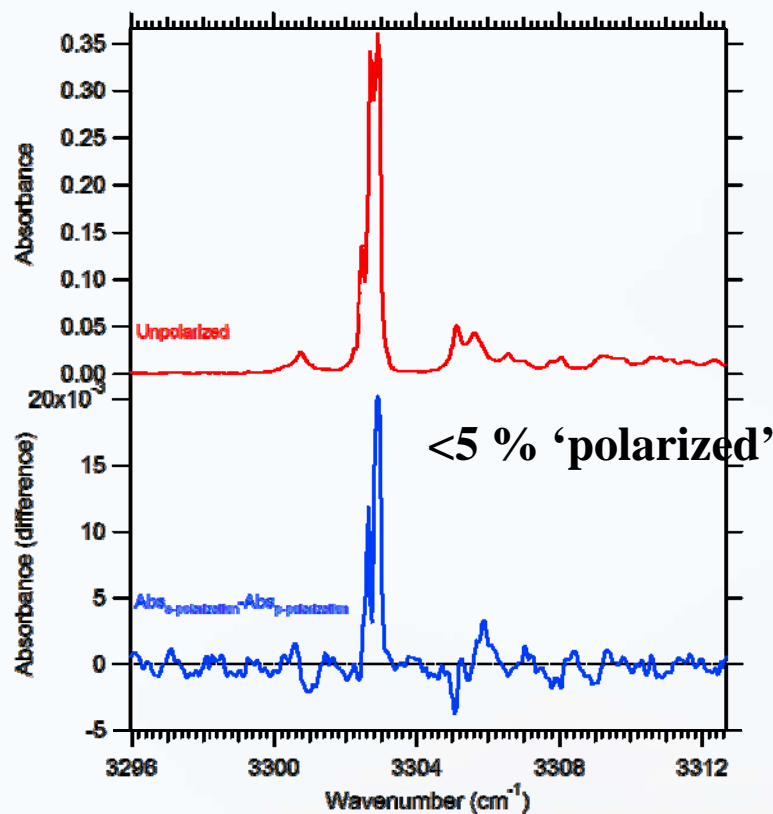
Polarization analysis provides:

- An assignment of the perpendicular and parallel components to the crystal field perturbed rotational structure (*i.e.* Δm)
- $Abs_{s-pol} - Abs_{p-pol} = \frac{1}{2} \mu_{\perp}^2 - \frac{1}{2} \mu_{\parallel}^2$

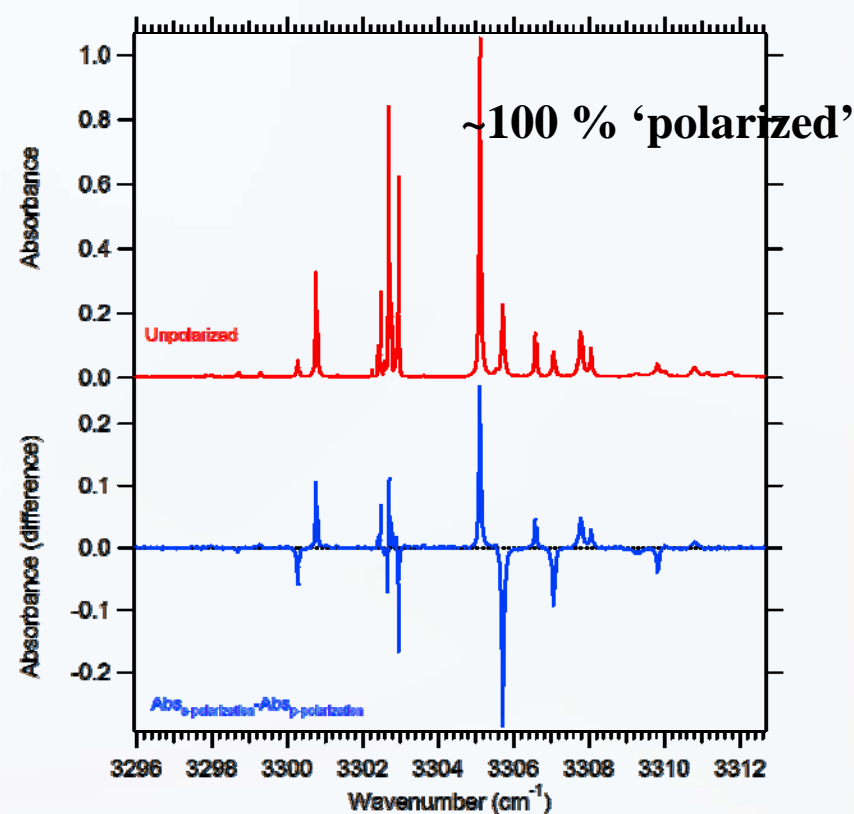


As Deposited Versus Annealed

As-deposited, 8 ppm HCN in p -H₂ @ 2.3 K



Annealed, 8 ppm HCN in p -H₂ @ 2.3 K



- Before annealing, less than 5% of the HCP features are oriented normal to the substrate.
 - After annealing, ~90% of the HCP features are oriented normal to substrate!!
- Upon deposition, HCP lattices randomly oriented, but upon annealing gain a macroscopic orientation to the laboratory frame.

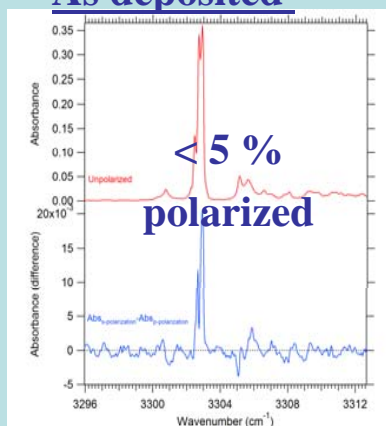




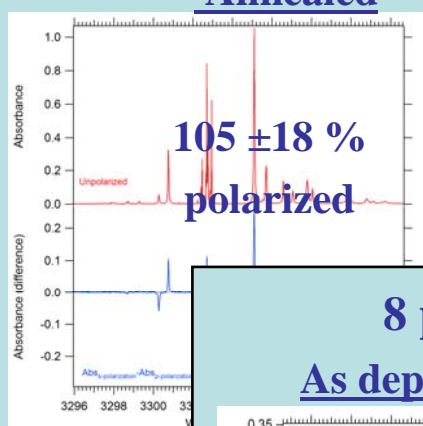
Multiple samples – HCN, CO, NO

8 ppm HCN in parahydrogen

As deposited

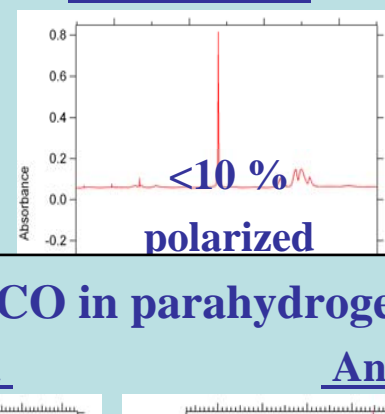


Annealed

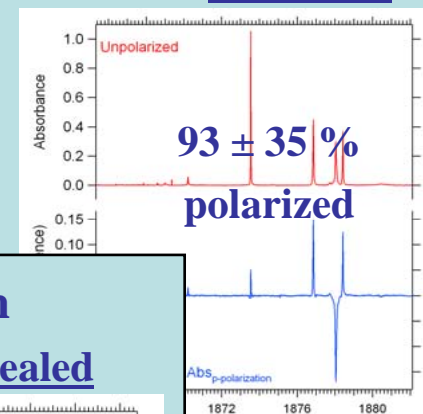


8 ppm NO in parahydrogen

As deposited

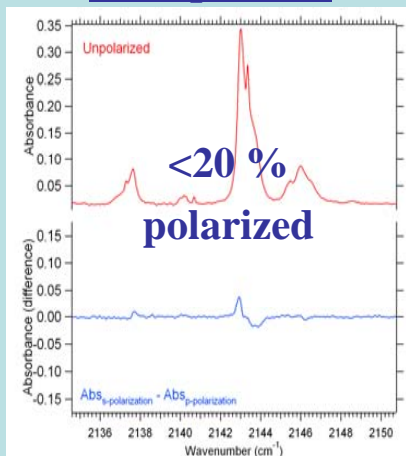


Annealed

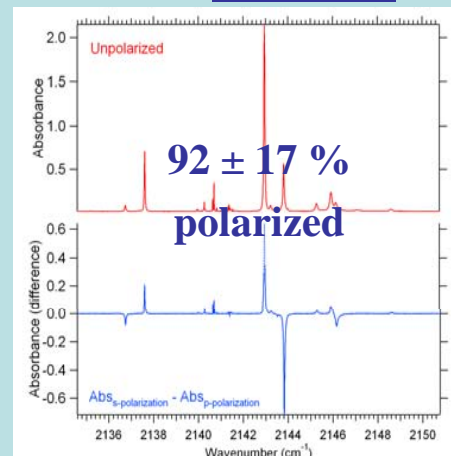


8 ppm CO in parahydrogen

As deposited



Annealed



- All exhibit virtually no alignment in as deposited samples

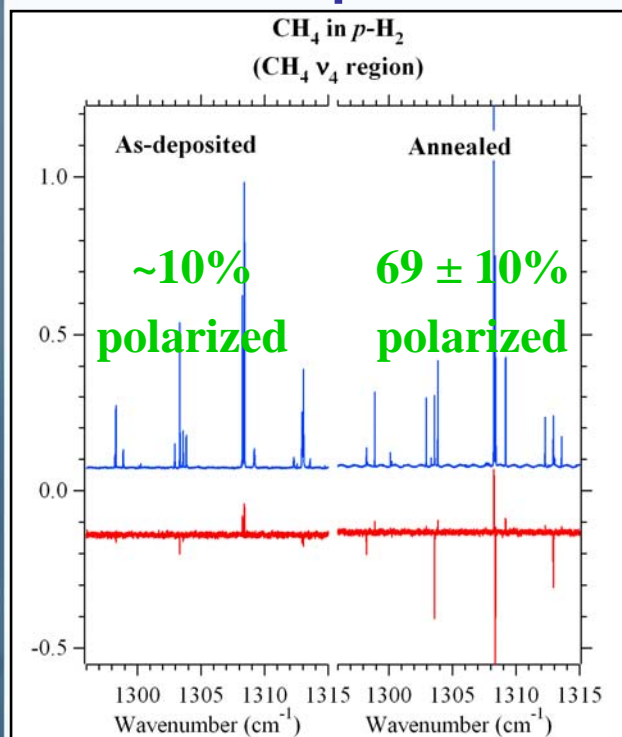
- All exhibit more than 90% alignment of crystal axis after annealing.



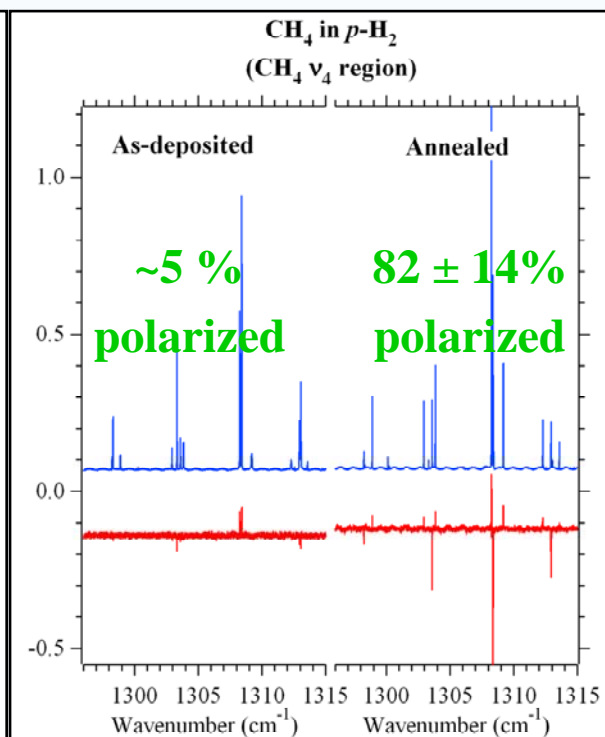


CH₄ in parahydrogen

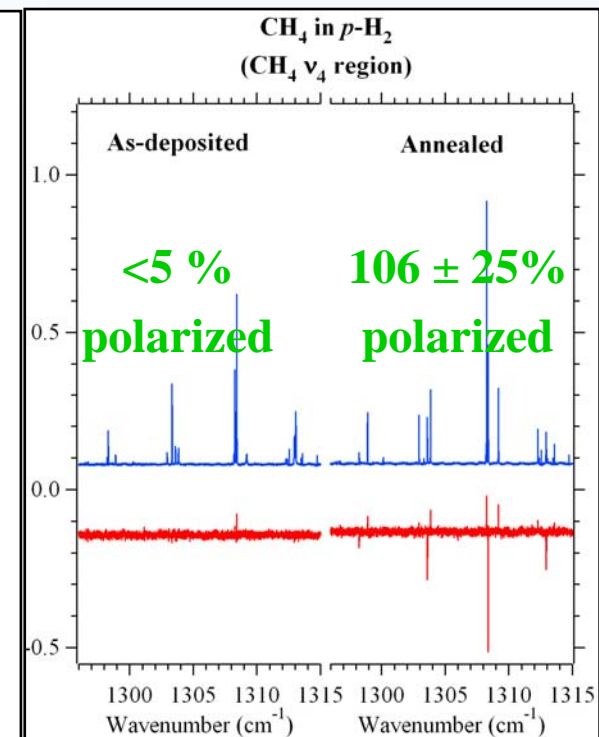
Sample 1



Sample 2



Sample 3

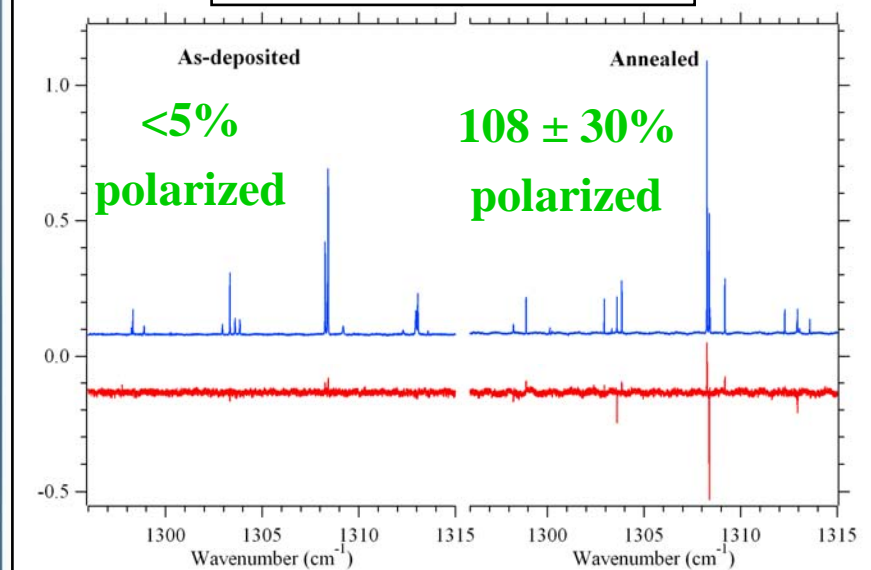


- Essentially no orientation in as deposited.
- Degree of polarization in annealed samples fluctuates for CH₄ from sample to sample.
- Dopant helps establish macroscopic orientation?

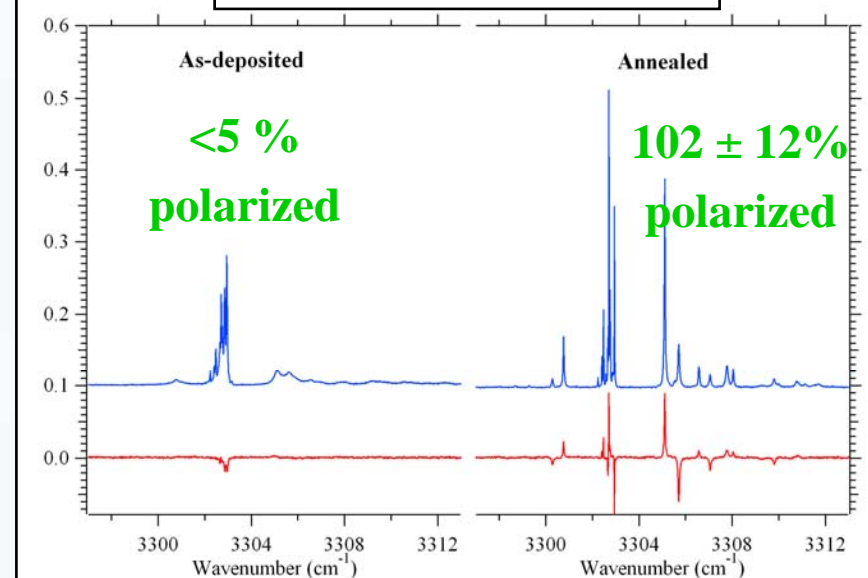


Mixed CH₄ and HCN (3.5 ppm/3.8 ppm)

CH₄ ν₄ Region



HCN ν₁ Region



- % orientation agrees in mixed samples
- HCN more influential than CH₄?



Conclusions

- Solid parahydrogen produced by Rapid Vapor Deposition is amenable to Polarization Spectroscopy:
 - Facilitates the assignment of the crystal field fine structure in the spectra of rotating dopants.
 - Sheds light on cluster formation in doped parahydrogen samples.
 - Provides new insight into the annealing behavior of the solid parahydrogen produced by RVD.

Electron and Positron irradiation of solid hydrogen presently underway

Acknowledgements:

Takamasa Momose, U. British Columbia (Crystal Field Theory)

David Anderson, U. Wyoming (NO and (HCl)₂ work)

David Moore, Lehigh U. (H₂-HCN *ab initio* potential)





Basic Research in Military

... It's alive and active

- Great job opportunities for recent grads
- Good, fundamental research efforts underway
- Opportunities for academia to help! The real challenge is in “selling” your work and providing a valid, realistic path towards an application... (more than just lip service is required)





A few final thoughts...

*“ Scientists do a great job with the details of the science.
Scientists must learn the art of the sound bite!”*

- Bill Nye (the science guy)

Interview with C&E News, 2006

“In this Worldwide economy our ability to create wealth is not/no longer bounded by physical limits/natural resources but by our ability to come up with KEY “new ideas”/Inventions. The More Education, the more Ideas and the More WEALTH, Education is THE KEY”

- Dennis Bushnell (2002)

Chief Scientist, NASA Langley

“The best way to predict the future is to invent it.”

- Alan Kay

Computer Scientist, 1991)





QUESTIONS?





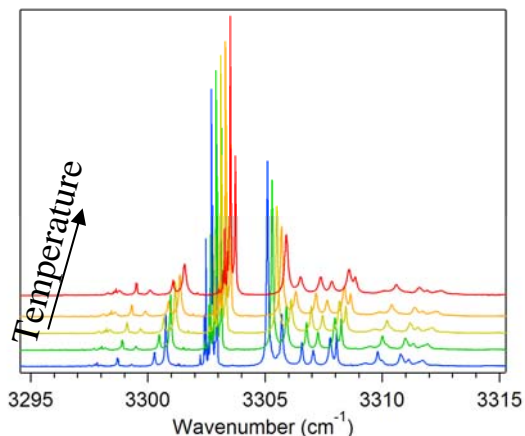
Back-up Slides



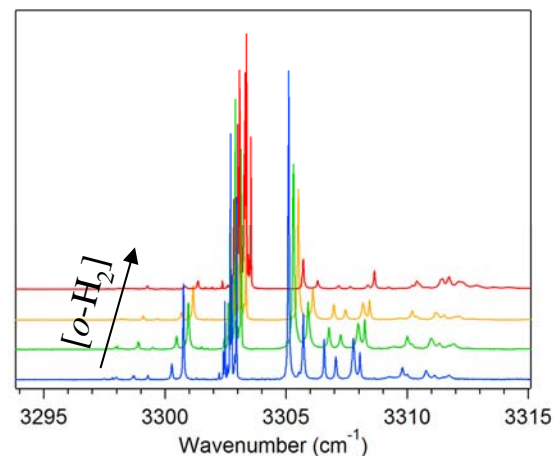


Spectral Assignments Tools

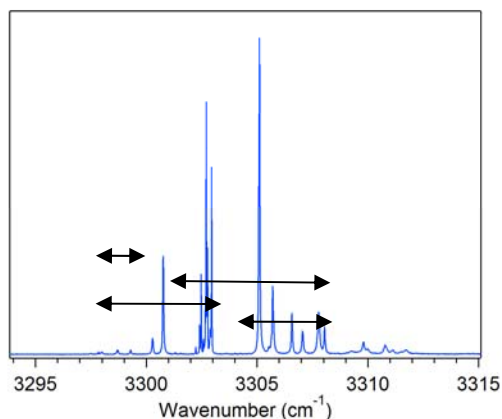
Temperature Dependence



Orthohydrogen Dependence



Combination Differences



Spectrum was interpreted by its:

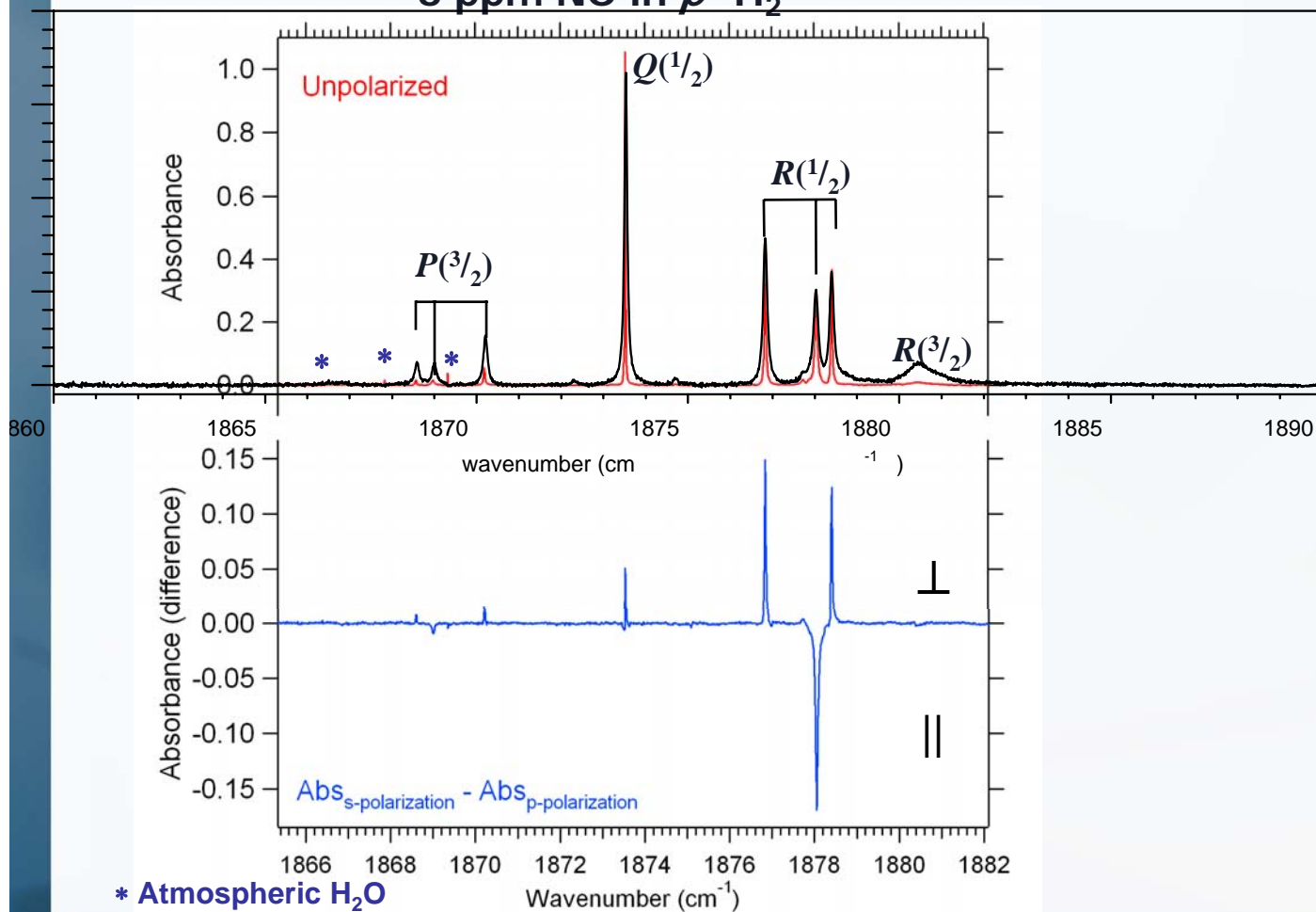
- Temperature dependence
- Orthohydrogen concentration dependence
- Transition frequency combination differences
- **Polarization dependence!**

AFRL



NO in solid parahydrogen

6 ppm NO in *p*-H₂



* Atmospheric H₂O

