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SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-VG-2001-130**
Fajardo, Mario, "Spectral Inhomogeneity as a Discrete, Countable Entity – The Role of Residual oH2 Molecules on the RoVibrational Spectra of Dopants in pH2 Solids"

56th International Symposium on Molecular Spectroscopy **(Statement A)**
Columbus OH, 11-15 June 2001) (Deadline:ASAP)

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PHILIP A. KESSEL Date
Technical Advisor
Space and Missile Propulsion Division

56th International Symposium on Molecular Spectroscopy, 11 - 15 June 2001, Ohio State University, Columbus, OH

Spectral Inhomogeneity as a Discrete, Countable Entity - The Role of Residual oH_2 Molecules on the RoVibrational Spectra of Dopants in pH_2 Solids

Mario E. Fajardo, and Simon Tam
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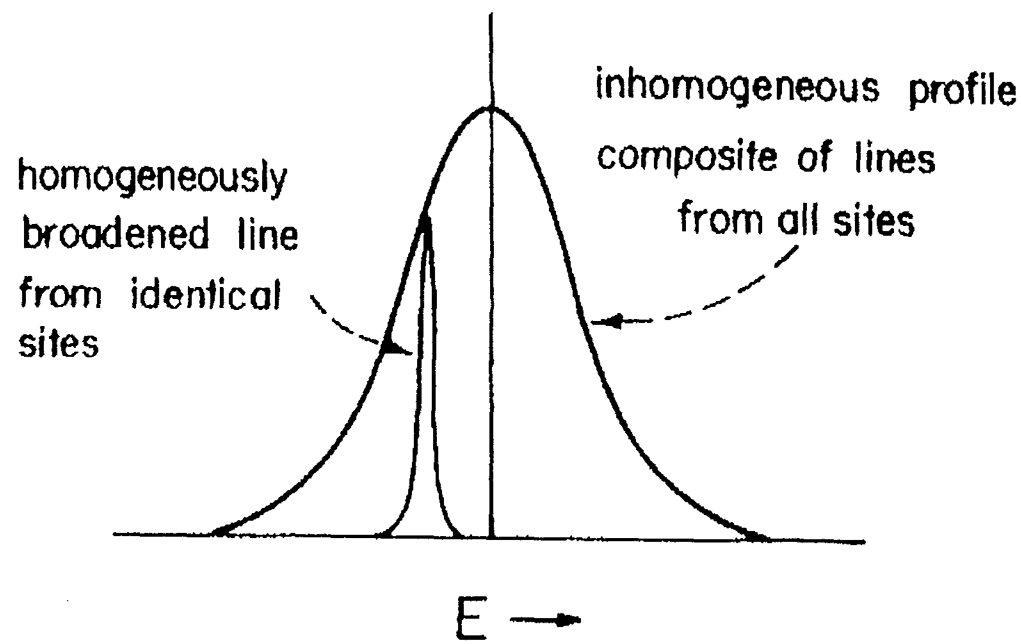
* Introduction
* Rapid Vapor Deposition of Transparent Parahydrogen (pH_2) Solids
* High Resolution IR Absorption Spectroscopy in Doped pH_2 Solids
  Rotating (CH_4) vs. Nonrotating (CO_2) Dopants
* Role of Residual oH_2 Molecules on Spectra of:
  CO_2 dopant
  H_2O dopant
* Summary

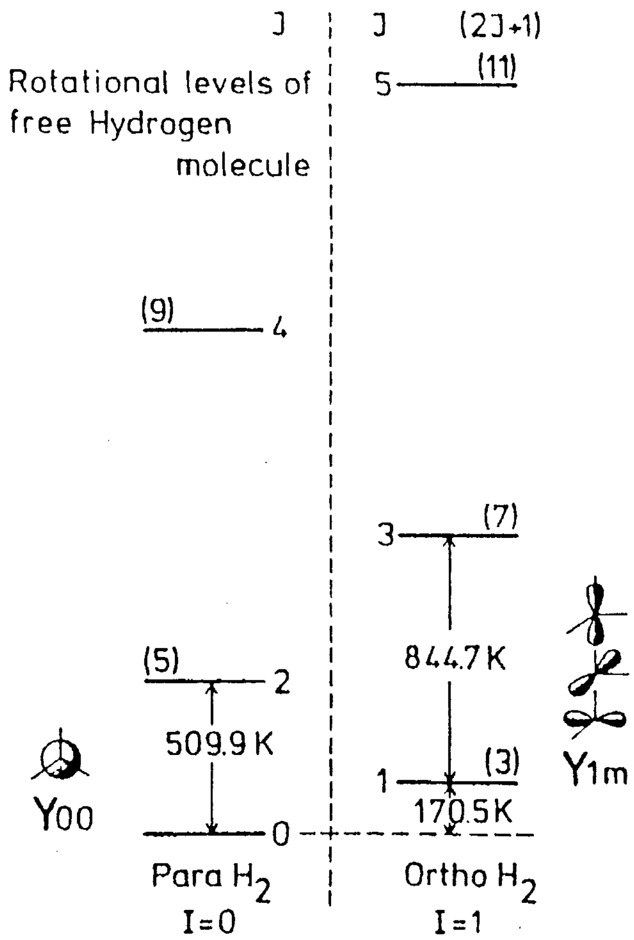
Textbook Inhomogeneous Broadening



* Assumes continuously variable peak energies for the homogeneous sub-population lines; due to imperfections e.g.: strains, dislocations, stacking faults, unintentional impurities, etc.

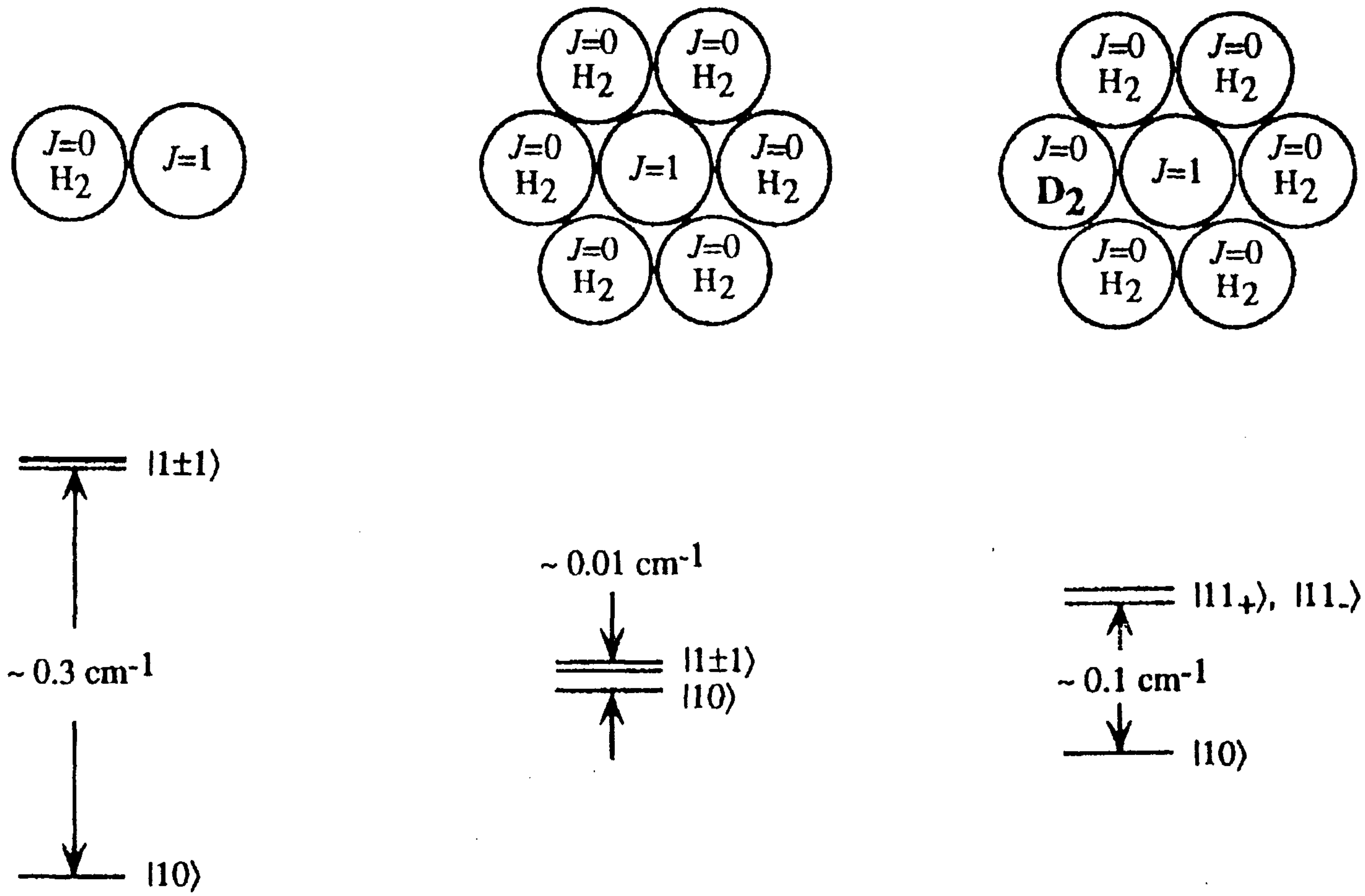
[G.F. Imbusch and R. Kopelman, "Optical Spectroscopy of Electronic Centers in Solids," in Laser Spectroscopy of Solids, edited by W.M. Yen and P.M. Selzer (Springer-Verlag, Berlin, 1986)]

ortho- and para-hydrogen



[I.F. Silvera, Rev. Mod. Phys. **52**, 393 (1980)]

oD_2-oH_2 pairs in solid pH_2



[D.P. Weliky, K.E. Kerr, T.J. Byers, Y. Zhang, T. Momose, and T. Oka, J. Chem. Phys. **105**, 4461 (1996)]

Optical Scattering in Solid Hydrogen

Crystal Growing and Quality (p. 81)

"There is a considerable art to growing hydrogen crystals of high quality. Good crystals are always grown slowly from the melt; a rapid freeze from the gas produces snow."

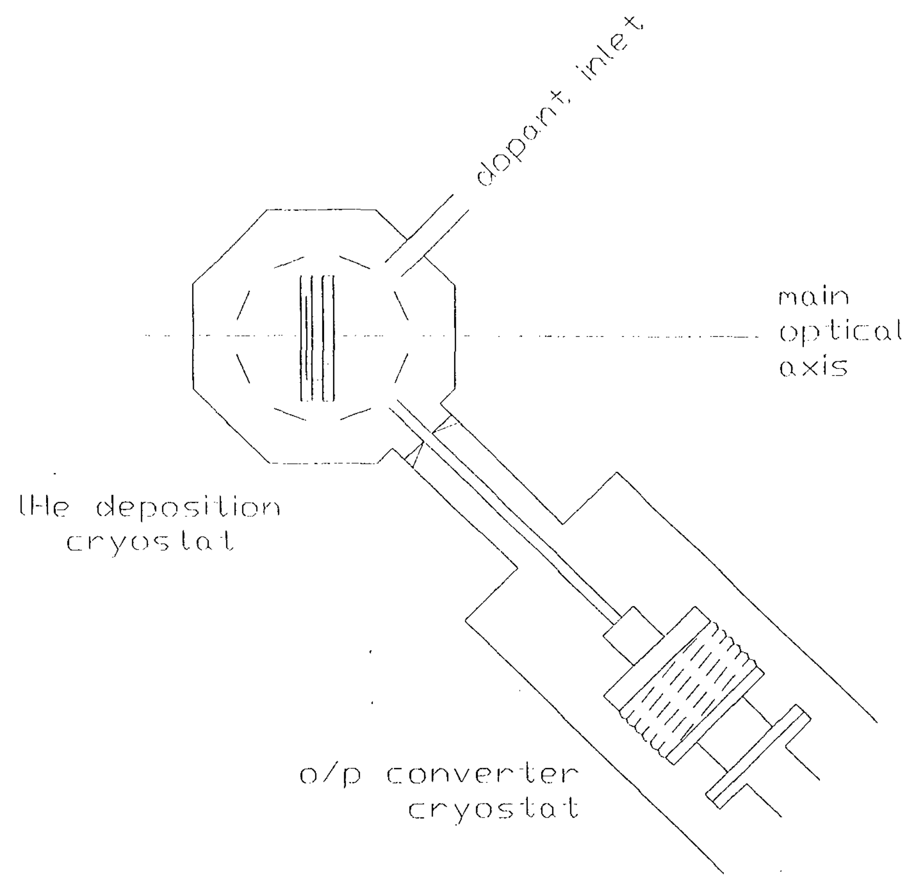
Crystallite Light Scattering (p. 83)

"The reason that a good hydrogen crystal is so hard to see is its low refractive index...an estimated 1.16!

Yet a 1 mm-thick layer of hydrogen crystallites can be a completely opaque brown-black."

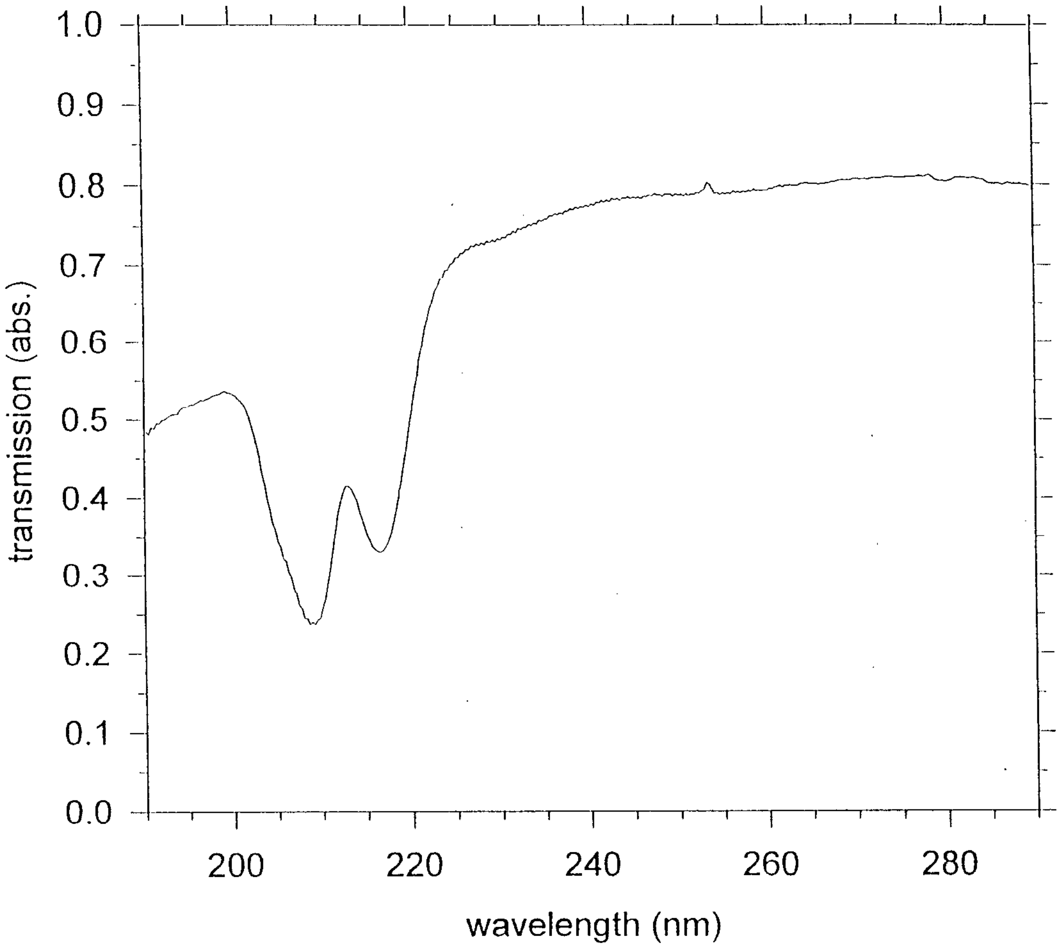
[P.C. Souers, Hydrogen Properties for Fusion Energy (UC Press, Berkeley, 1986)]

Experimental Diagram (c1997)



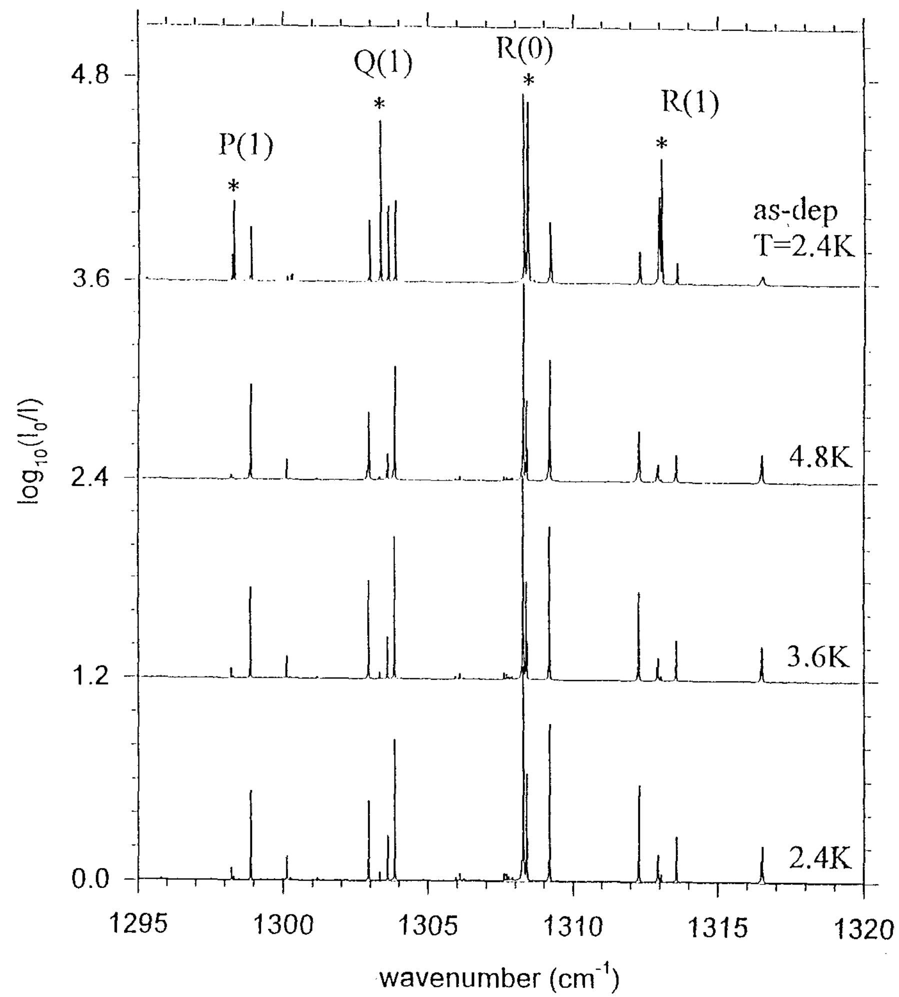
M.E. Fajardo and S. Tam, J. Chem. Phys. **108**, 4237 (1998).
S. Tam and M.E. Fajardo, Rev. Sci. Instrum. **70**, 1926 (1999).

Transmission Spectrum of B/pH_2 d≈1mm



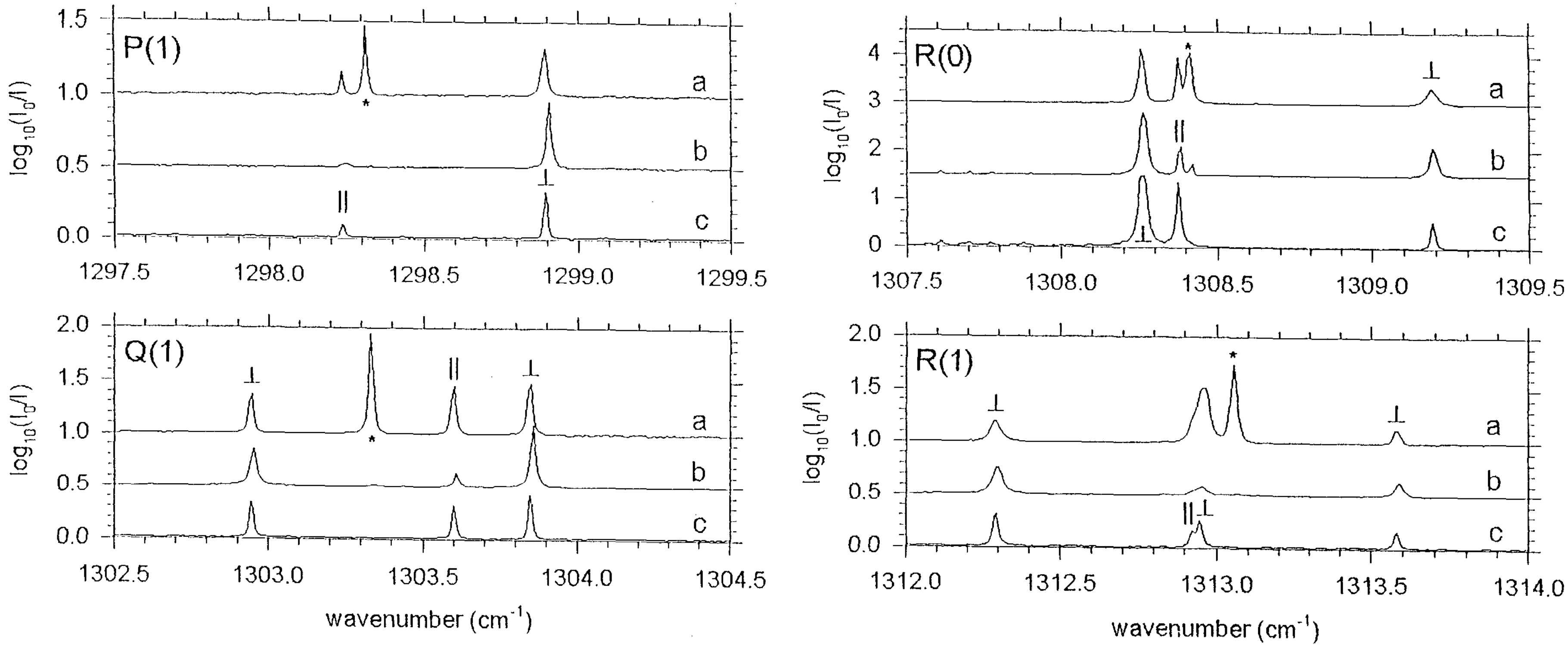
M.E. Fajardo and S. Tam, J. Chem. Phys. **108**, 4237 (1998).
S. Tam, M. Macler, M.E. DeRose, and M.E. Fajardo, J. Chem. Phys. **113**, 9067 (2000).

ν_4 CH_4/pH_2 IR Absorptions (res = 0.01 cm^{-1})



S. Tam, M.E. Fajardo, H. Katsuki, H. Hoshina, T. Wakabayashi, and T. Momose, J. Chem. Phys. **111**, 4191 (1999).

ν_4 CH_4/pH_2 IR Absorptions



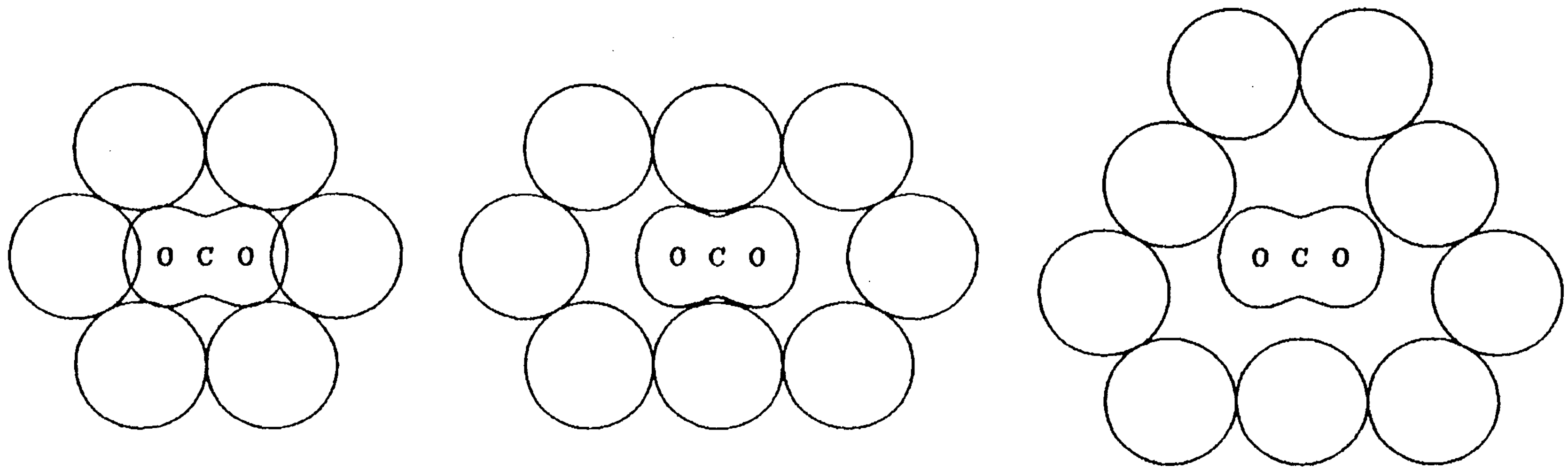
(a) Rapid Vapor Deposited sample: as-deposited at 2.4 K

(b) Rapid Vapor Deposited sample: annealed to 4.8 K

(c) Enclosed Cell Condensed sample: cooled to 4.8 K

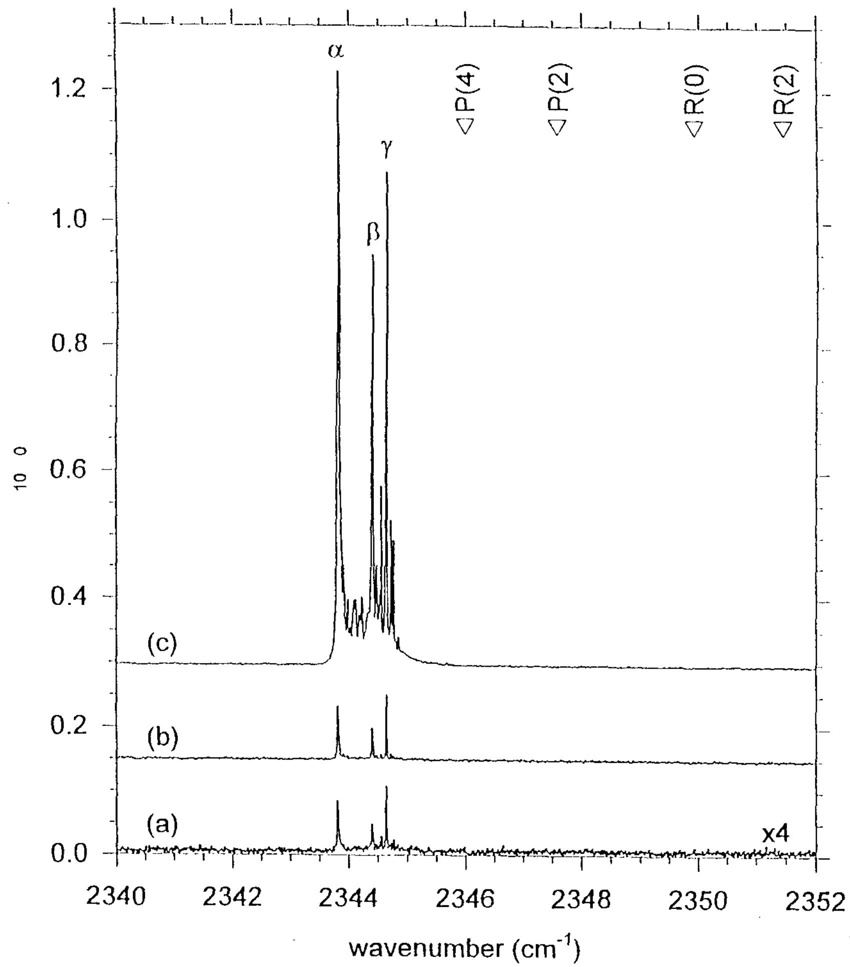
S. Tam, M.E. Fajardo, H. Katsuki, H. Hoshina, T. Wakabayashi, and T. Momose, J. Chem. Phys. **111**, 4191 (1999).

CO_2/pH_2 Trapping Sites



S. Tam and M.E. Fajardo, Fiz. Nizk. Temp. **26**, 889 (2000) {Low Temp. Phys. **26**, 653 (2000)}.

CO_2/pH_2 IR Absorptions



as-deposited at T = 2.4 K

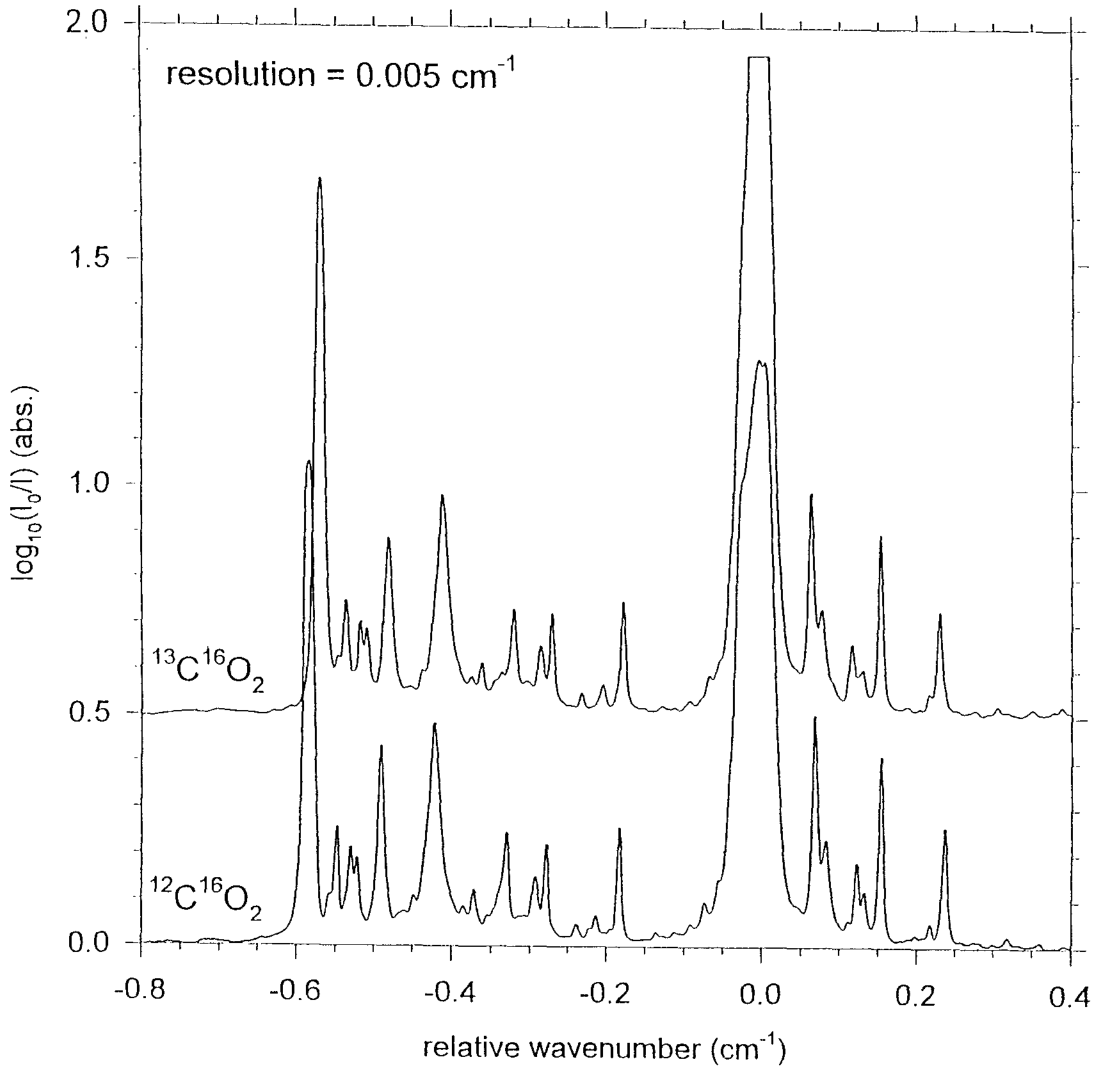
d ≈ 1 mm

res = 0.008 cm^{-1}

(c) 1.2 ppm CO_2/pH_2
(b) 0.04 ppm CO_2/pH_2
(a) 0.01 ppm CO_2/pH_2

S. Tam and M.E. Fajardo, Fiz. Nizk. Temp. **26**, 889 (2000) {Low Temp. Phys. **26**, 653 (2000)}.

$^{13}C^{16}O_2/^{12}C^{16}O_2/pH_2$

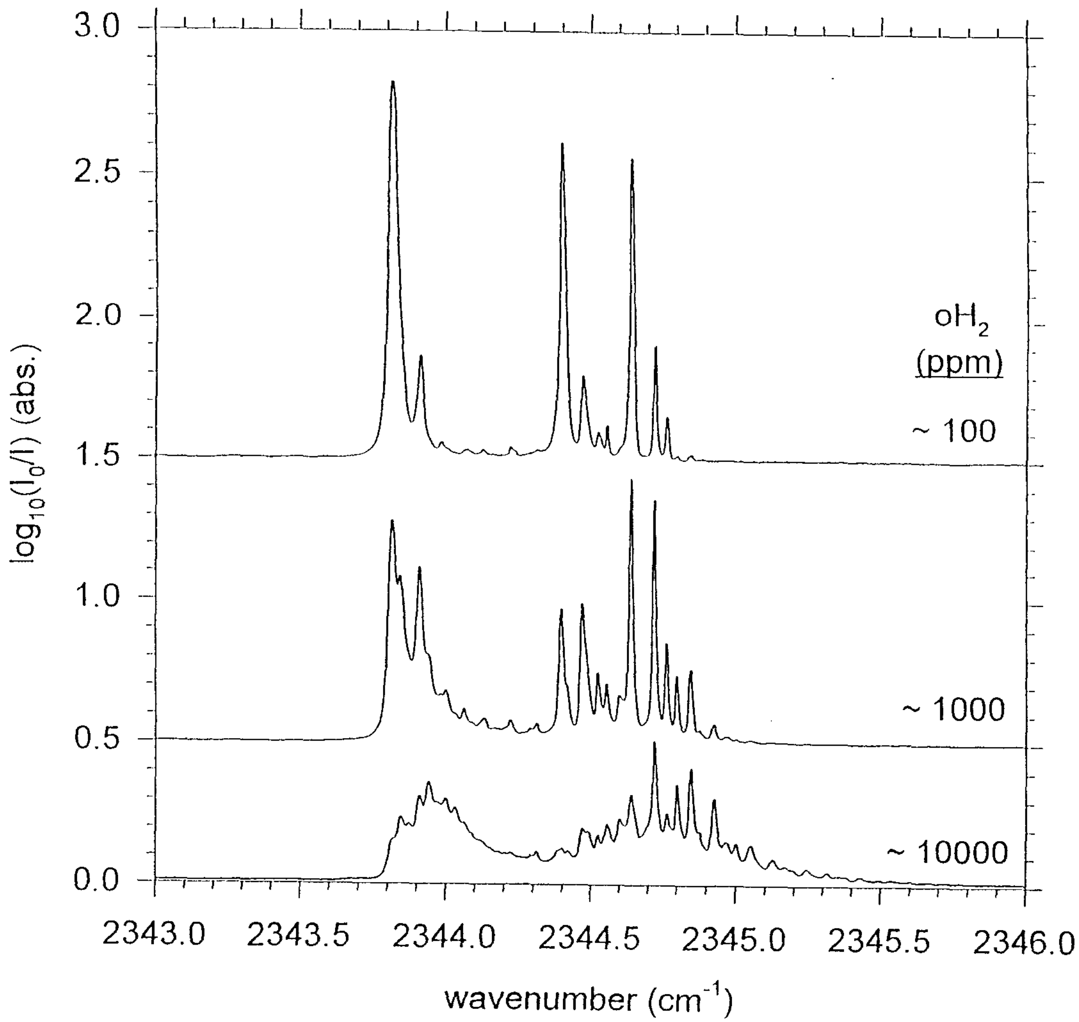


annealed, T = 2.4 K

d = 1.0 mm

2 ppm $^{13}C^{16}O_2$ and
2 ppm $^{12}C^{16}O_2$

$(oH_2)_n$ - CO_2 clusters



as-deposited

T = 2.4 K

d ≈ 1 mm

CO_2-$(oH_2)_n$ Counting Scheme

* $CO_2/oH_2/pH_2$ peaks start out as well separated, discrete features
  ⇒ try counting them!

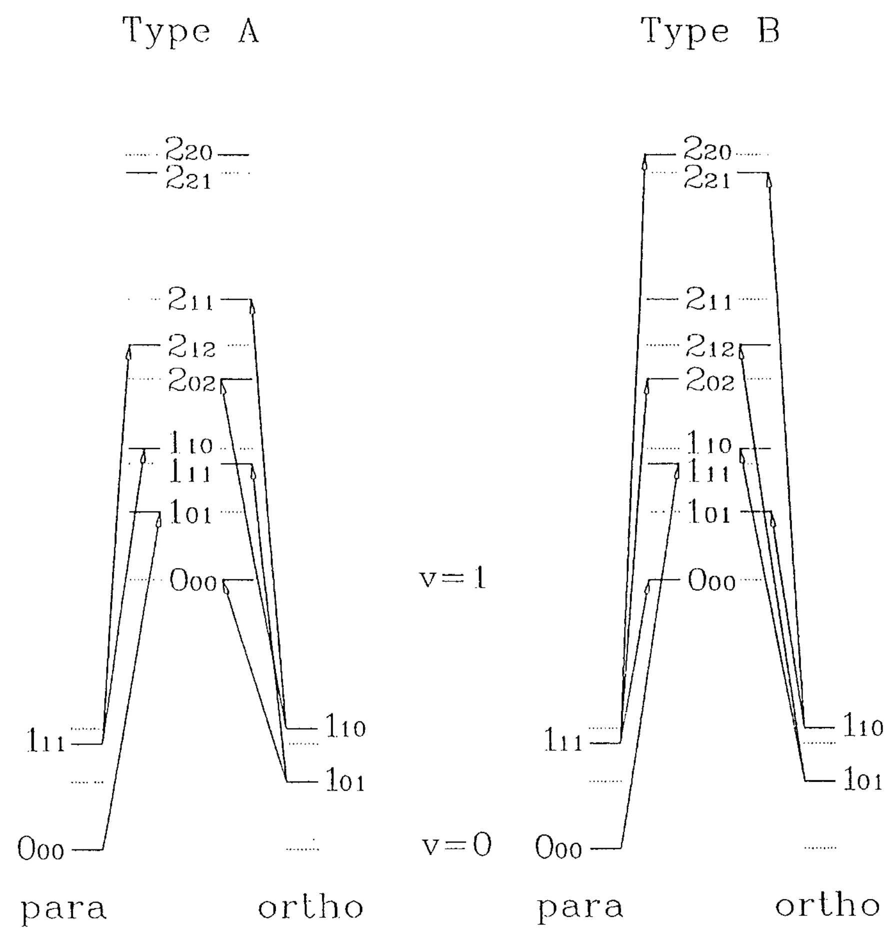
* CO_2-oH_2: nn ip, nn oop, nnn

* CO_2-$(oH_2)_2$:
  nn ip + nn ip (3x)
  nn oop + nn oop (3x)
  nn ip + nn oop (3x)
  nn + nnn, nnn + nnn

* CO_2-$(oH_2)_3$:
  nn ip + nn ip + nn ip (3x)
  nn oop + nn oop + nn oop (3x)
  nn ip + nn ip + nn oop (9x)
  nn ip + nn oop + nn oop (9x)
  nn^2 + nnn, nn + nnn^2, nnn^3

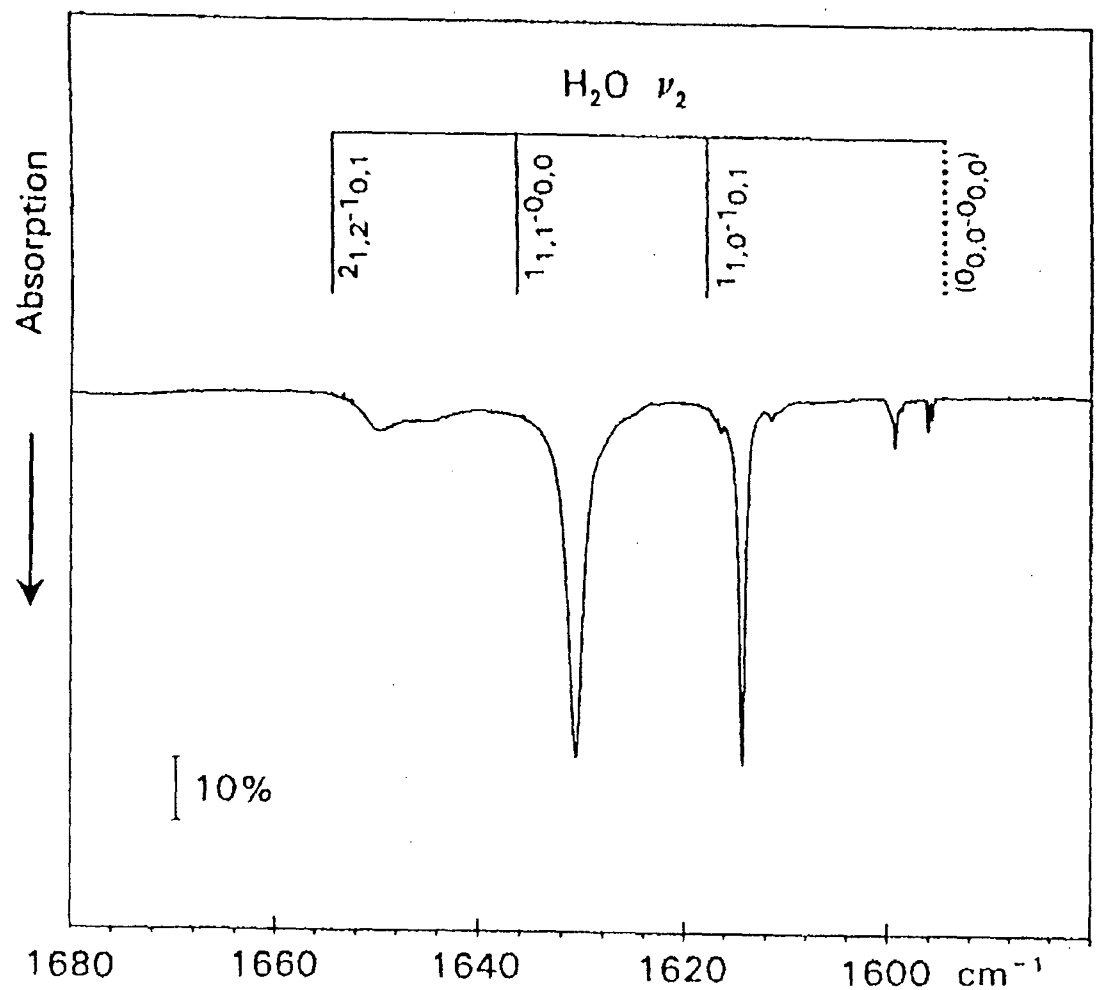
* CO_2-$(oH_2)_n$…

Allowed IR Transitions of gas-phase H_2O



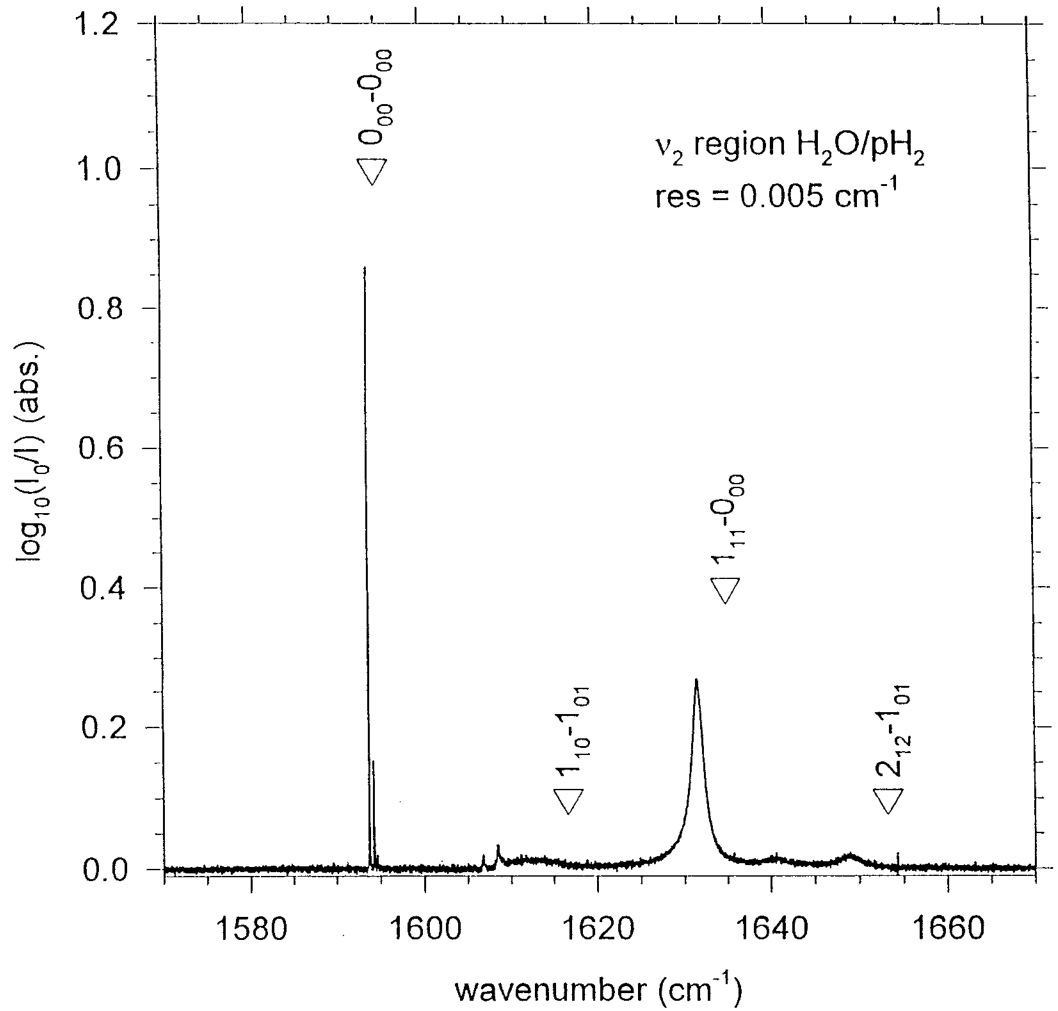
[J.A. Glasel, J. Chem. Phys. **33**, 252 (1960)]
[G. Herzberg, Molecular Spectra and Molecular Structure, Vol. II (Krieger, Malabar, FL, 1991)]

Matrix Isolated H_2O/Ne

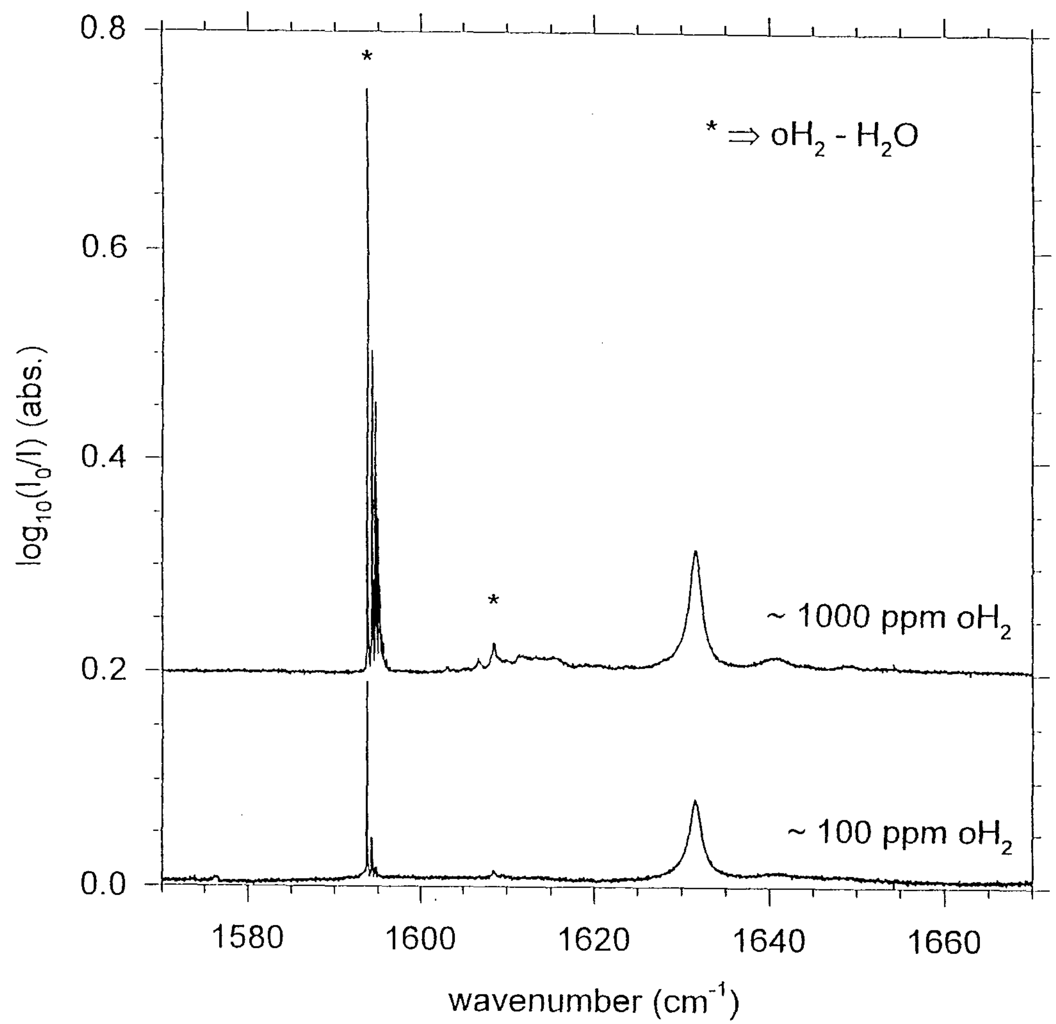


[D. Forney, M.E. Jacox, W.E. Thompson, J. Mol. Spec. **157**, 479 (1993)]

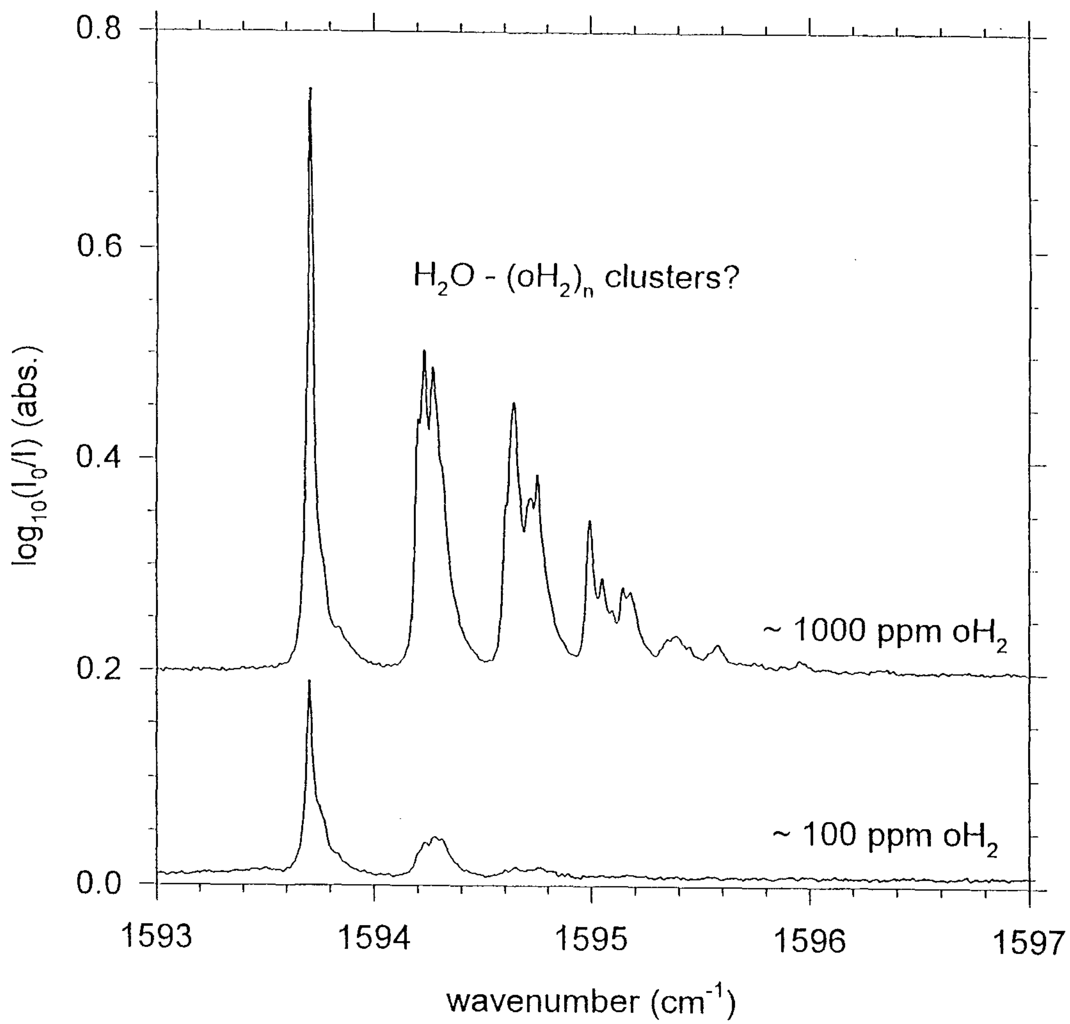
15 ppm H_2O/pH_2 d ≈ 3 mm



$H_2O/oH_2/pH_2$


* ⇒ oH2 - H2O
~ 1000 ppm oH2
~ 100 ppm oH2
log10(I0/I) (abs.)
wavenumber (cm-1)
0.8
0.6
0.4
0.2
0.0
1580
1600
1620
1640
1660

$H_2O/oH_2/pH_2$ detail



Summary

* Demonstrated suitability of Rapid Vapor Deposited pH_2 solids as hosts for high resolution IR absorption spectroscopy of chemically interesting dopants.

* Fine structure in IR spectra of CO_2/pH_2 solids is due to CO_2-$(oH_2)_n$ clusters.

* Initially well-separated CO_2-oH_2 peaks
  $\Rightarrow$ interesting system for hole-burning studies (?)

* oH_2 impurities can stop the rotation of H_2O dopants in solid pH_2

* Speculate that IR spectra of $H_2O/oH_2/pH_2$ solids may provide sensitive measure of anisotropy of H_2O-oH_2 interaction potential [analysis ala Weliky et al., JCP (1996)].

Collaborators

* Mr. Simon Tam and Ms. Michelle E. DeRose, AFRL/PRSP
  responsible for our experimental data.

* Prof. Takamasa Momose, Kyoto U.
  spectroscopy of CH_4, C_{60}, and CO doped pH_2 solids.

* Prof. Robert J. Hinde, U. Tennessee at Knoxville
  dopant-induced IR absorptions.

* Prof. David T. Anderson, U. Wyoming
  spectroscopy of HCl and $(HCl)_2$ in solid pH_2.