



23031208 TP-FY99-0110

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✓ DTS

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MEMORANDUM FOR PRR (Contractor/In-House Publication)

1 June 1999

FROM: PROI (TI) (STINFO)

SUBJECT: Authorization for Release of Technical Information, Control Number: AFRL-PR-ED-TP-FY99-0110  
Fajardo and Tam, "High Resolution Infrared Absorption Spectroscopy of Molecular Dopants in Cryogenic Solid Parahydrogen"

(Public Release)

Poster Session HEDM CONFERENCE

# High Resolution Infrared Absorption Spectroscopy of Molecular Dopants in Cryogenic Solid Parahydrogen

Mario E. Fajardo and Simon Tam

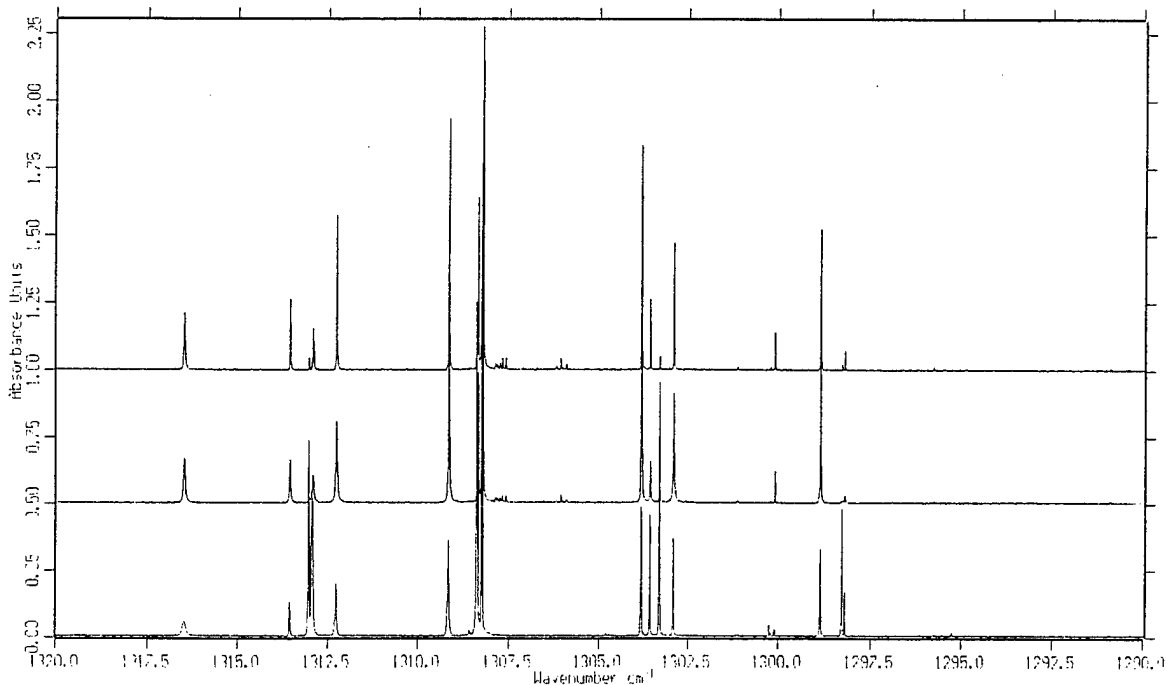
US Air Force Research Laboratory, Propulsion Directorate  
(AFRL/PRSP Bldg. 8451, Edwards AFB, CA 93524-7680) mario\_fajardo@ple.af.mil

Premature claims of successful energy storage in cryogenic solids date back to the National Bureau of Standards' Free Radicals program. Such errors typically result from reliance on unsupplemented calorimetric data, which shed little light on the mechanism of energy storage, *i.e.*, chemical identities of the energetic species and microscopic structures within the trapping medium. **Only spectroscopic measurements provide the species and structure specific information required for directed incremental progress towards higher stored energy densities.**

In HEDM program funded studies, Oka and co-workers pioneered the use of high resolution spectroscopic techniques in solid parahydrogen ( $pH_2$ ). Our rapid vapor deposition sample preparation technique now enables us to trap virtually any volatilizable species in solid  $pH_2$ . We present results of high resolution infrared absorption experiments on  $pH_2$  solids doped with isolated molecules and small clusters.

**DISTRIBUTION STATEMENT A**  
Approved for Public Release  
Distribution Unlimited

## 13 PPM $CH_4/pH_2$ $d \approx 3mm$



st27011.8      annealed    T=2.4K  
st27011.4      annealing    T=4.8K  
st27011.2      as deposited T=2.4K

resolution = 0.0075 cm<sup>-1</sup>

20021121 033

## OBJECTIVE

Develop infrared (IR) absorption spectroscopic diagnostics for HEDM doped cryogenic parahydrogen (pH<sub>2</sub>) solids.

## APPROACH

Collect high resolution IR spectra of pH<sub>2</sub> solids doped with non-energetic species: prototypical diatomic, triatomic, linear polyatomic, symmetric top, and spherical top dopant molecules.

Model data as "matrix-perturbed" gas phase spectra, if possible. Develop new spectroscopic models in collaboration with AFRL/Edwards Theory group, as necessary.

## SUMMARY

Many, but not all, molecular dopants exhibit very sharp ( $\sim 0.01$  cm<sup>-1</sup> FWHM) IR absorption lines in solid pH<sub>2</sub>, providing an extremely detailed window into trapping site structures and dynamics.

Model for spherical top molecules trapped in single substitutional sites in fcc and hcp solid pH<sub>2</sub> developed in collaboration with Prof. T. Momose of Kyoto U. is completely successful in explaining spectra of CH<sub>4</sub>/pH<sub>2</sub> system. Model of trapped diatomic molecules forthcoming.

## FUTURE DIRECTIONS

Develop model for dopants trapped in multi-substitutional vacancies.

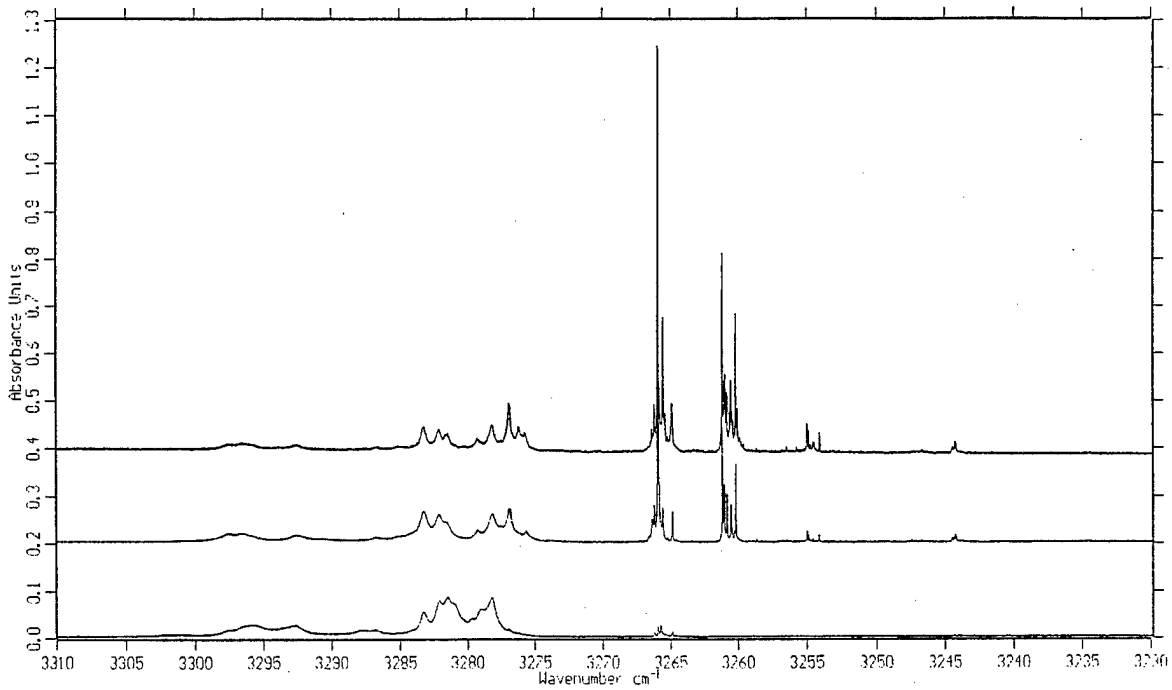
Include effects of lattice relaxation via quantum Monte Carlo methods.

Flow

2 Surveys

Back

ppm  
~~9 PPM~~ C<sub>2</sub>H<sub>2</sub>/pH<sub>2</sub> d≈3mm

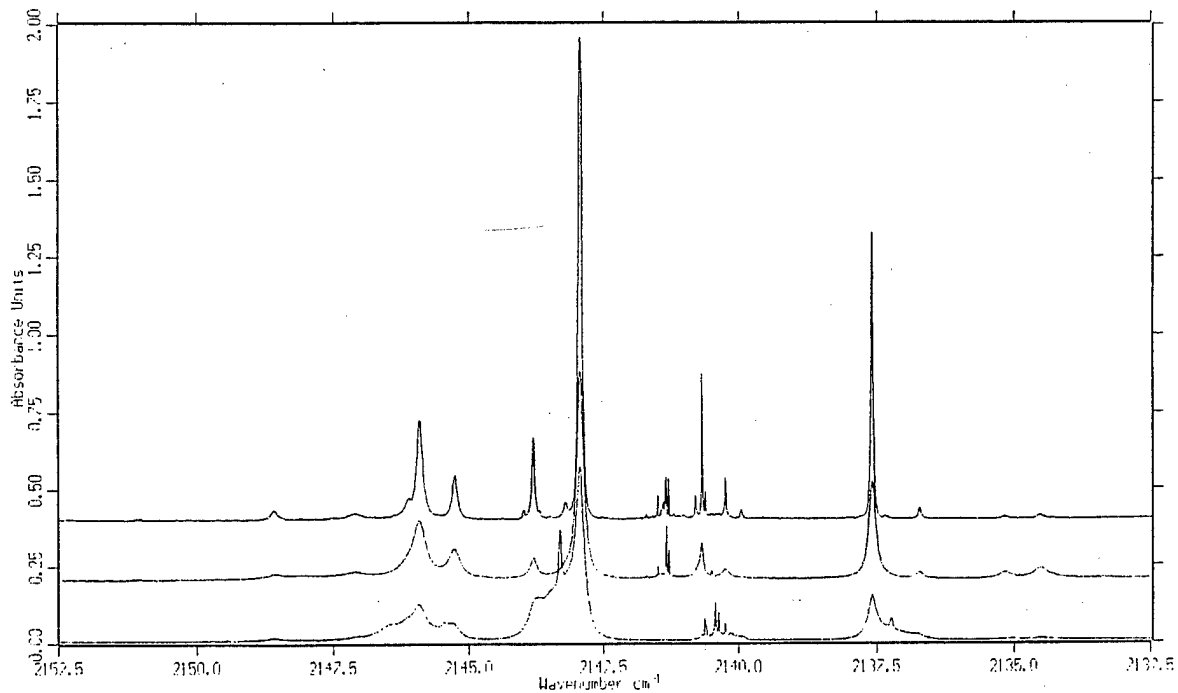


st28034.13     annealed     T=2.4K  
 st28034.7     annealing     T=4.8K  
 st28034.5     as deposited     T=2.4K

resolution = 0.005 cm<sup>-1</sup>

ST28034.5

ppm  
~~13 PPM~~ CO/pH<sub>2</sub> d≈3mm

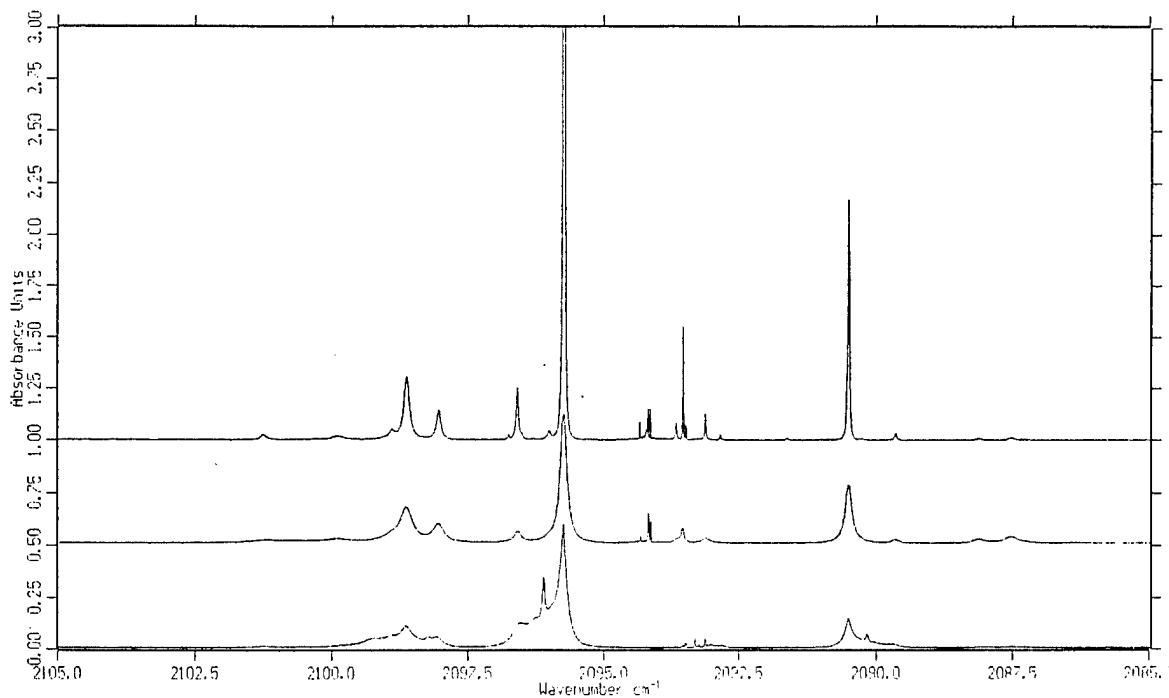


st27017.18     annealed     T=2.4K  
 st27017.14     annealing     T=4.8K  
 st27017.10     as deposited     T=2.4K

resolution = 0.0075 cm<sup>-1</sup>

ST27017.18

# $^{13}\text{C}^{16}\text{O}/\text{pH}_2$ $d \approx 3\text{mm}$

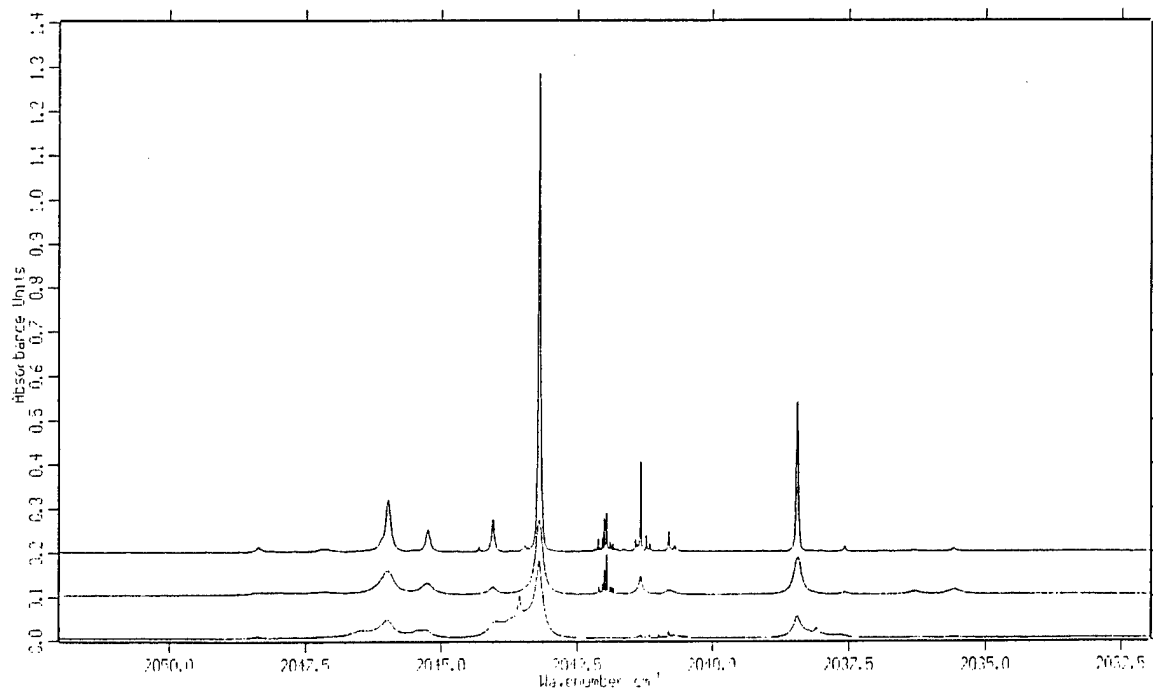


st28082.6 annealed T=2.4K  
st28082.4 annealing T=4.8K  
st28082.2 as deposited T=2.4K

11 PPM  $^{13}\text{CO}/\text{pH}_2$  resolution =  $0.005\text{ cm}^{-1}$

ST28082.2

# $^{13}\text{C}^{18}\text{O}/\text{pH}_2$ $d \approx 3\text{mm}$

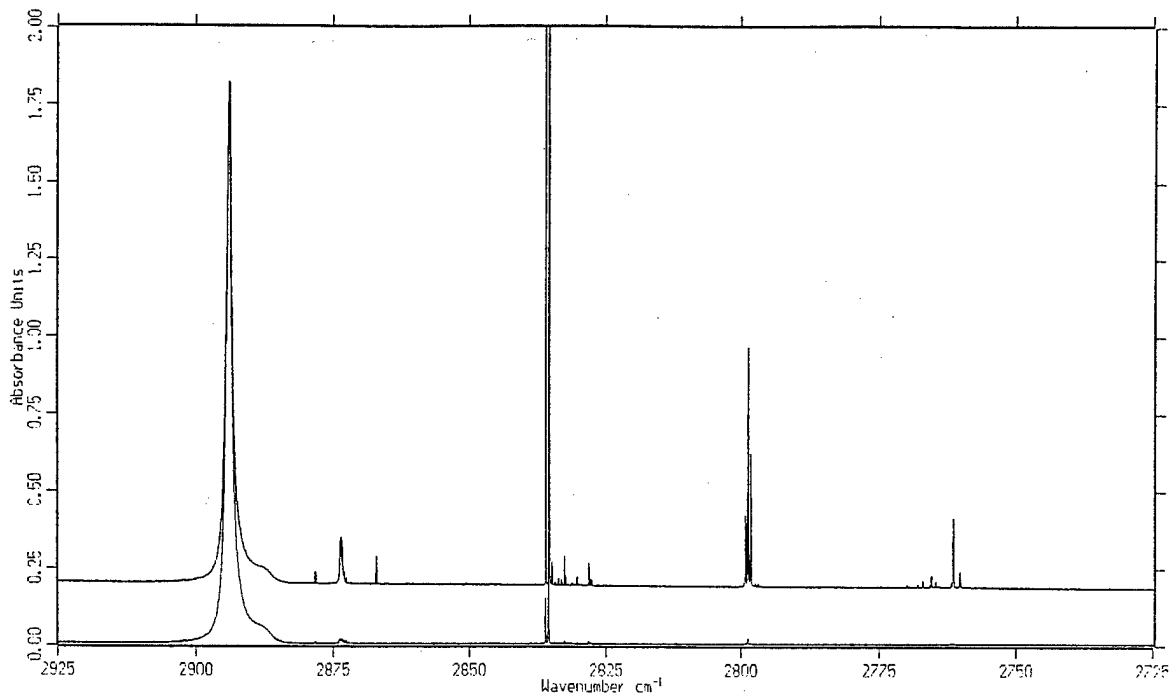


st28085.5 annealed T=2.4K  
st28085.3 annealing T=4.8K  
st28085.1 as deposited T=2.4K

29 PPM  $^{13}\text{CO}/\text{pH}_2$  resolution =  $0.005\text{ cm}^{-1}$

ST28085.1

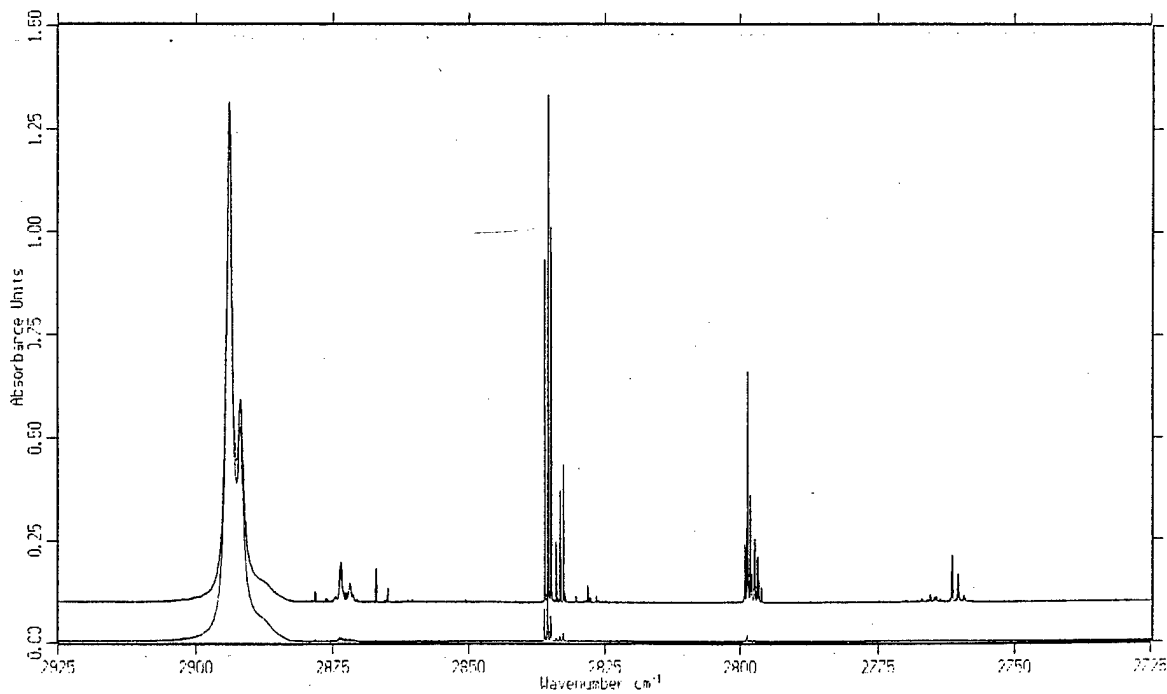
ppm  
90 PPM  $\text{H}^{35}\text{Cl}/\text{pH}_2$   $d \approx 3\text{mm}$



st27079.11 annealed T=2.4K  
st27079.7 as deposited T=2.4K  
resolution = 0.005  $\text{cm}^{-1}$

st27079.7

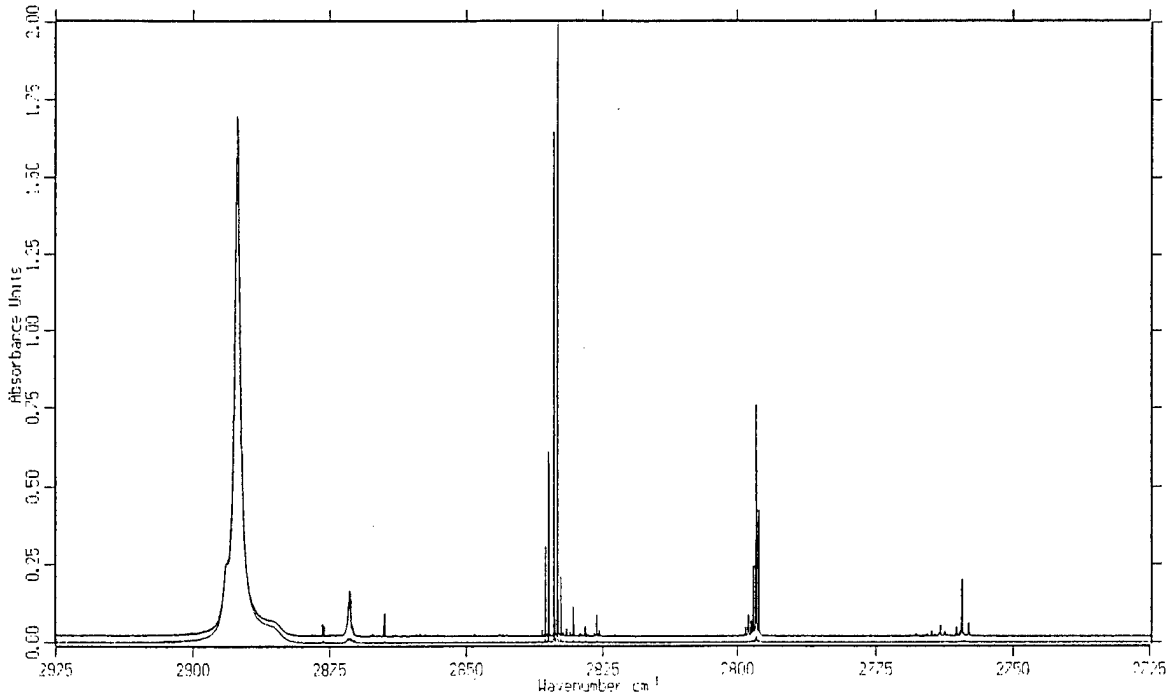
ppm  
88 PPM  $\text{HCl}/\text{pH}_2$   $d \approx 3\text{mm}$



st27061.11 annealed T=2.4K  
st27061.7 as deposited T=2.4K  
resolution = 0.0075  $\text{cm}^{-1}$

st27061.7

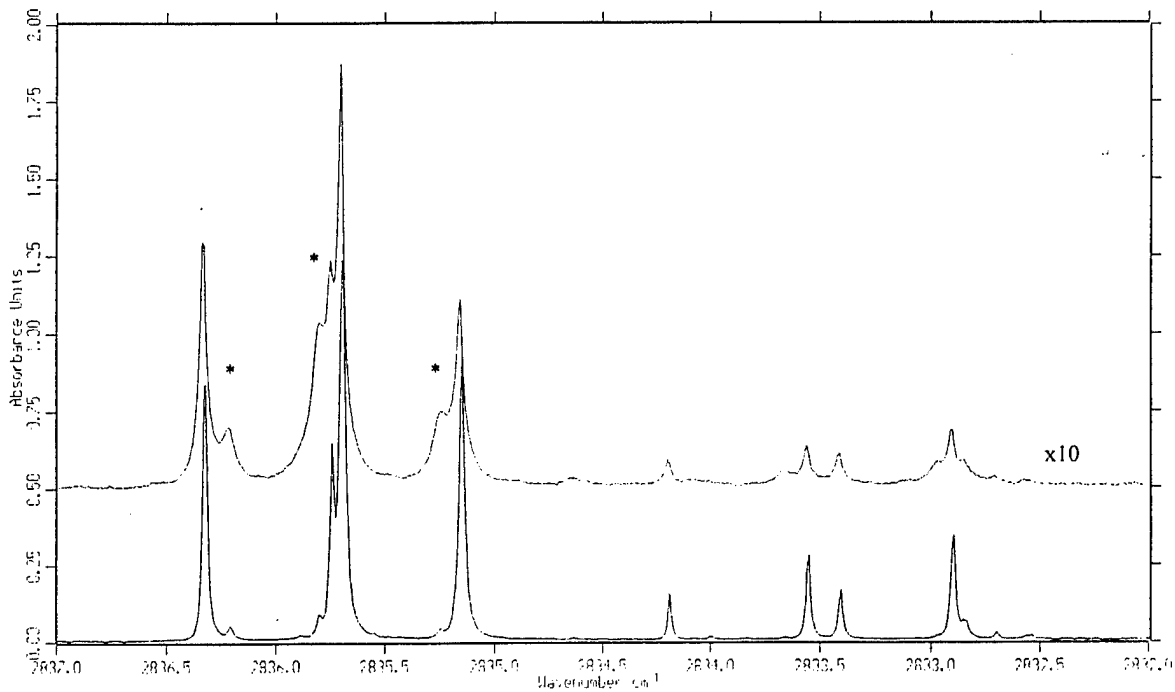
ppm  
94 PPM  $H^{37}Cl/pH_2$   $d \approx 3mm$



st27103.6 annealed T=2.4K  
st27103.2 as deposited T=2.4K  
resolution = 0.005 cm<sup>-1</sup>

st27103.0

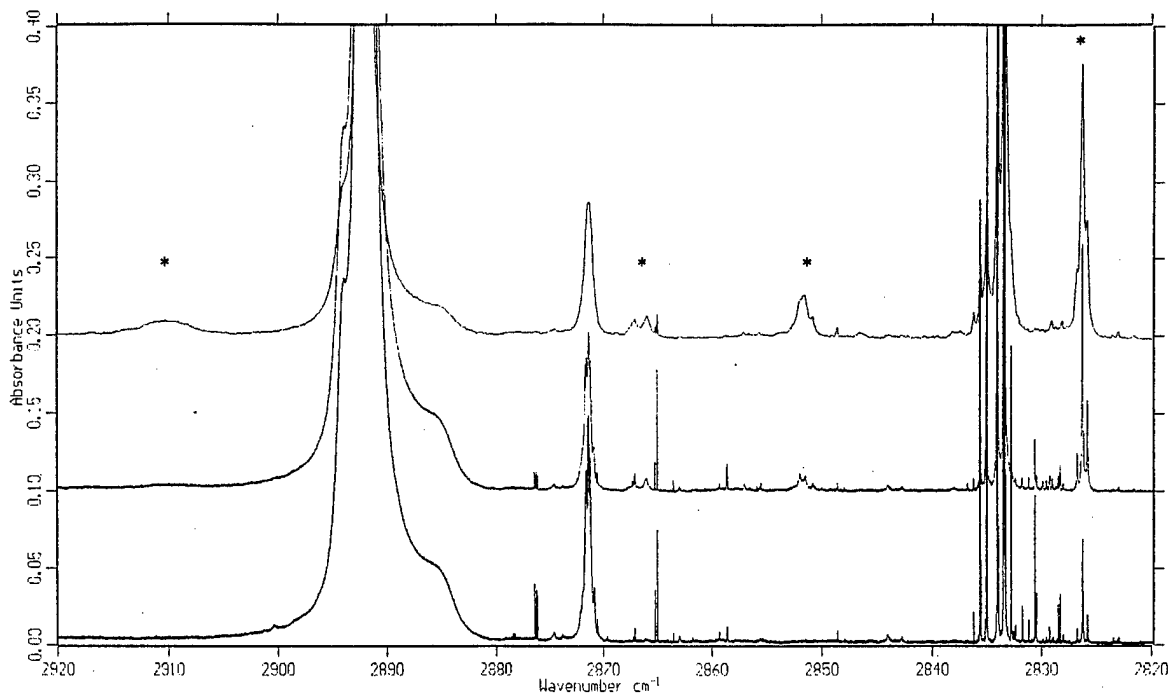
irreversible T dependences



88 PPM  $HCl/pH_2$   $d \approx 3mm$   
st27061.7 as deposited T=2.4K  
st27061.11 annealed T=2.4K

st27061.0

# reversible T dependences

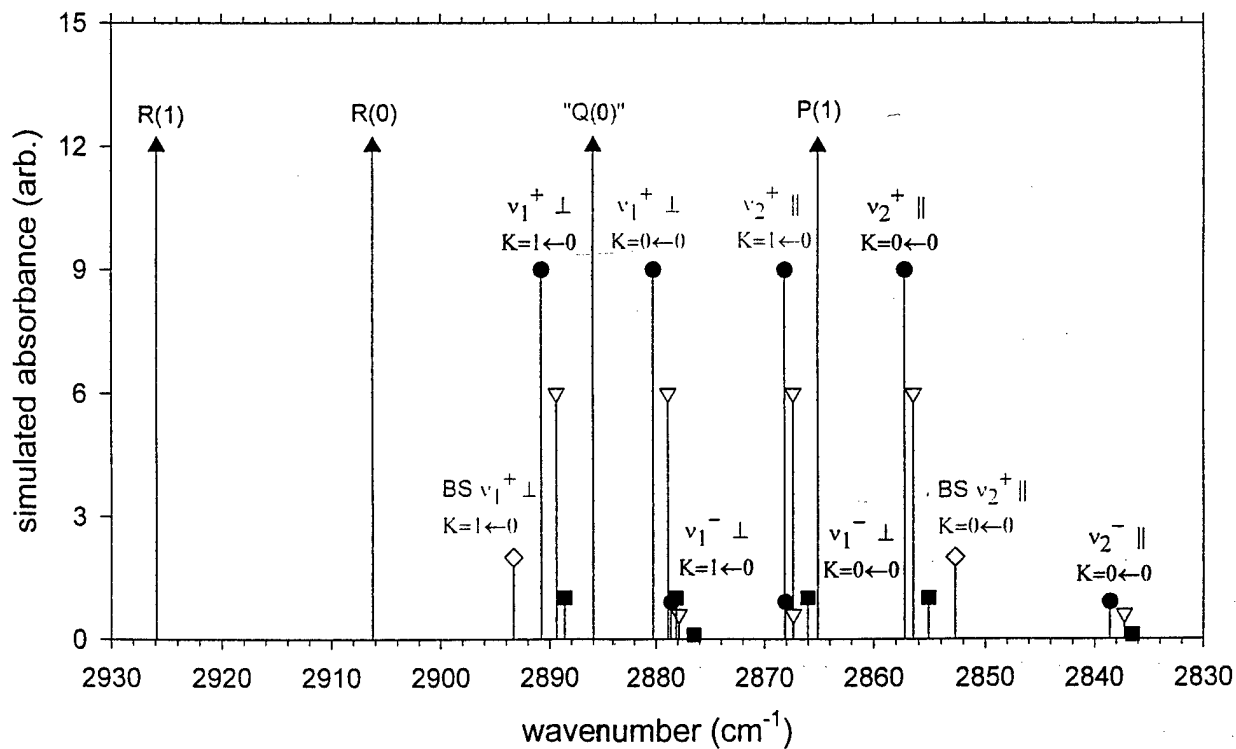


st27103.13 evaporating T ≈ 10K  
 st27103.4 annealing T = 4.8K  
 st27061.11 annealed T = 2.4K

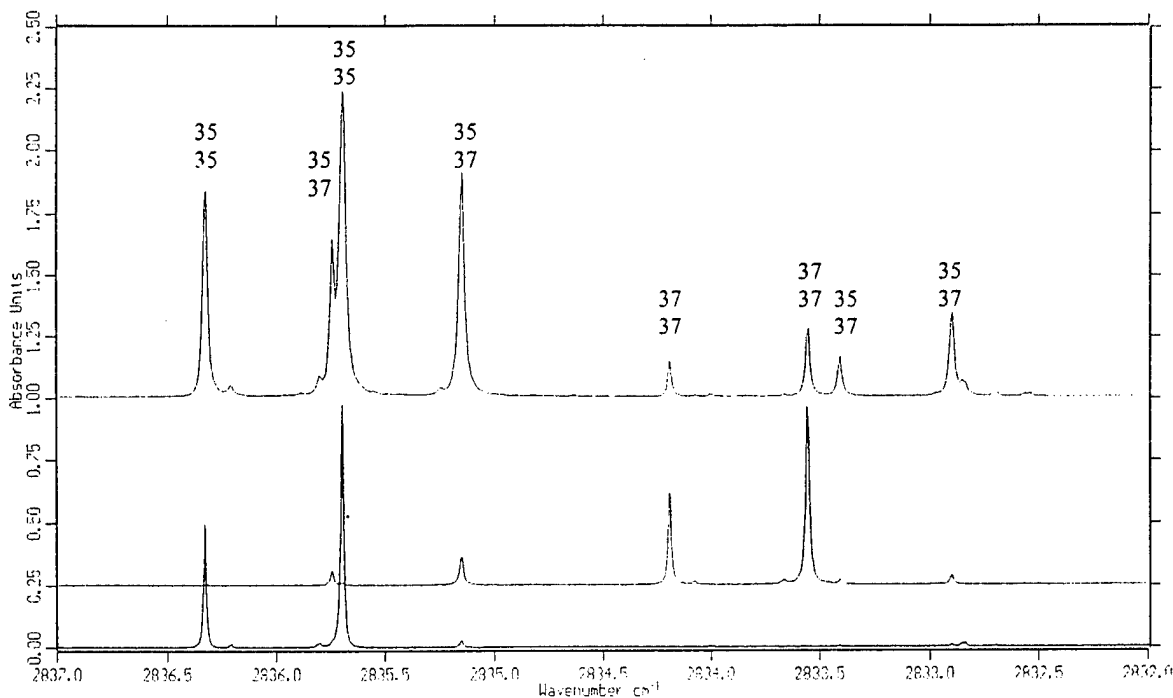
94 PPM H<sup>37</sup>Cl

ST27103.4

## gas phase HCl and (HCl)<sub>2</sub> transitions



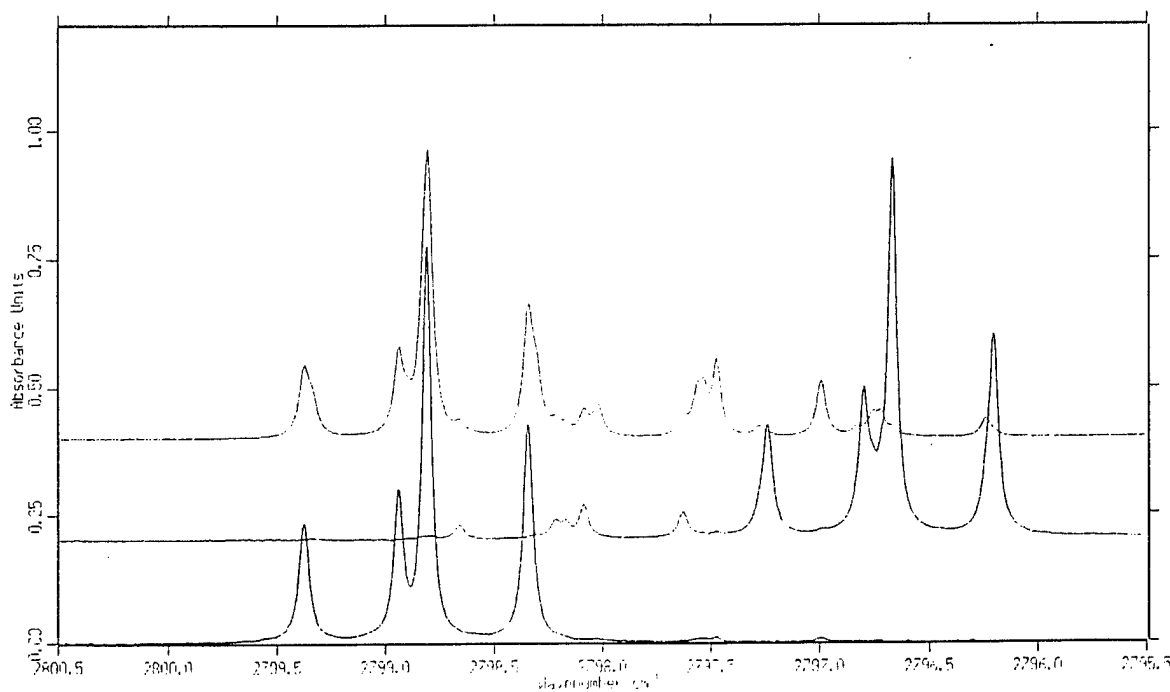
# $(\text{HCl})_2 \nu_2^+$ region



st27061.11	annealed	T=2.4K	88 PPM HCl
st27097.6	annealed	T=2.4K	33 PPM $\text{H}^{37}\text{Cl}$
st27073.17	annealed	T=2.4K	30 PPM $\text{H}^{35}\text{Cl}$

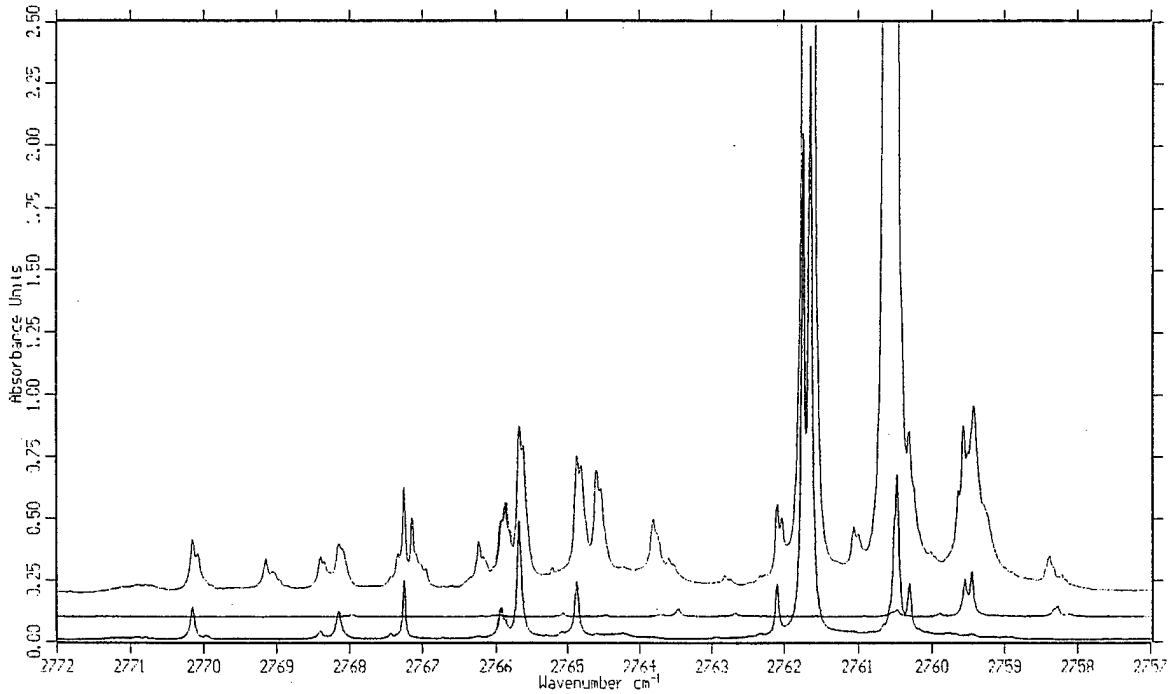
ST27073.17

# $(\text{HCl})_3$



st27061.11	annealed	T=2.4K	88 PPM HCl
st27103.6	annealed	T=2.4K	94 PPM $\text{H}^{37}\text{Cl}$
st27079.11	annealed	T=2.4K	90 PPM $\text{H}^{35}\text{Cl}$

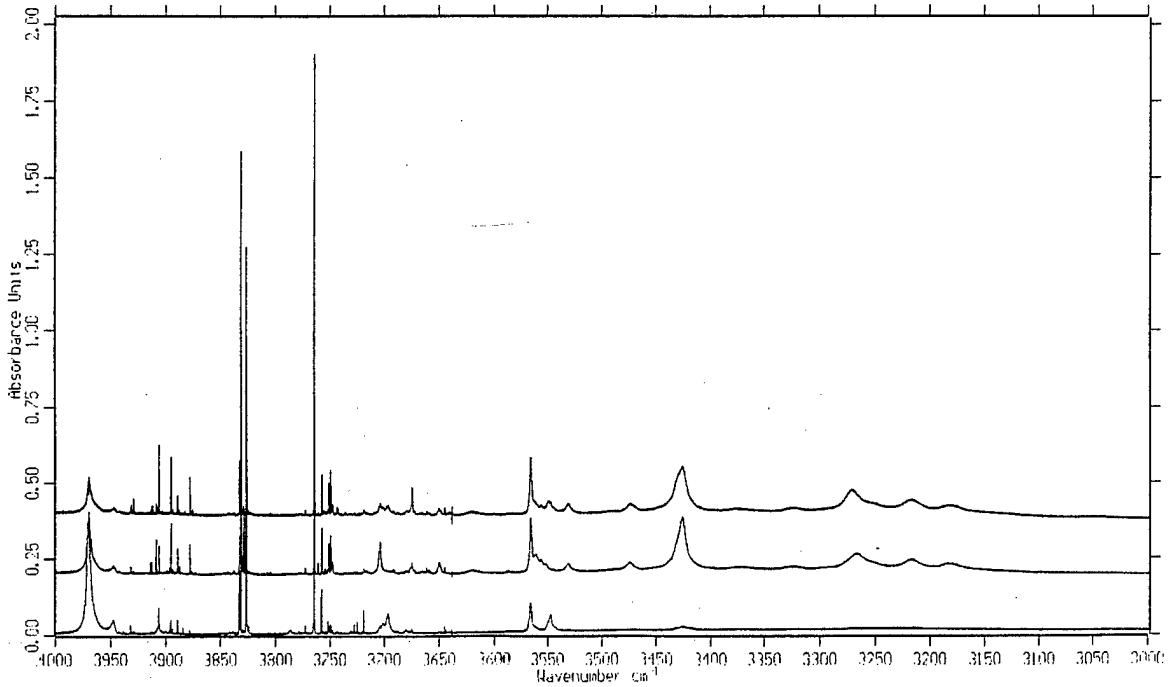
ST27103.6



st27067.10 annealed T=2.4K 494 PPM HCl  
st27103.6 annealed T=2.4K 94 PPM H<sup>37</sup>Cl  
st27085.9 annealed T=2.4K 284 PPM H<sup>35</sup>Cl

ST27103.6

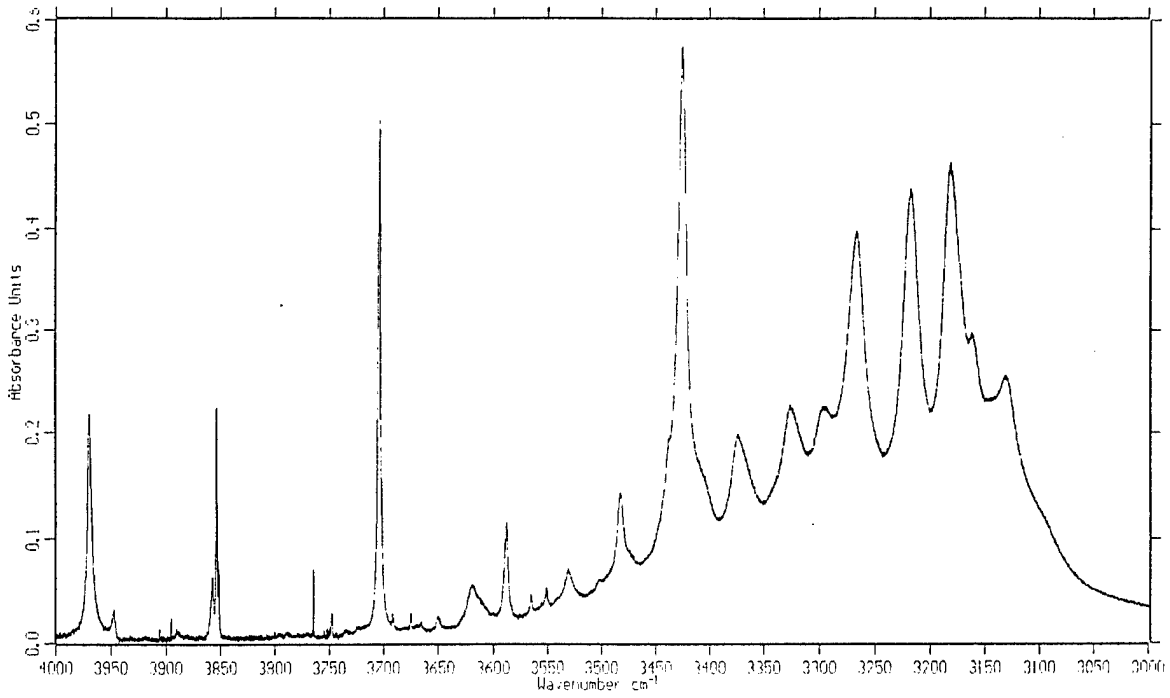
ppm  
123 PPM HF/pH<sub>2</sub> d≈3mm



st27115.15 annealed T=2.4K  
st27115.13 annealing T=4.8K  
st271215.9 as deposited T=2.4K

resolution = 0.005 cm<sup>-1</sup>

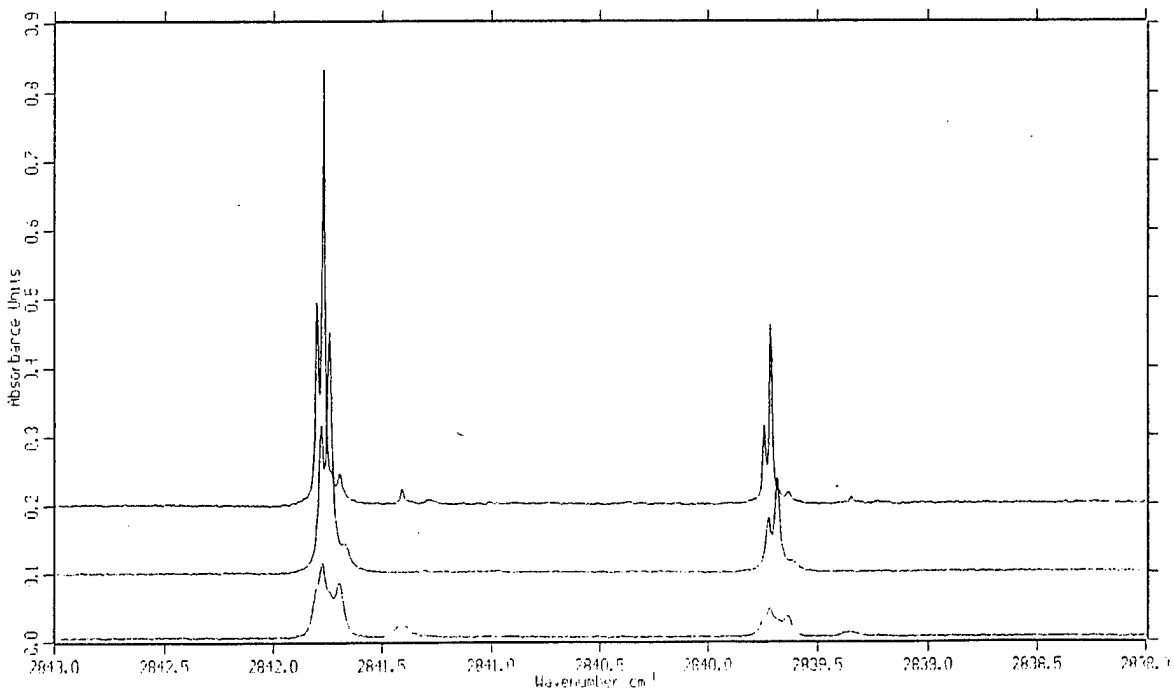
# $(\text{HF})_n/\text{pH}_2$



st27133.15    sample burnoff    T~10K    268 PPM HF/pH<sub>2</sub>    resolution = 0.1  $\text{cm}^{-1}$

st27133.15

# HF-HCl/pH<sub>2</sub>



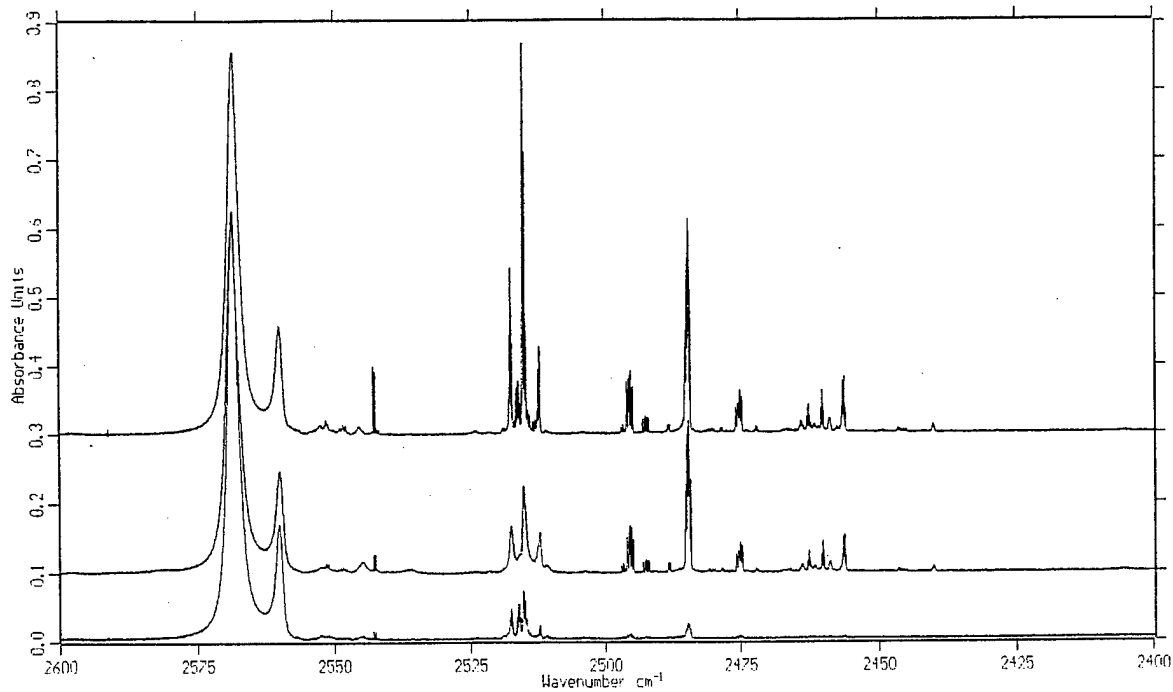
st27115.15    annealed    T=2.4K  
st27115.13    annealing    T=4.8K  
st27115.9    as deposited    T=2.4K

123 PPM HF/pH<sub>2</sub>    d≈3mm

resolution = 0.005  $\text{cm}^{-1}$

st27115.9

ppm  
**260 PPM HBr/pH<sub>2</sub> d≈3mm**

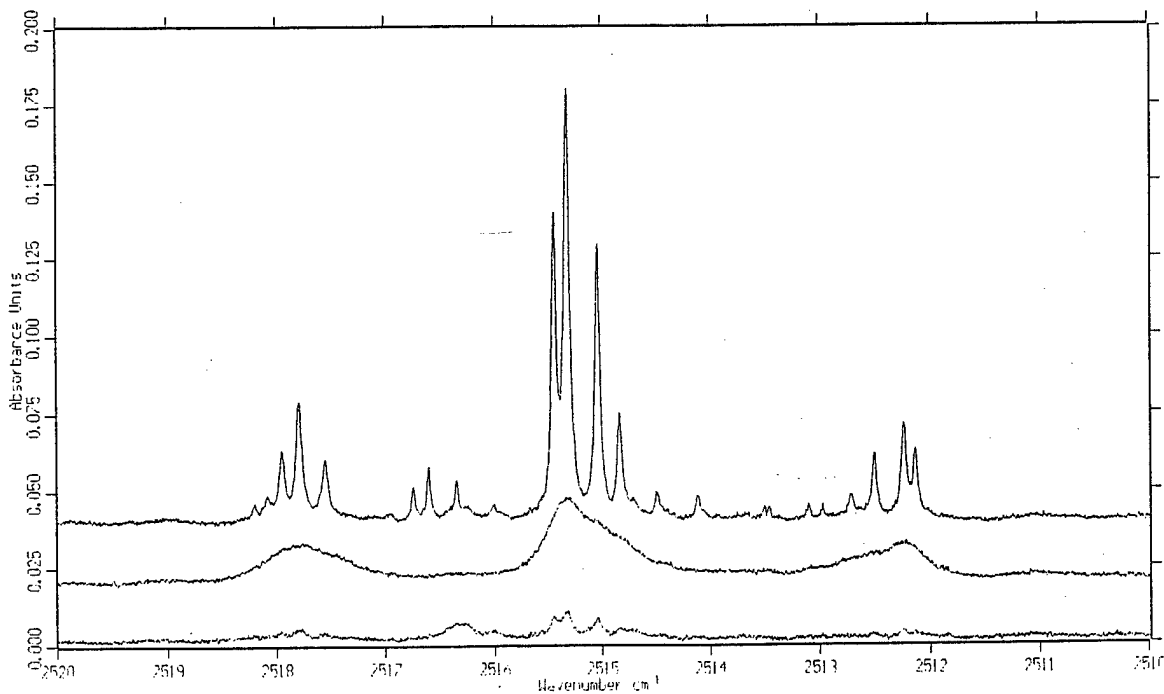


st27145.9      annealed    T=2.4K  
 st27145.7      annealing   T=4.8K  
 st27145.5      as deposited T=2.4K

resolution = 0.005 cm<sup>-1</sup>

ST27145.5

**(HBr)<sub>2</sub>/pH<sub>2</sub>**



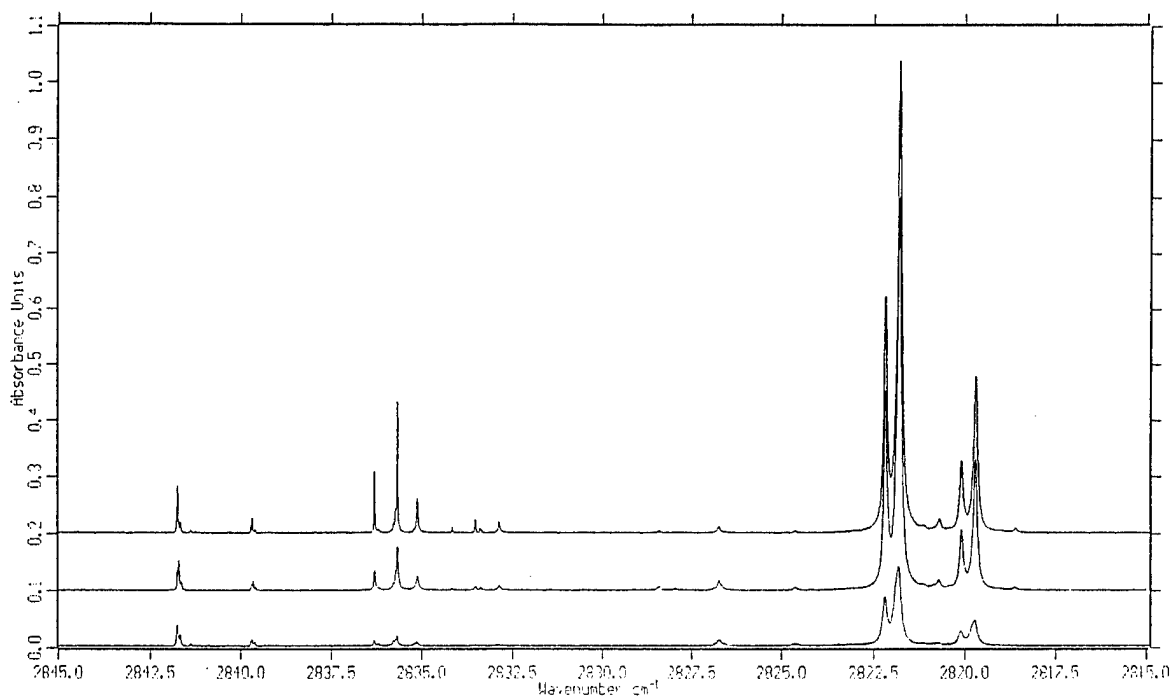
st27140.9      annealed    T=2.4K  
 st27140.7      annealing   T=4.8K  
 st27140.5      as deposited T=2.4K

80 PPM HBr/pH<sub>2</sub> d≈3mm

resolution = 0.005 cm<sup>-1</sup>

ST27140.5

# HCl-(HF, HCl, HBr)/pH<sub>2</sub>



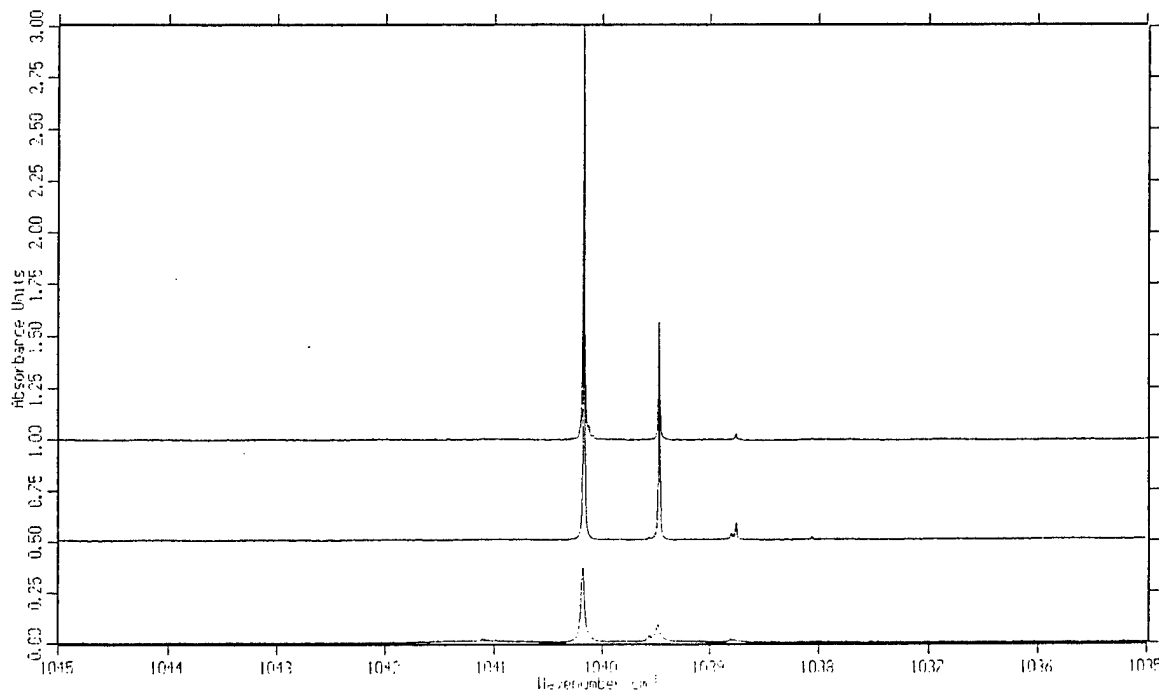
st27145.9      annealed    T=2.4K  
st27145.7      annealing    T=4.8K  
st27145.5      as deposited T=2.4K

260 PPM HBr/pH<sub>2</sub> d≈3mm

resolution = 0.005 cm<sup>-1</sup>

ST27145.5

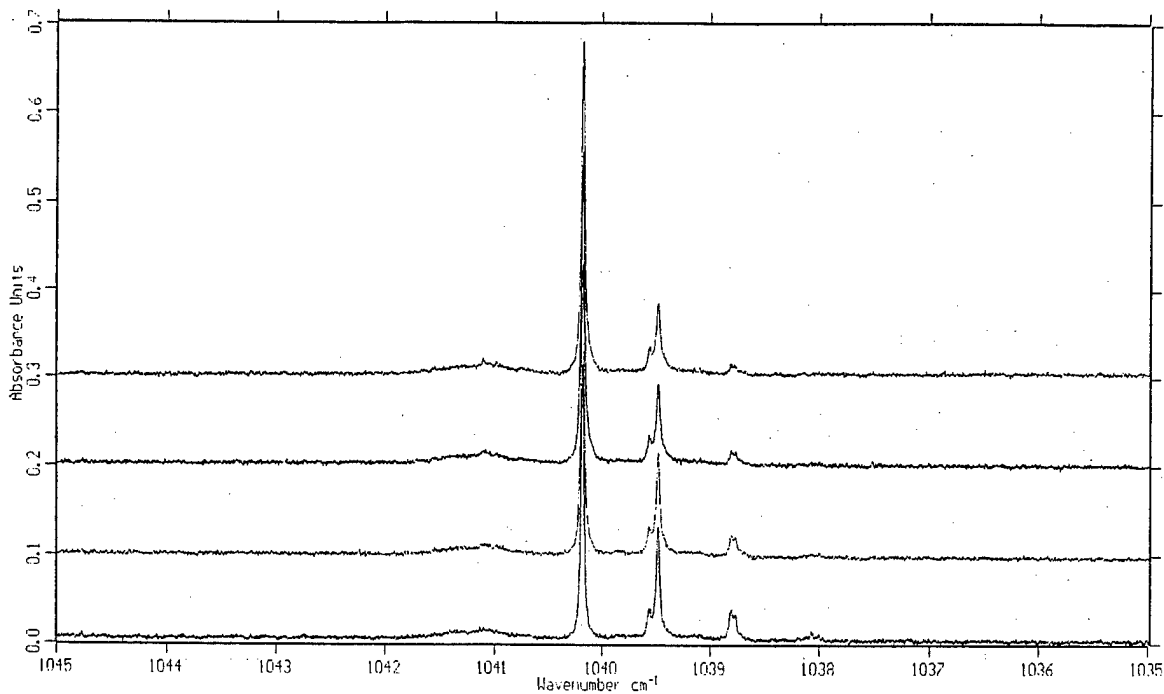
# 2.4 PPM CH<sub>3</sub>F/pH<sub>2</sub> d≈3mm



st28060.15      annealed    T=2.4K  
st28060.11      annealing    T=4.8K  
st28060.6+7      as deposited T=2.4K

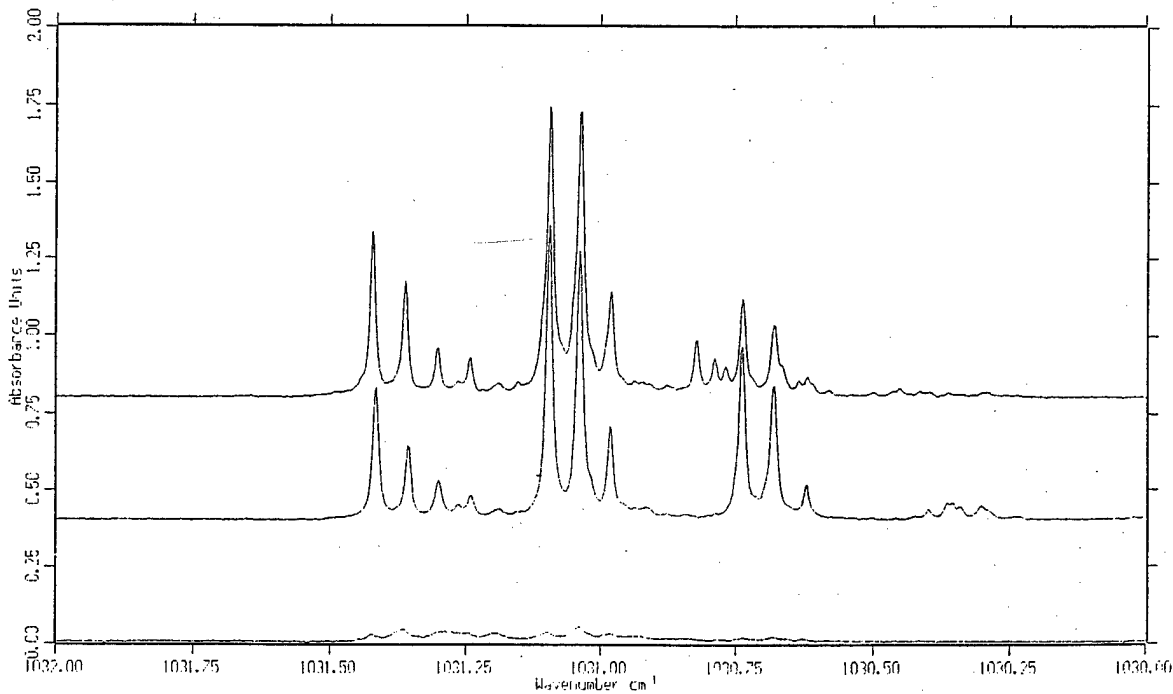
resolution = 0.005 cm<sup>-1</sup>

# $^1\text{H}$ Spin Relaxation in $\text{CH}_3\text{F}/\text{pH}_2$



st28060.7 after 100 min T=2.4K    st28060.3 after 30 min T=2.4K  
 st28060.6 after 70 min T=2.4K    st28060.2 as deposited T=2.4K    resolution = 0.005  $\text{cm}^{-1}$   
ST28060.2

## $(\text{CH}_3\text{F})_2/\text{pH}_2$



st28044.11 annealed T=2.4K  
 st28044.7 annealing T=4.8K  
 st28044.3 as deposited T=2.4K    30 PPM  $\text{CH}_3\text{F}/\text{pH}_2$     resolution = 0.005  $\text{cm}^{-1}$

ST28044.7

# SUPPLEMENTAL MATERIALS

for the poster:

HIGH ENERGY DENSITY MATTER CONTRACTORS CONFERENCE  
Cocoa Beach, FL 8-11 June 1999

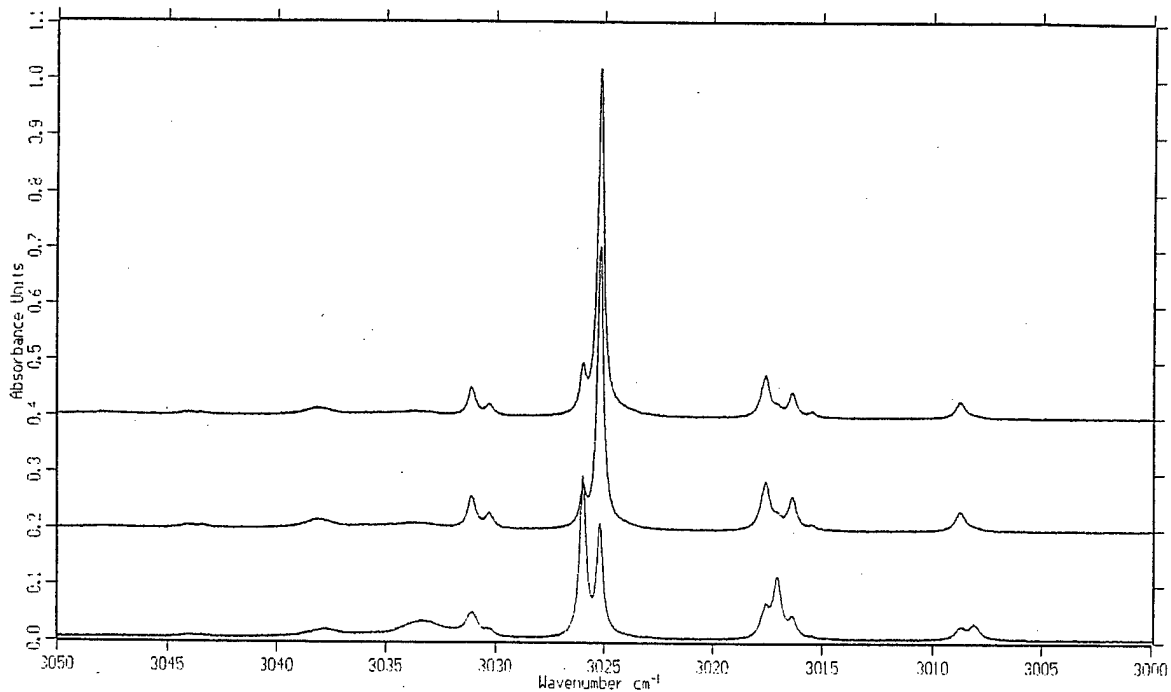
## High Resolution Infrared Absorption Spectroscopy of Molecular Dopants in Cryogenic Solid Parahydrogen

Mario E. Fajardo and Simon Tam

US Air Force Research Laboratory, Propulsion Directorate  
(AFRL/PRSP Bldg. 8451, Edwards AFB, CA 93524-7680) mario\_fajardo@ple.af.mil

Consisting of spectra of NON-ENERGETIC species trapped in solid hydrogen at low concentrations. These data encompass prototypical diatomic (CO, HCl, HF, HBr), triatomic (CO<sub>2</sub>, N<sub>2</sub>O, H<sub>2</sub>O), linear polyatomic (C<sub>2</sub>H<sub>2</sub>), symmetric top (NH<sub>3</sub>, CH<sub>3</sub>F), and spherical top (CH<sub>4</sub>) molecular dopants. The basic research activity of understanding these spectra will aid in the future characterization of HEDM cryosolid propellants.

ppm  
13 PPM CH<sub>4</sub>/pH<sub>2</sub> d≈3mm

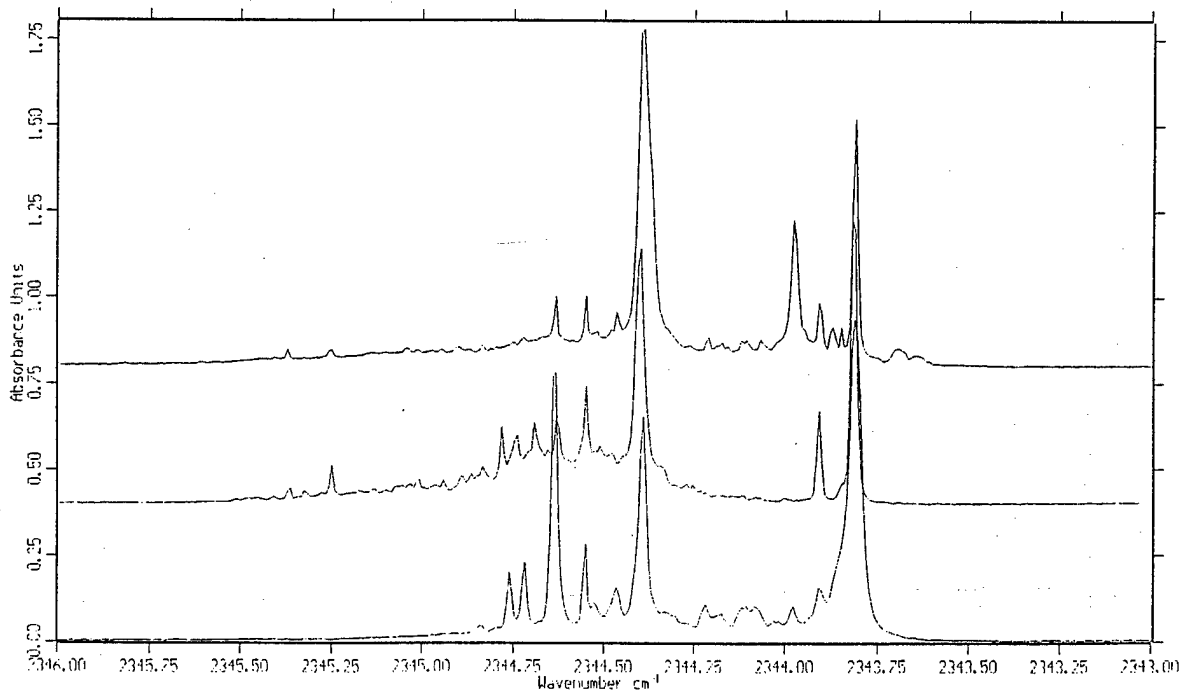


st27011.8      annealed    T=2.4K  
st27011.4      annealing   T=4.8K  
st27011.2      as deposited T=2.4K

resolution = 0.0075 cm<sup>-1</sup>

ST27011.2

ppm  
1 PPM CO<sub>2</sub>/pH<sub>2</sub> d≈3mm

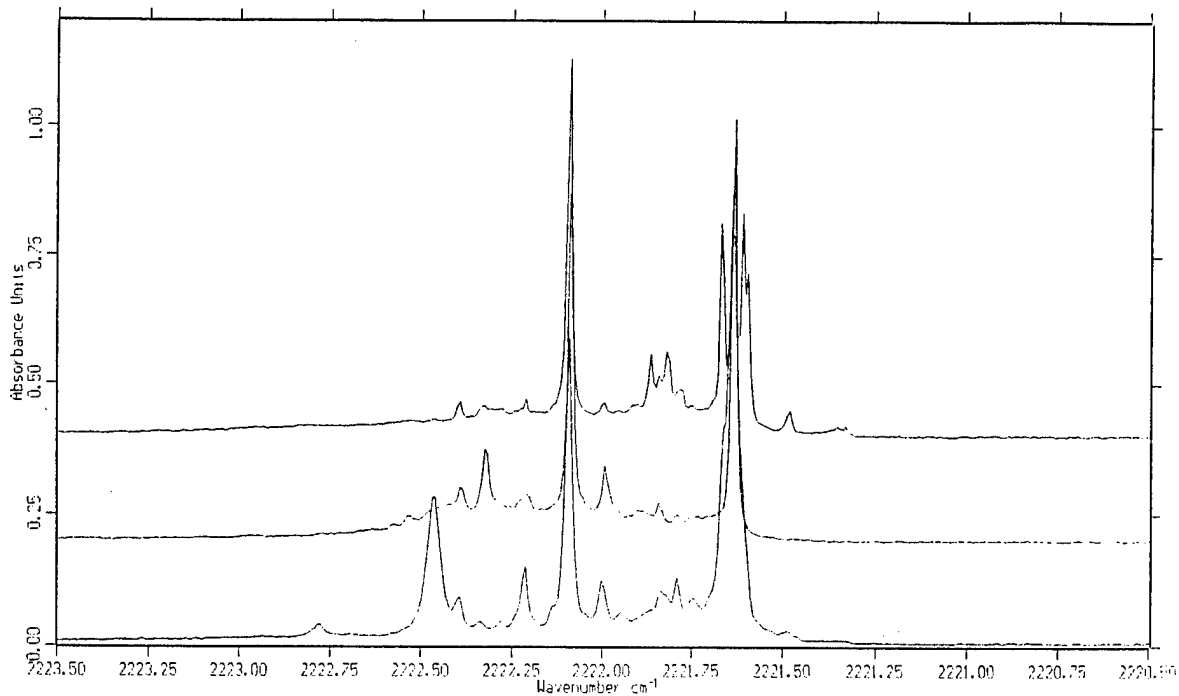


st27025.11      annealed    T=2.4K  
st27025.9      annealing   T=4.8K  
st27025.7      as deposited T=2.4K

resolution = 0.005 cm<sup>-1</sup>

ST27025.7

ppm  
1 PPM  $N_2O/pH_2$   $d \approx 3mm$

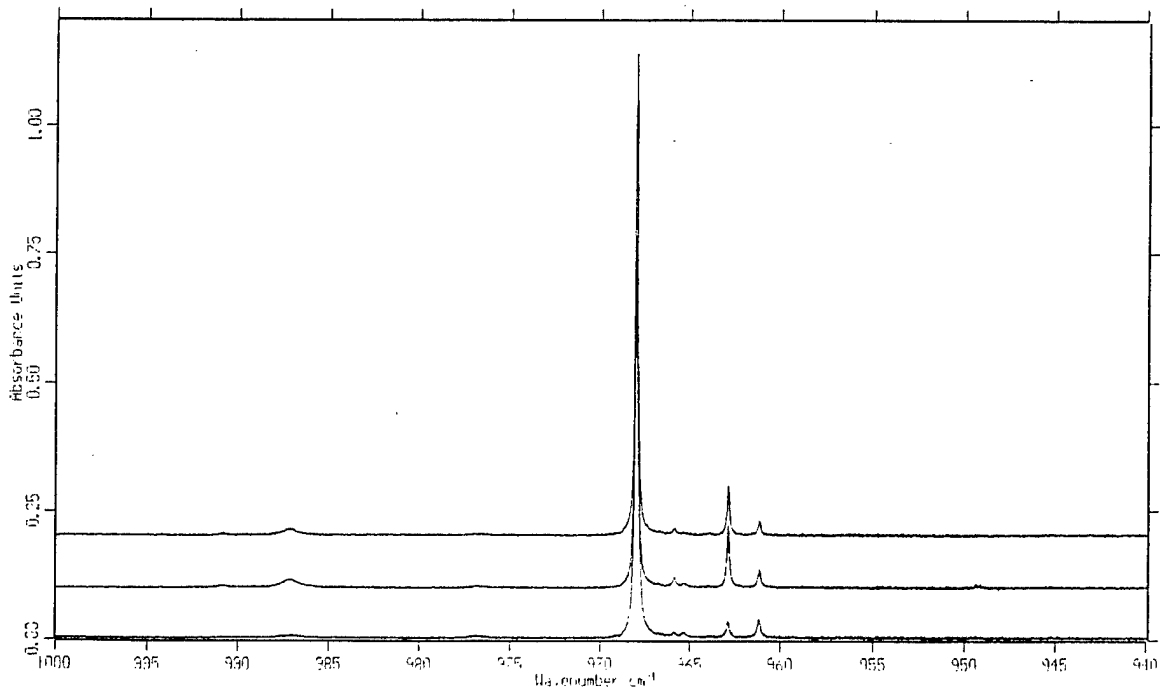


st27025.14     annealed    T=2.4K  
st27025.12     annealing    T=4.8K  
st27025.6       as deposited T=2.4K

resolution = 0.005  $cm^{-1}$

ST27001.0

ppm  
4 PPM  $NH_3/pH_2$   $d \approx 3mm$

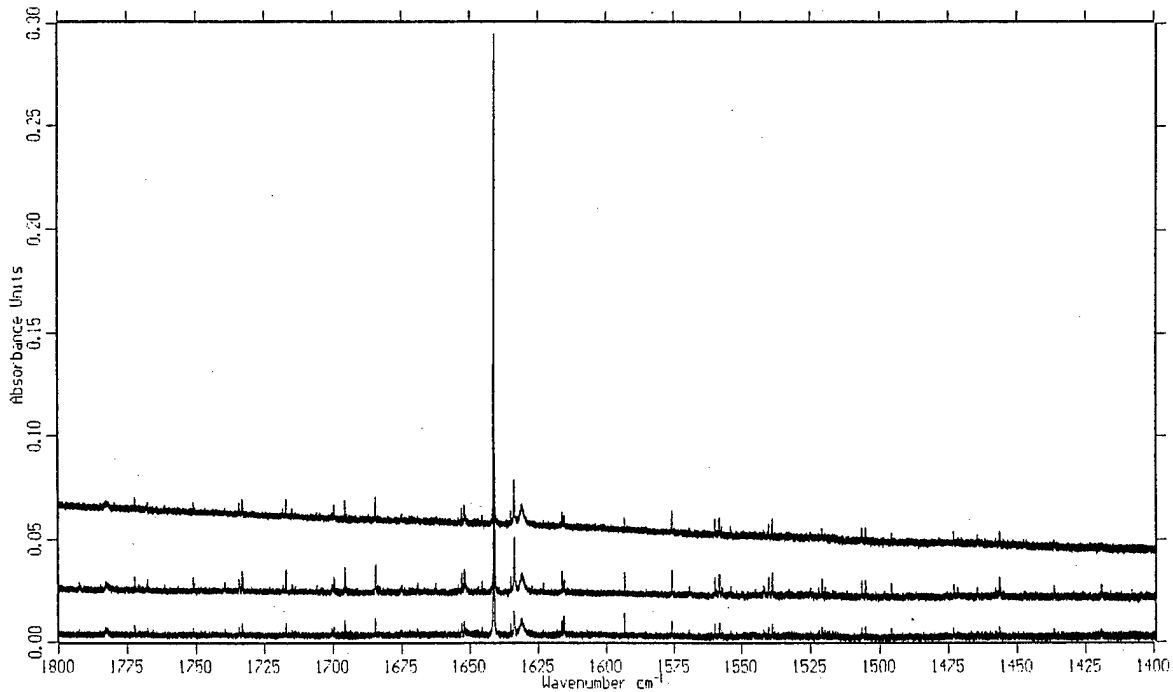


st27036.12     annealed    T=2.4K  
st27036.10     annealing    T=4.8K  
st27036.8       as deposited T=2.4K

resolution = 0.005  $cm^{-1}$

ST27001.0

ppm  
4 PPM NH<sub>3</sub>/pH<sub>2</sub> d≈3mm

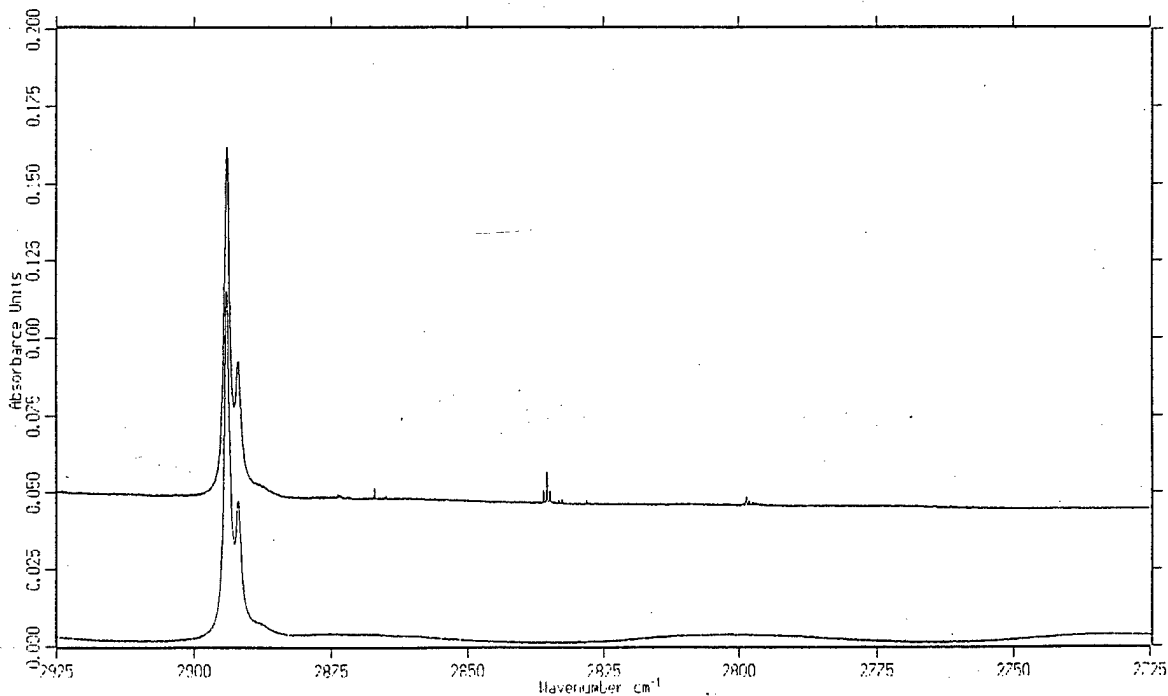


st27036.12 annealed T=2.4K  
st27036.10 annealing T=4.8K  
st27036.8 as deposited T=2.4K

resolution = 0.005 cm<sup>-1</sup>

ST27036.8

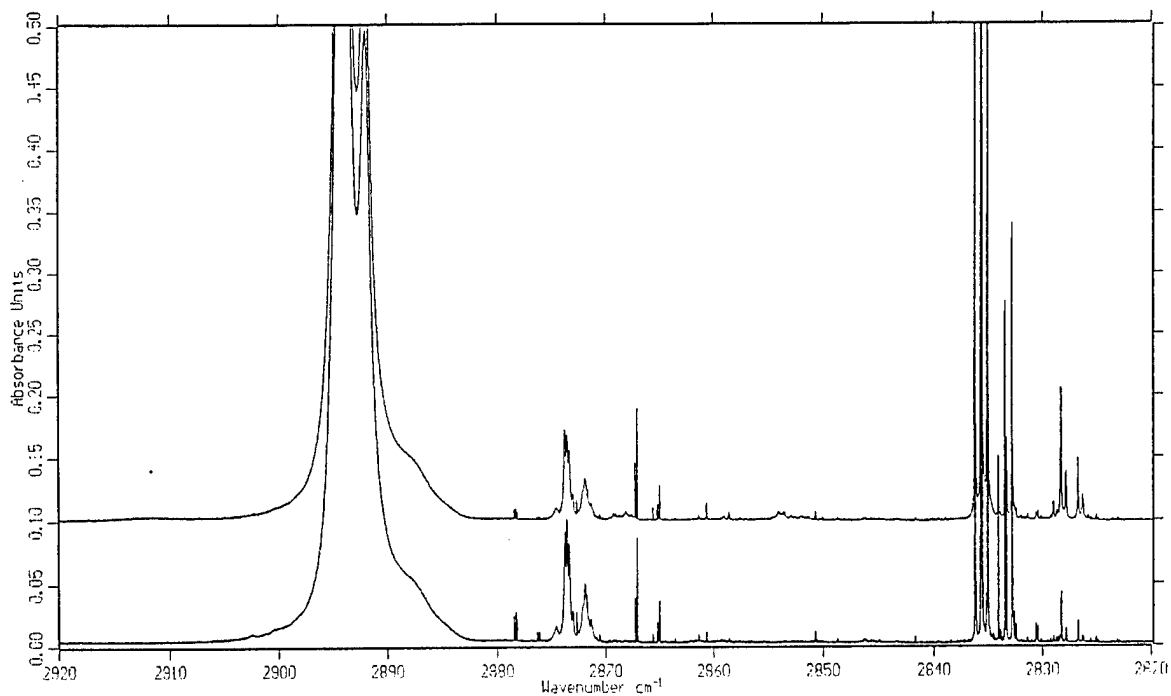
ppm  
8 PPM HCl/pH<sub>2</sub> d≈3mm



st27055.11 annealed T=2.4K  
st27055.4 as deposited T=2.4K  
resolution = 0.05 cm<sup>-1</sup>

ST27055.4

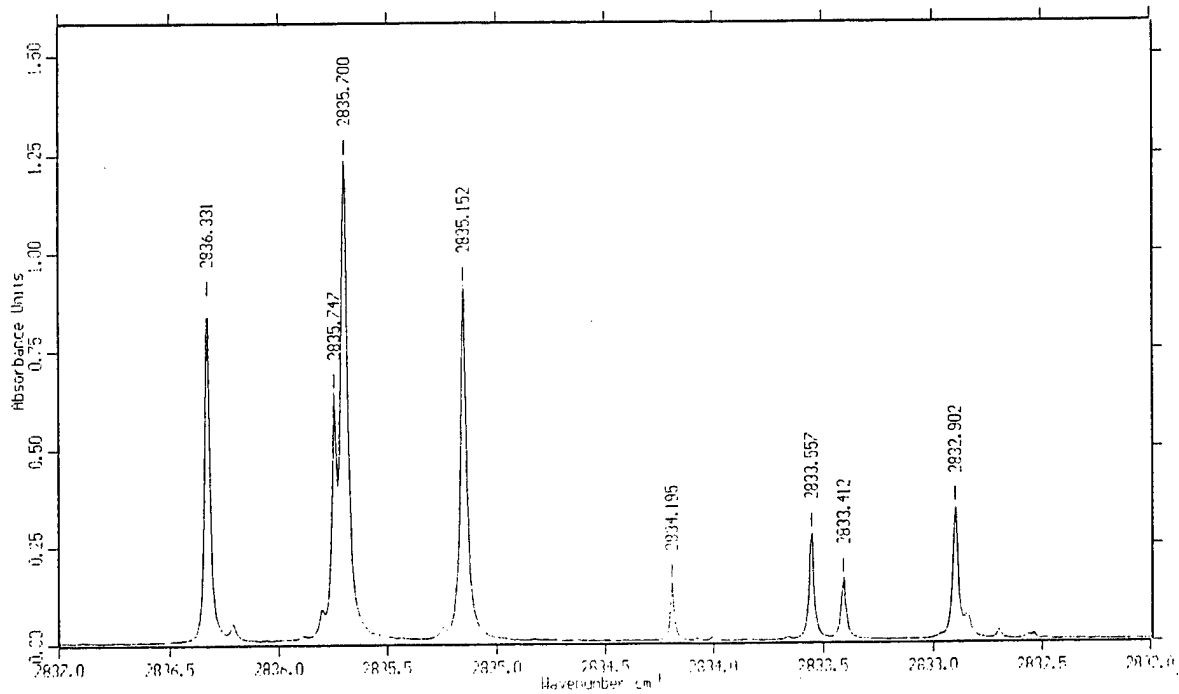
# reversible T dependences



88 PPM HCl  
st27061.9 annealing T=4.8K  
st27061.11 annealed T=2.4K

st27061.9

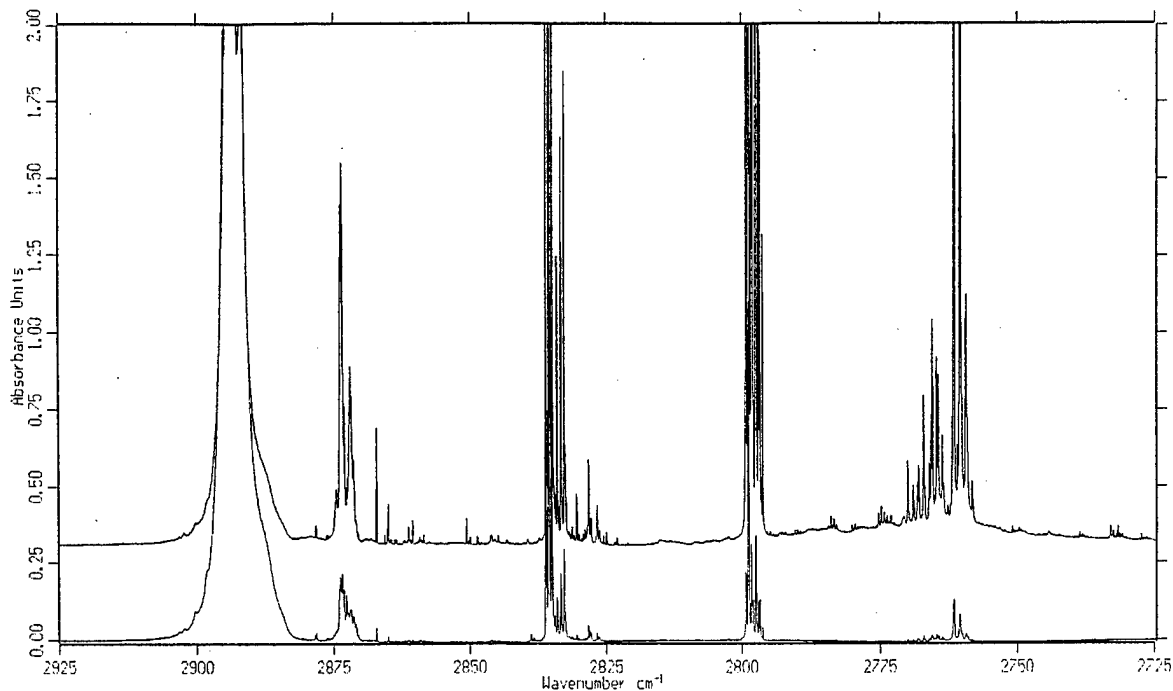
## $(\text{HCl})_2 \nu_2^+$ region



st27061.11 annealed T=2.4K 88 PPM HCl

st27061.11

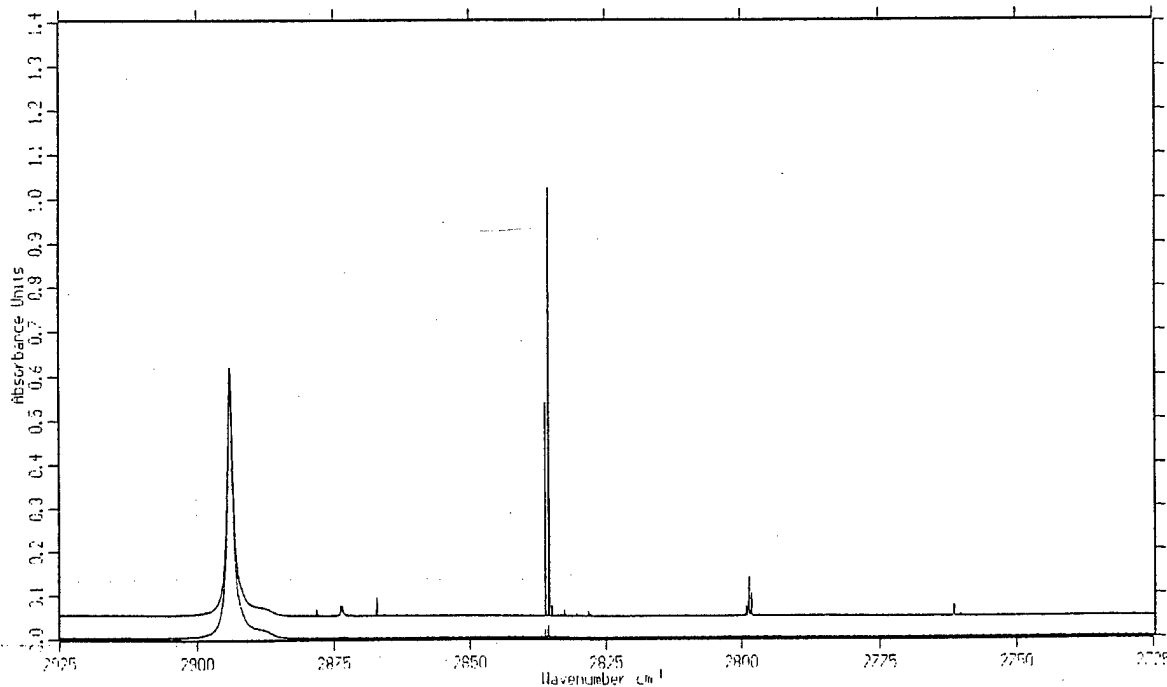
ppm  
494 PPM HCl/pH<sub>2</sub> d≈3mm



st27067.10 annealed T=2.4K  
st27067.6 as deposited T=2.4K  
resolution = 0.0075 cm<sup>-1</sup>

st27067.6

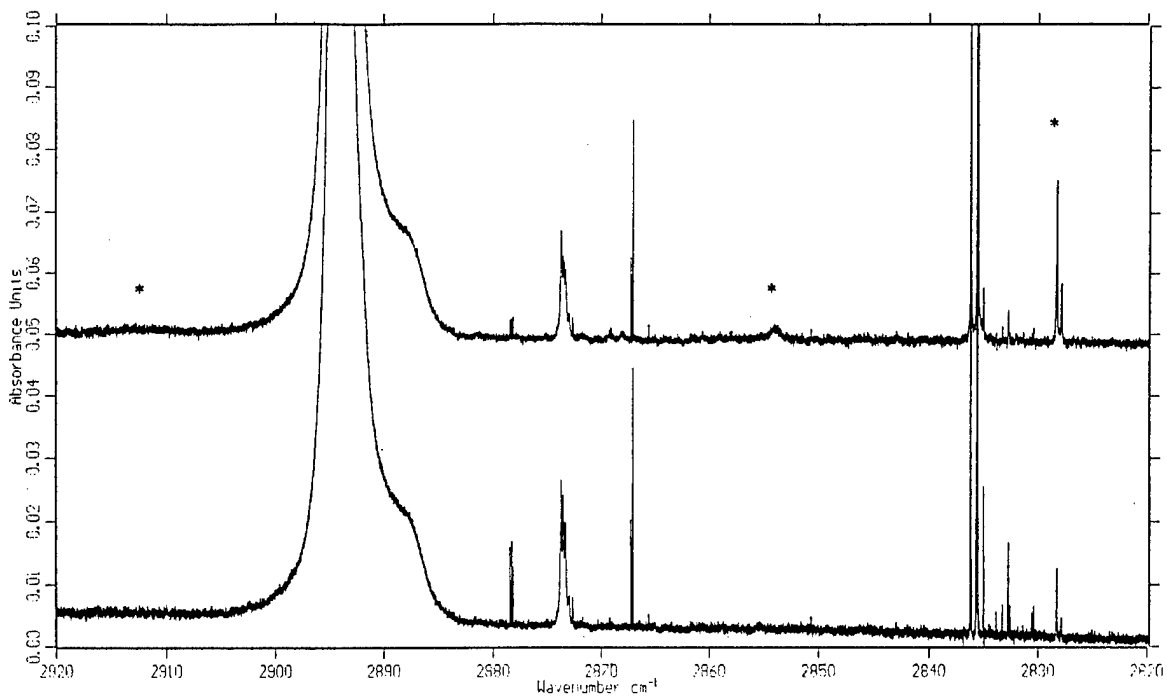
ppm  
30 PPM H<sup>35</sup>Cl/pH<sub>2</sub> d≈3mm



st27073.17 annealed T=2.4K  
st27073.9 as deposited T=2.4K  
resolution = 0.005 cm<sup>-1</sup>

st27073.9

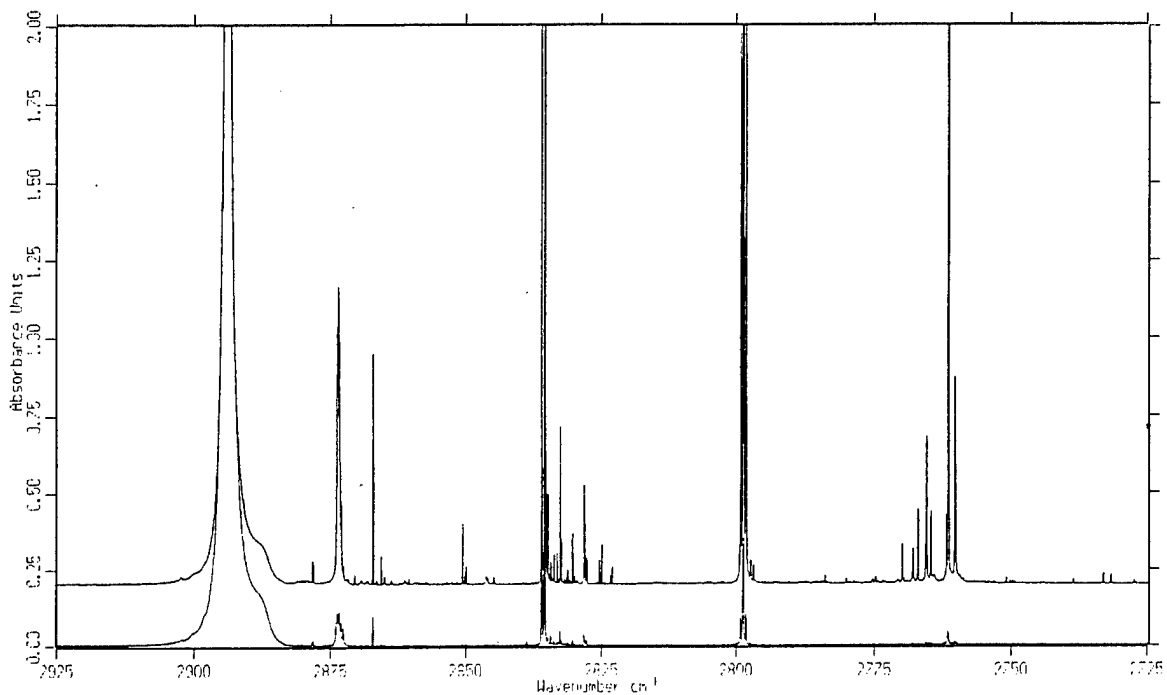
# reversible T dependences



30 PPM H<sup>35</sup>Cl  
st27073.11 annealing T=4.8K  
st27073.17 annealed T=2.4K

ST27073.11

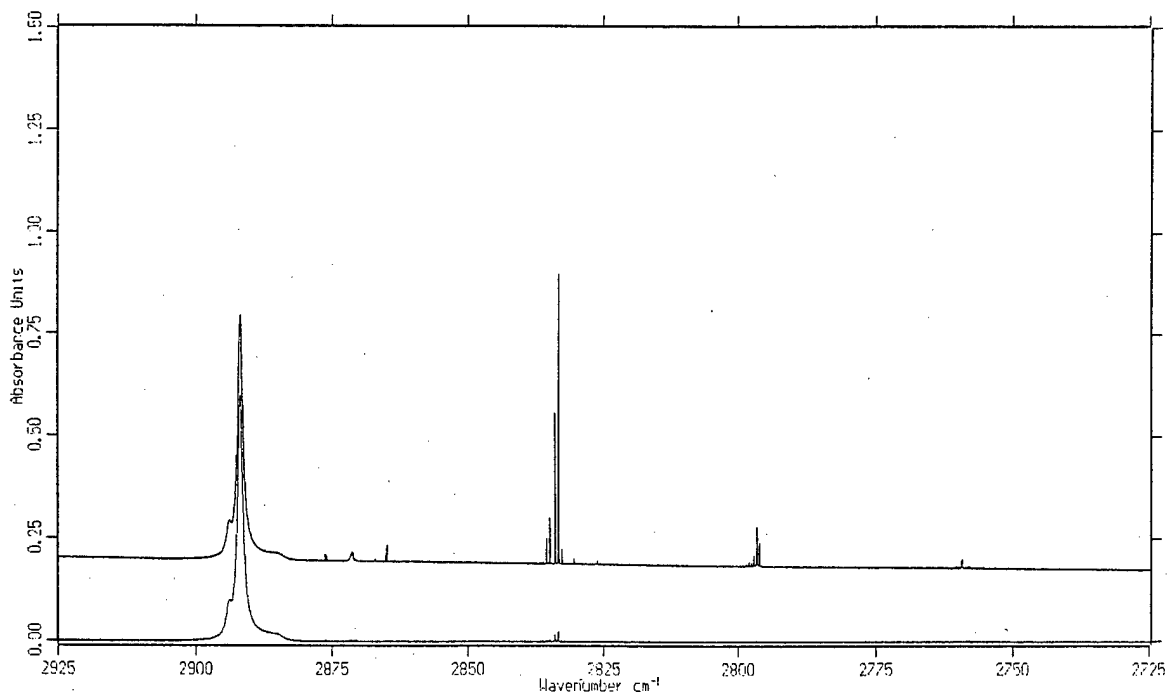
ppm  
284 PPM H<sup>35</sup>Cl/pH<sub>2</sub> d<sub>r</sub> ≈ 3mm



st27085.9 annealed T=2.4K  
st27085.5 as deposited T=2.4K  
resolution = 0.005 cm<sup>-1</sup>

ST27085.9

33 <sup>ppm</sup> PPM H<sup>37</sup>Cl/pH<sub>2</sub> d≈3mm



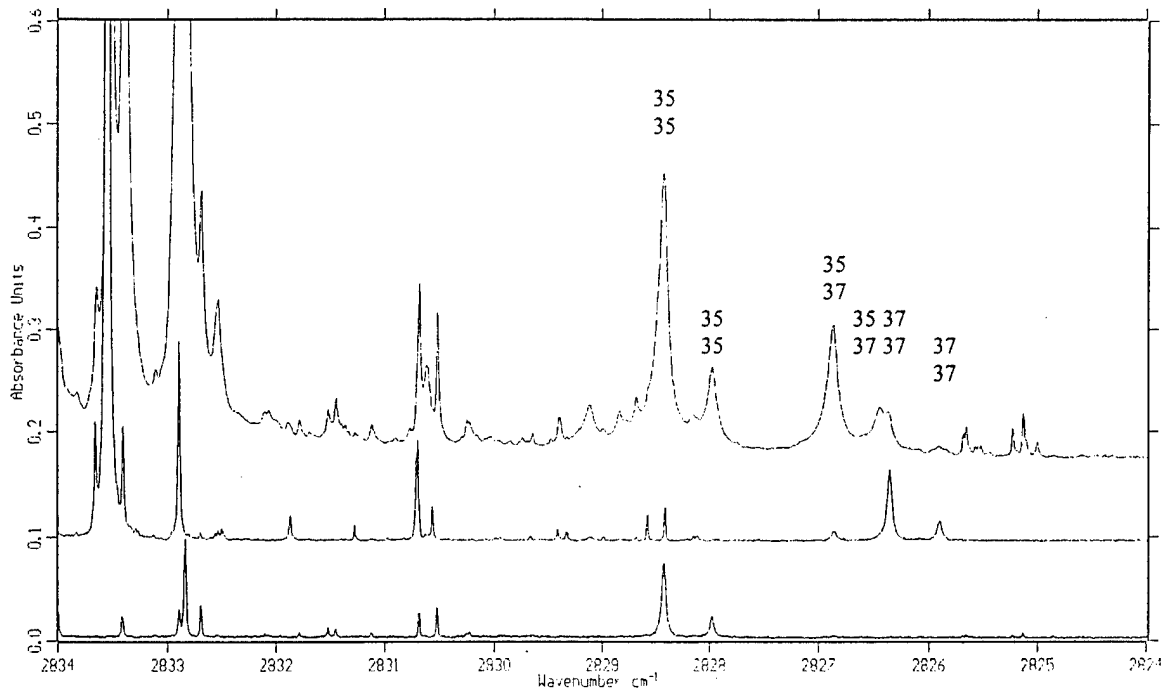
st27097.6 annealed T=2.4K  
 st27097.2 as deposited T=2.4K  
 resolution = 0.005 cm<sup>-1</sup>

ST27097.2

## HCl monomer shifts

<u>species</u>	<u>line/band</u>	<u>gas phase (cm<sup>-1</sup>)</u>	<u>solid pH<sub>2</sub></u>	<u>gas-matrix</u>
H <sup>35</sup> Cl	R(1)	2925.8961	2912	14
	R(0)	2906.2464	2894.2	12.1
	"Q(0)"	2885.67	2873.86	
			2873.67	12.0
			2873.46	
	P(1)	2865.0977	2873.14	
2854.12				
2853.58			11.5	
2852.95				
H <sup>37</sup> Cl	R(1)	2923.7315	2910.2	13.5
	R(0)	2904.1104	2892.1	12.0
	"Q(0)"	2883.57	2871.69	
			2871.48	12.1
			2871.31	
	P(1)	2863.0231	2870.97	
2852.07				
2851.55			11.5	
			2850.89	

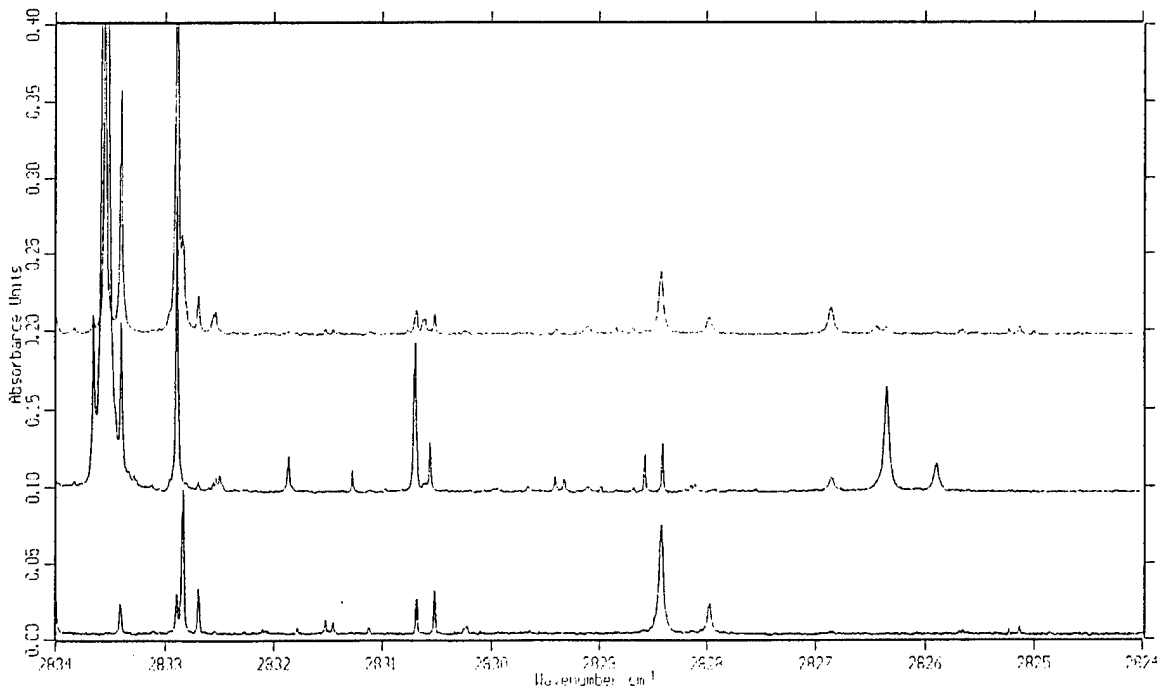
# (HCl)<sub>2</sub> v<sub>2</sub><sup>-</sup> region



st27067.10 annealed T=2.4K 494 PPM HCl  
 st27103.6 annealed T=2.4K 94 PPM H<sup>37</sup>Cl  
 st27079.11 annealed T=2.4K 90 PPM H<sup>35</sup>Cl

st27067.10

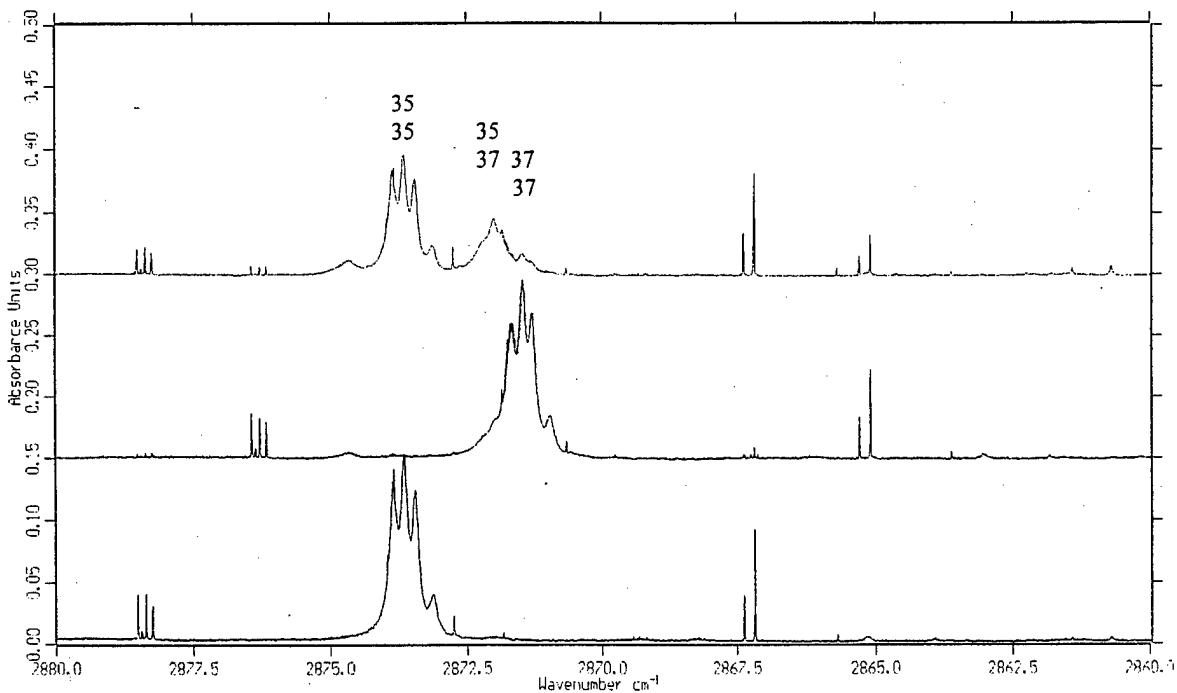
# (HCl)<sub>2</sub> v<sub>2</sub><sup>-</sup> region



st27061.11 annealed T=2.4K 88 PPM HCl  
 st27103.6 annealed T=2.4K 94 PPM H<sup>37</sup>Cl  
 st27079.11 annealed T=2.4K 90 PPM H<sup>35</sup>Cl

st27061.11

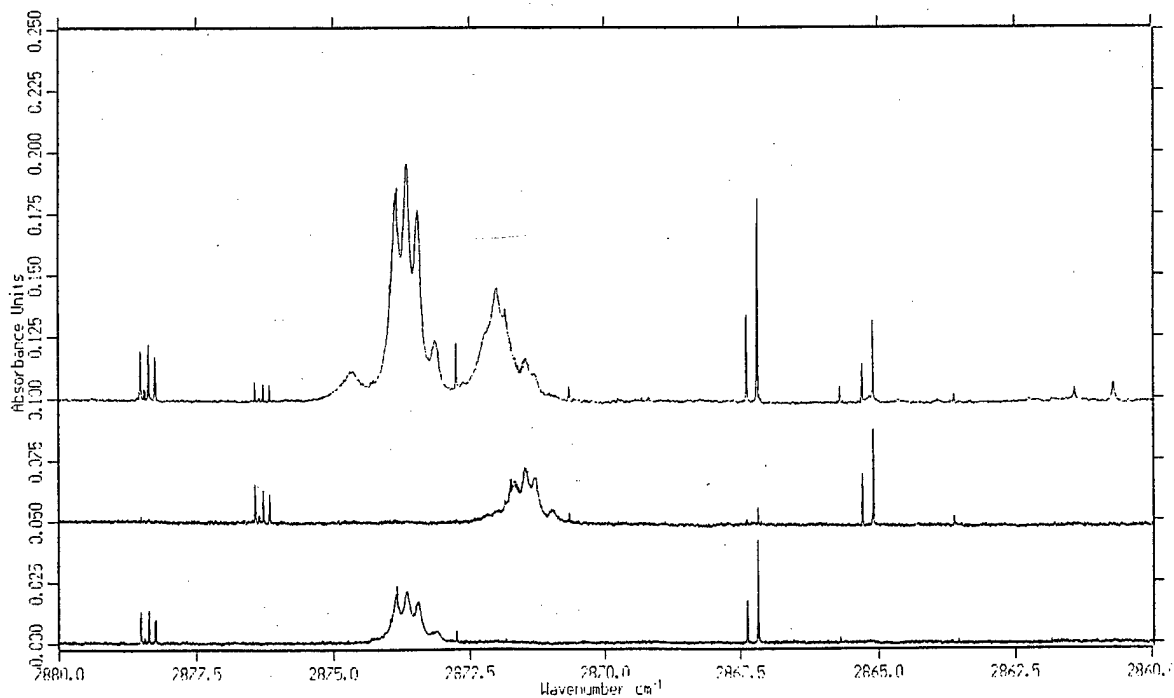
# (HCl)<sub>2</sub> v<sub>1</sub><sup>+</sup> region



st27061.11 annealed T=2.4K 88 PPM HCl  
st27103.6 annealed T=2.4K 94 PPM H<sup>37</sup>Cl  
st27079.11 annealed T=2.4K 90 PPM H<sup>35</sup>Cl

st27103.6

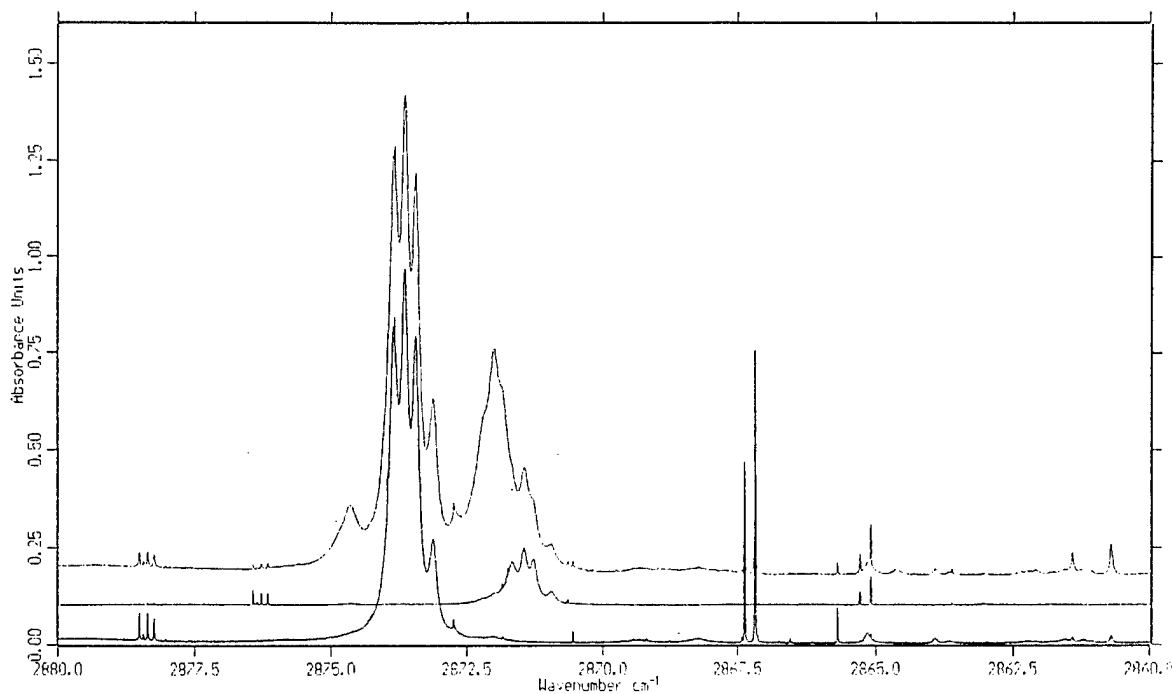
# (HCl)<sub>2</sub> v<sub>1</sub><sup>+</sup> region



st27061.11 annealed T=2.4K 88 PPM HCl  
st27097.6 annealed T=2.4K 33 PPM H<sup>37</sup>Cl  
st27073.17 annealed T=2.4K 30 PPM H<sup>35</sup>Cl

st27097.6

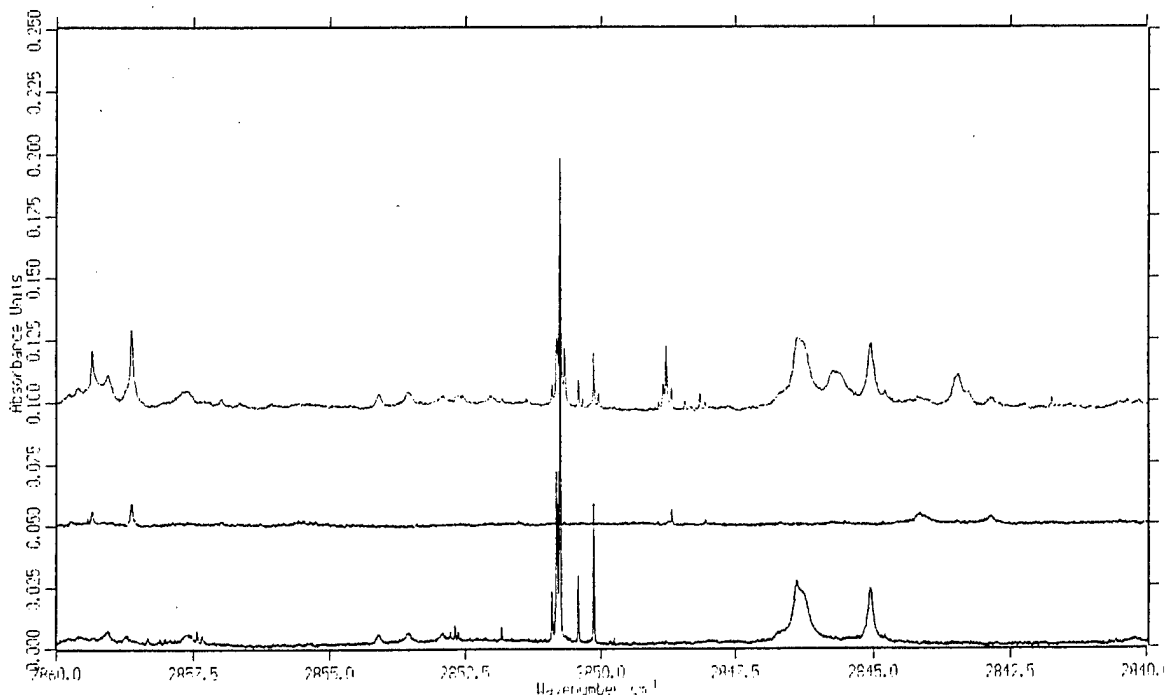
# $(\text{HCl})_2 \nu_1^+$ region



st27067.10	annealed	T=2.4K	494 PPM HCl
st27103.6	annealed	T=2.4K	94 PPM $\text{H}^{37}\text{Cl}$
st27085.9	annealed	T=2.4K	284 PPM $\text{H}^{35}\text{Cl}$

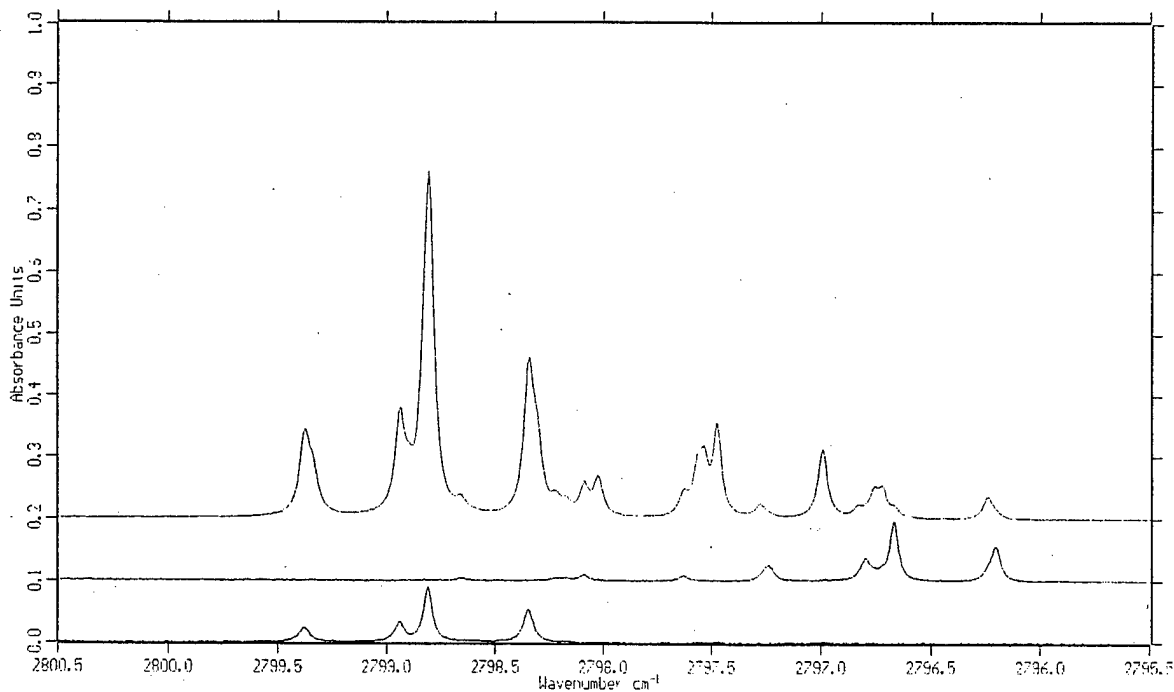
ST27103.6

# $(\text{HCl})_n$



st27067.10	annealed	T=2.4K	494 PPM HCl
st27103.6	annealed	T=2.4K	94 PPM $\text{H}^{37}\text{Cl}$
st27085.9	annealed	T=2.4K	284 PPM $\text{H}^{35}\text{Cl}$

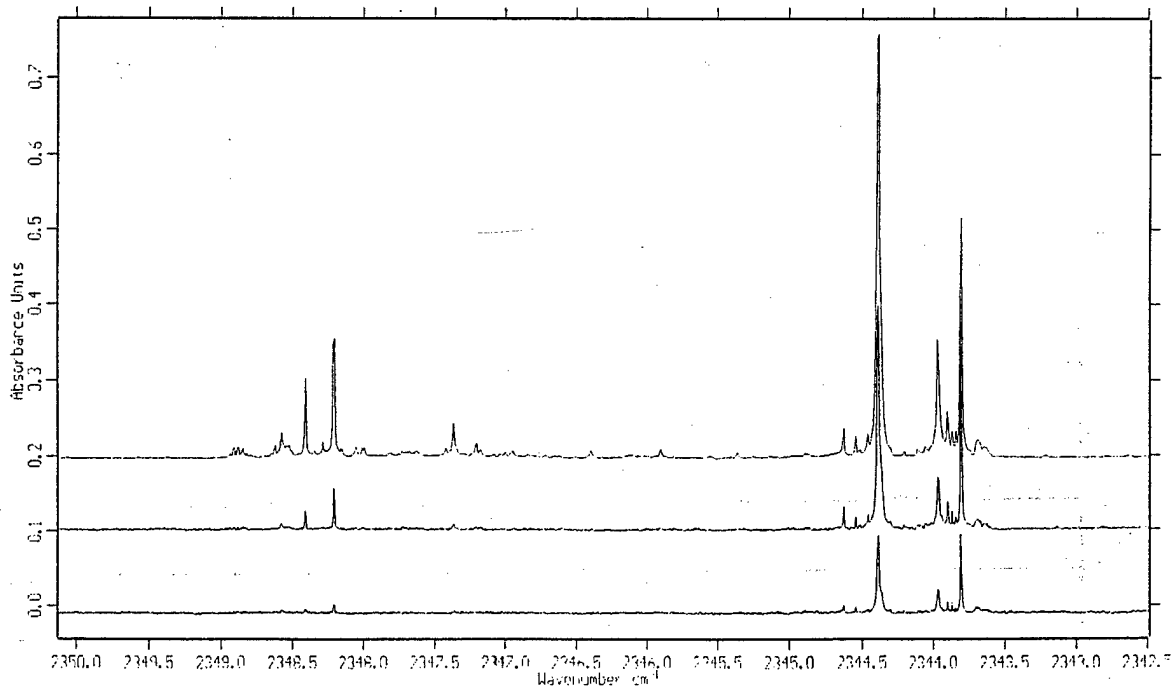
ST27103.6



st27061.11 annealed T=2.4K 88 PPM HCl  
st27097.6 annealed T=2.4K 33 PPM H<sup>37</sup>Cl  
st27073.17 annealed T=2.4K 30 PPM H<sup>35</sup>Cl

st27061.11

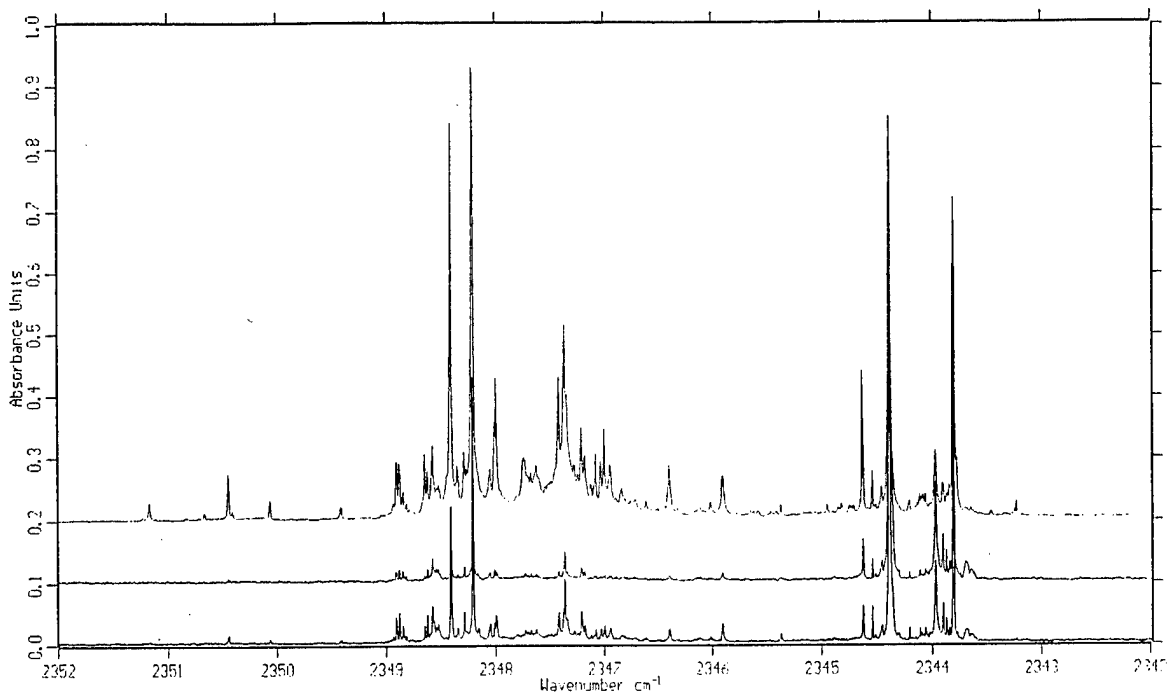
## $\nu_3$ CO<sub>2</sub>/(HCl)<sub>n</sub> clusters



st27061.11 annealed T=2.4K 88 PPM HCl  
st27097.6 annealed T=2.4K 33 PPM H<sup>37</sup>Cl  
st27073.17 annealed T=2.4K 30 PPM H<sup>35</sup>Cl

st27061.11

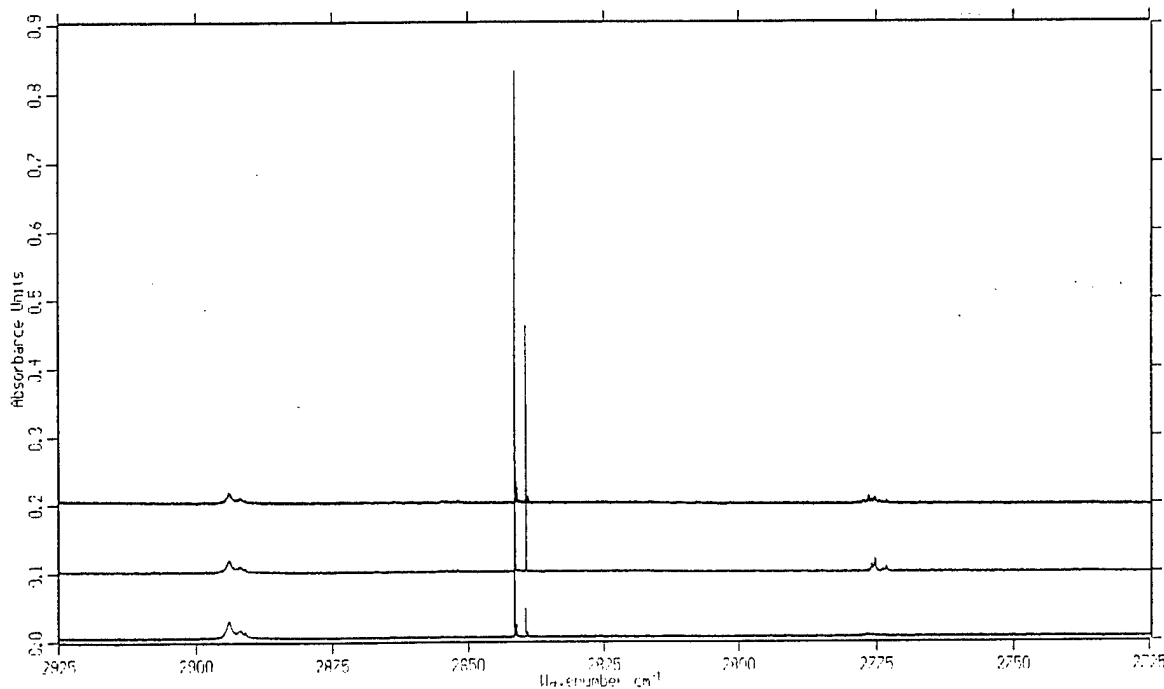
# $\nu_3$ CO<sub>2</sub>/(HCl)<sub>n</sub> clusters



st27067.10 annealed T=2.4K 494 PPM HCl  
 st27103.6 annealed T=2.4K 94 PPM H<sup>37</sup>Cl  
 st27085.9 annealed T=2.4K 284 PPM H<sup>35</sup>Cl

st27103.6

# HF-HCl/pH<sub>2</sub>

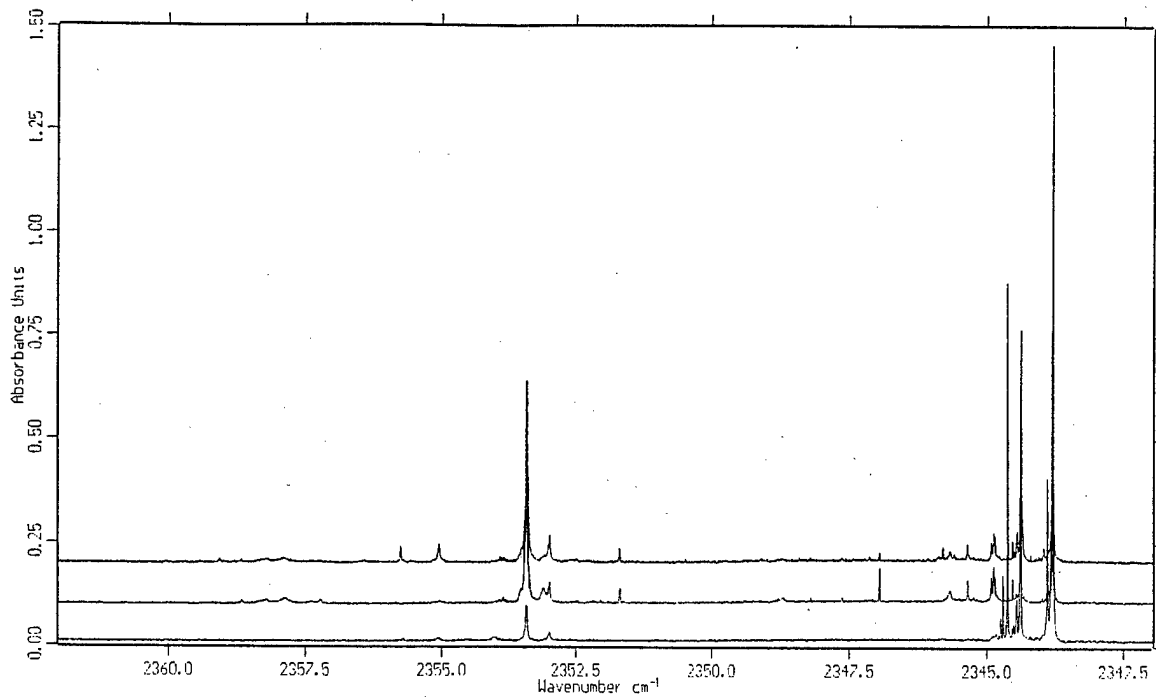


st27115.15 annealed T=2.4K  
 st27115.13 annealing T=4.8K  
 st27115.9 as deposited T=2.4K

123 PPM HF/pH<sub>2</sub> d≈3mm

resolution = 0.005 cm<sup>-1</sup>

# CO<sub>2</sub>-HF/pH<sub>2</sub>



st27115.15  
st27115.13  
st27115.9

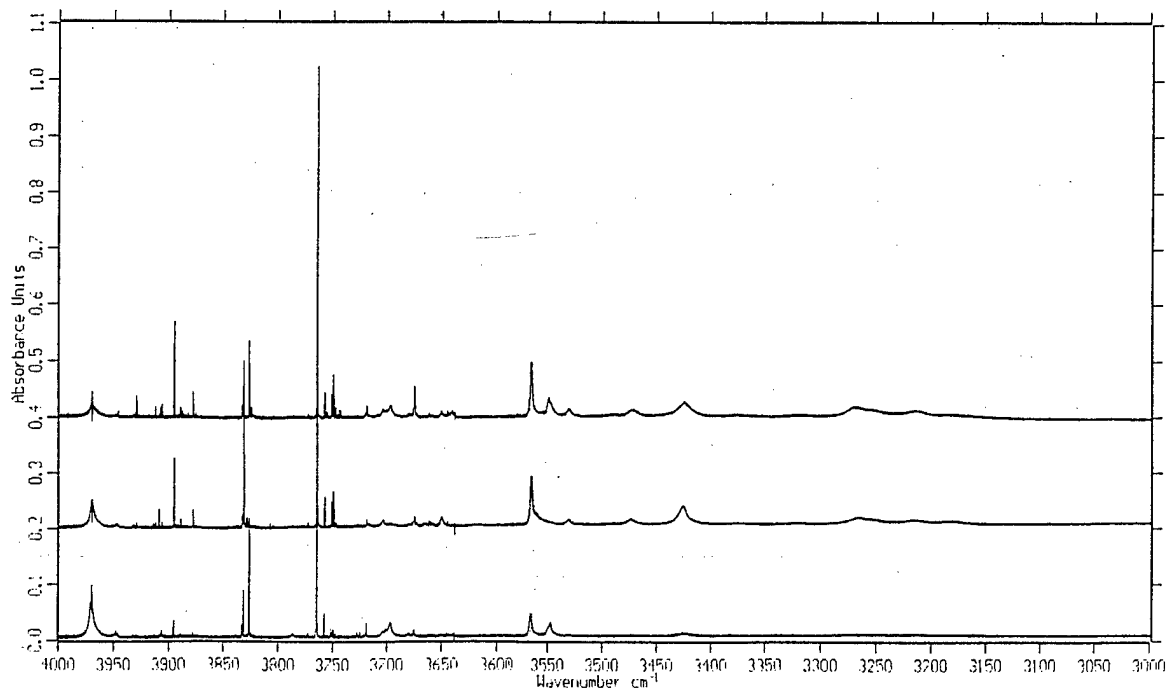
annealed T=2.4K  
annealing T=4.8K  
as deposited T=2.4K

123 PPM HF/pH<sub>2</sub> d≈3mm

resolution = 0.005 cm<sup>-1</sup>

ST27115.9

## 27 PPM HF/pH<sub>2</sub> d≈3mm



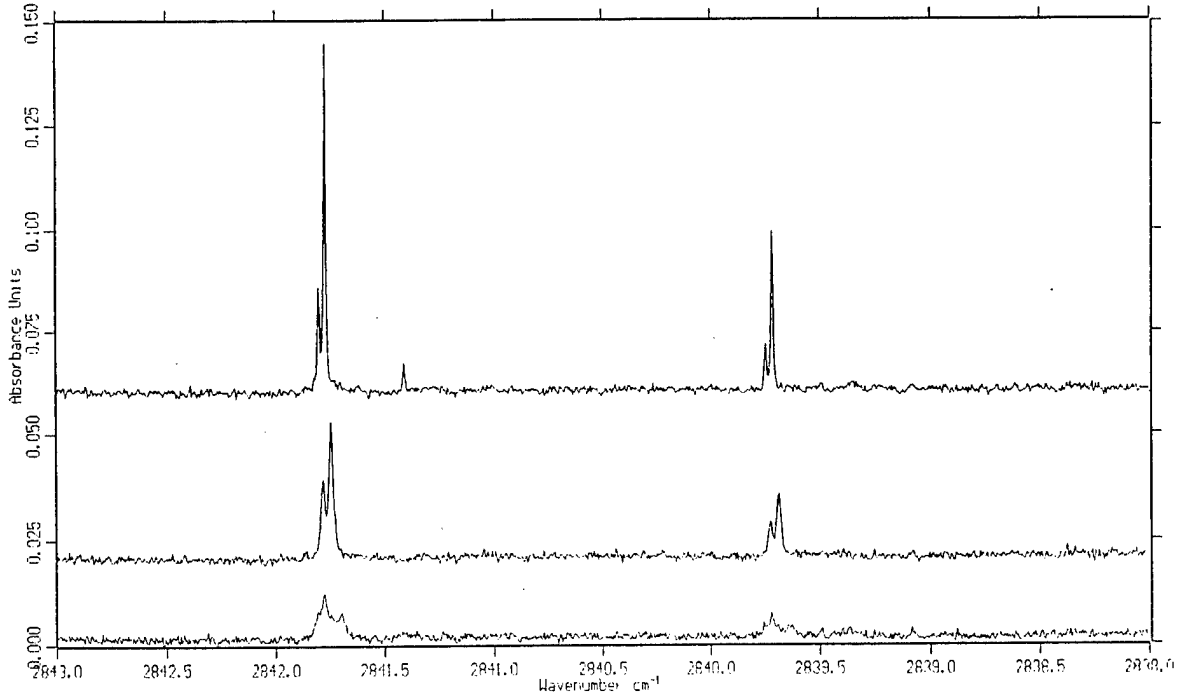
st27121.9  
st27121.7  
st27121.5

annealed T=2.4K  
annealing T=4.8K  
as deposited T=2.4K

resolution = 0.005 cm<sup>-1</sup>

ST27121.5

# HF-HCl/pH<sub>2</sub>



st27121.9  
st27121.7  
st27121.5

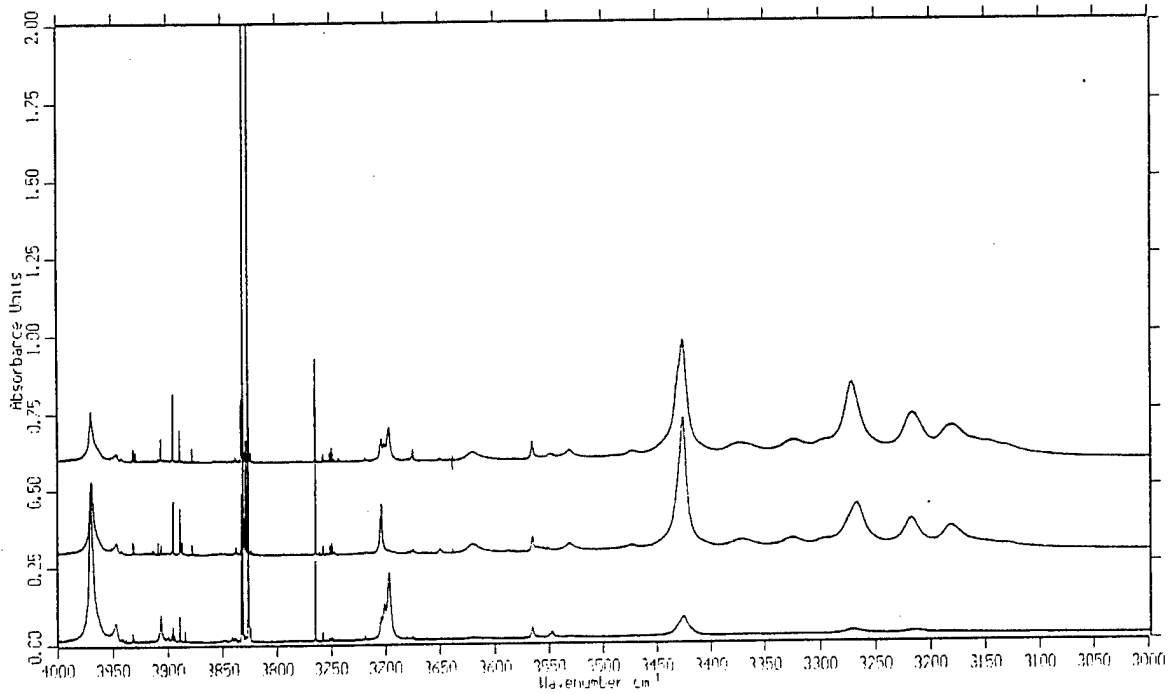
annealed T=2.4K  
annealing T=4.8K  
as deposited T=2.4K

27 PPM HF/pH<sub>2</sub> d≈3mm

resolution = 0.005 cm<sup>-1</sup>

st27121.5

## 91 <sup>ppm</sup> PPM HF/pH<sub>2</sub> d≈3mm



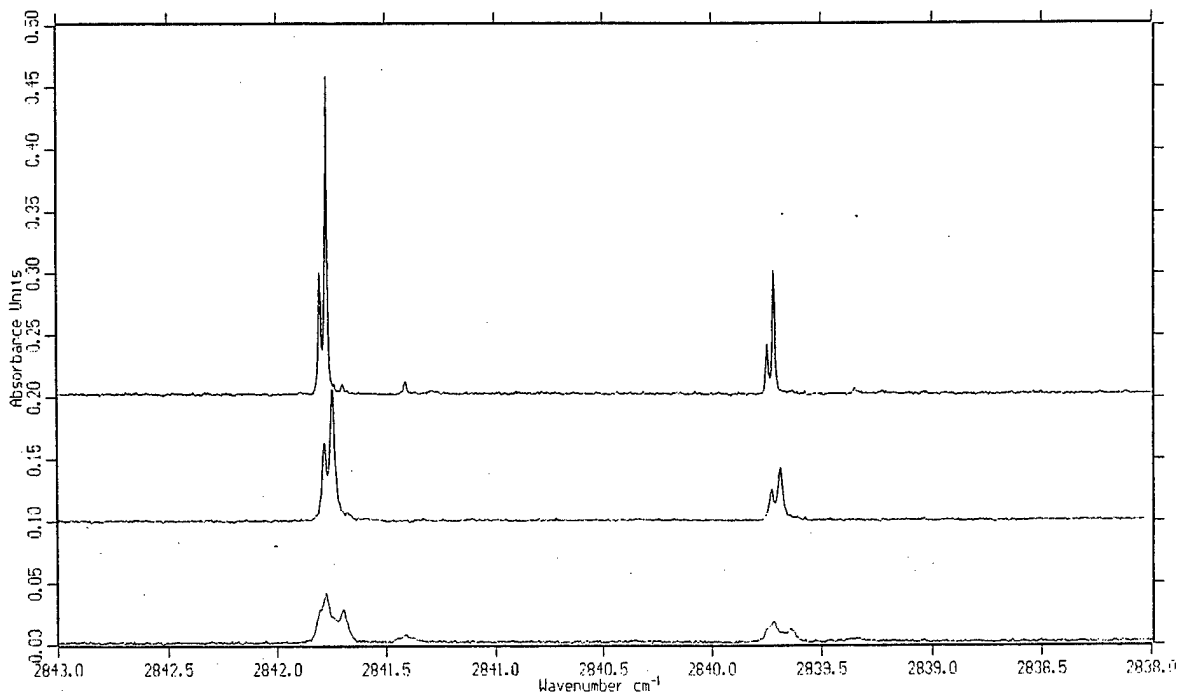
st27127.9  
st27127.7  
st27127.5

annealed T=2.4K  
annealing T=4.8K  
as deposited T=2.4K

resolution = 0.005 cm<sup>-1</sup>

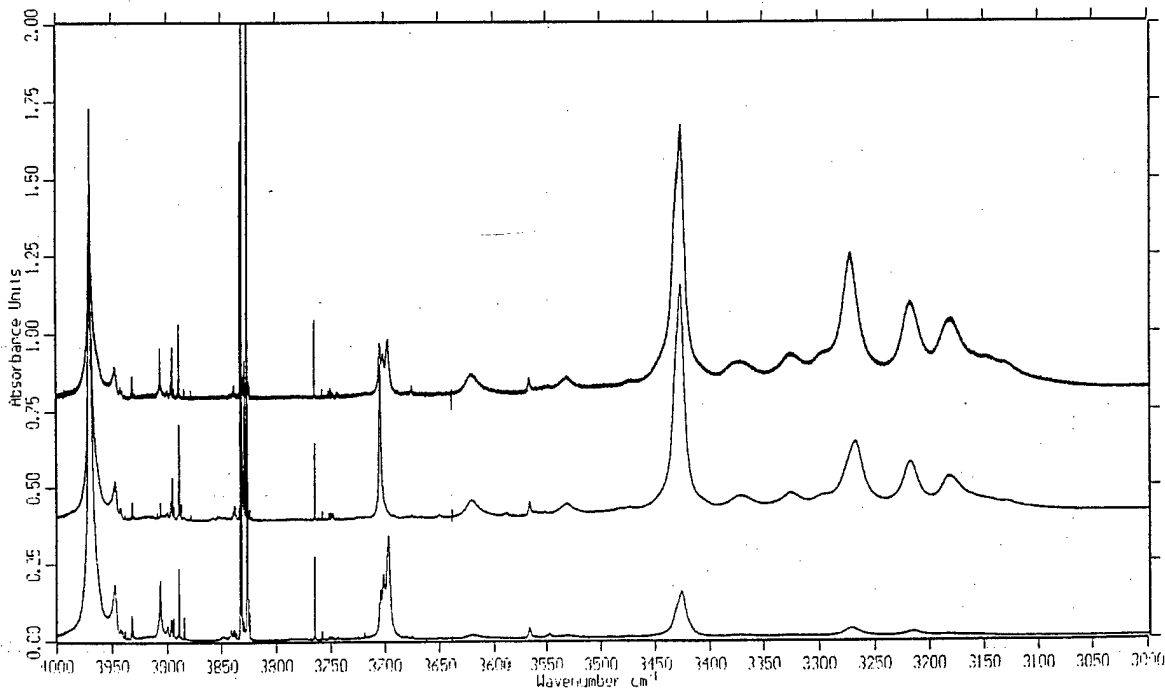
st27127.5

# HF-HCl/pH<sub>2</sub>



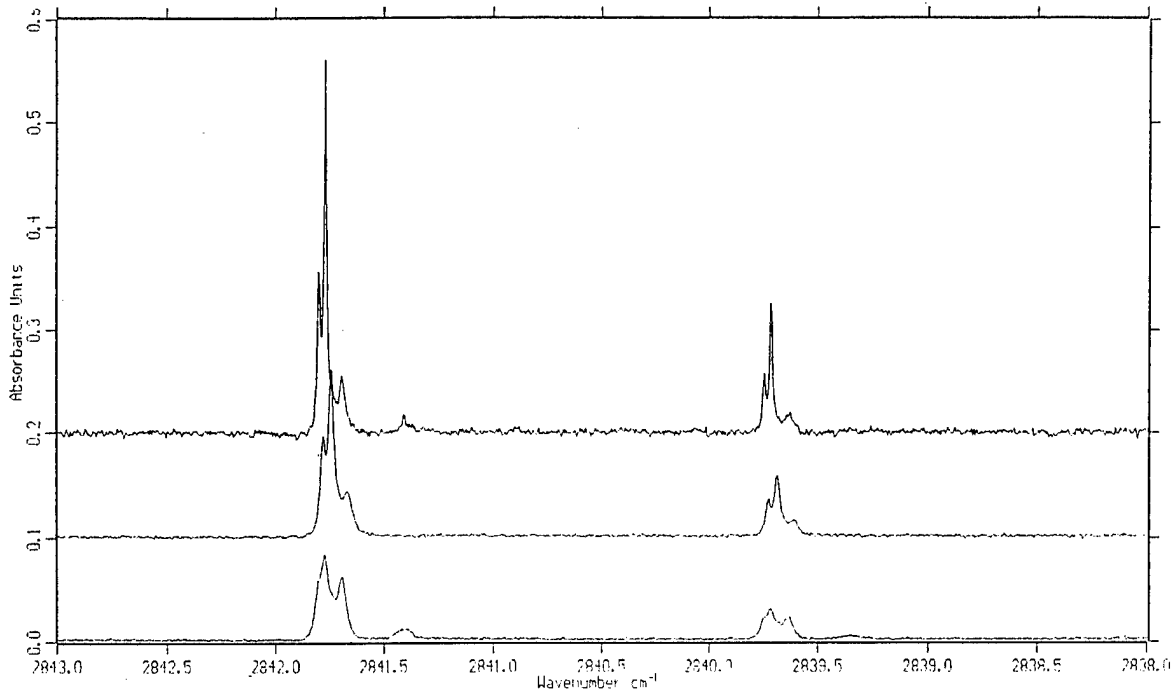
st27127.9      annealed    T=2.4K  
st27127.7      annealing    T=4.8K  
st27127.5      as deposited T=2.4K      91 PPM HF/pH<sub>2</sub> d≈3mm      resolution = 0.005 cm<sup>-1</sup>      st27127.5

# 268 PPM HF/pH<sub>2</sub> d≈3mm



st27133.9      annealed    T=2.4K  
st27133.7      annealing    T=4.8K  
st27133.5      as deposited T=2.4K      resolution = 0.005 cm<sup>-1</sup>      st27133.5

# HF-HCl/pH<sub>2</sub>



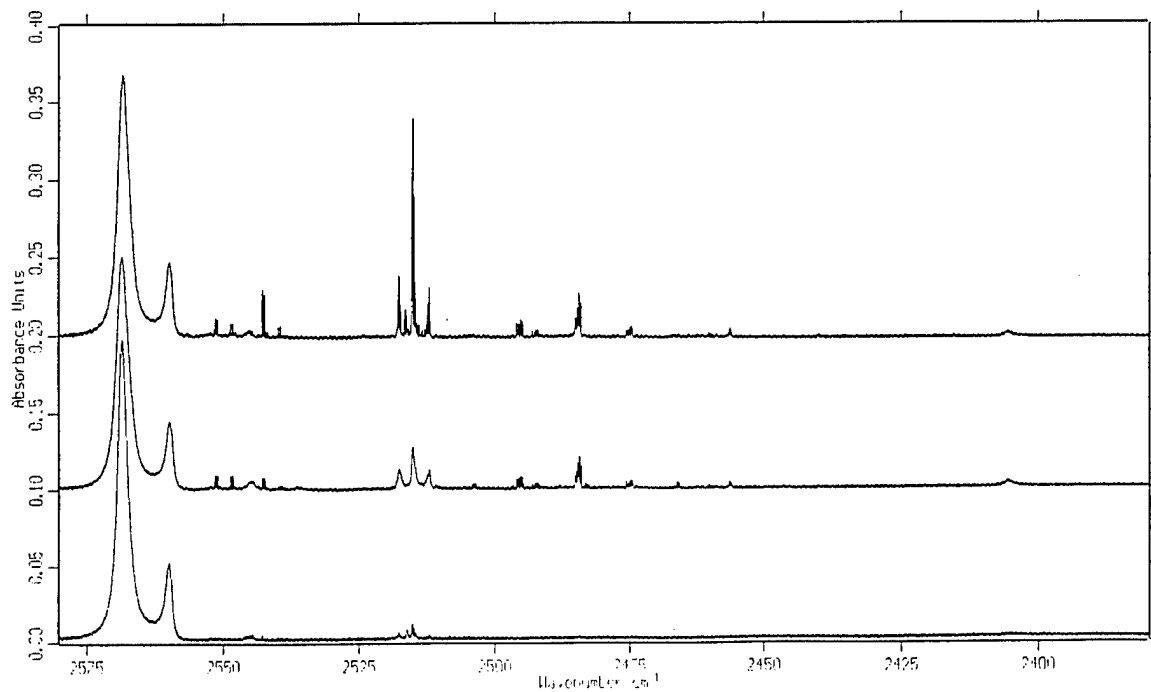
st27133.9      annealed    T=2.4K  
st27133.7      annealing    T=4.8K  
st27133.5      as deposited T=2.4K

268 PPM HF/pH<sub>2</sub> d≈3mm

resolution = 0.005 cm<sup>-1</sup>

st27133.5

# 80 PPM HBr/pH<sub>2</sub> d≈3mm

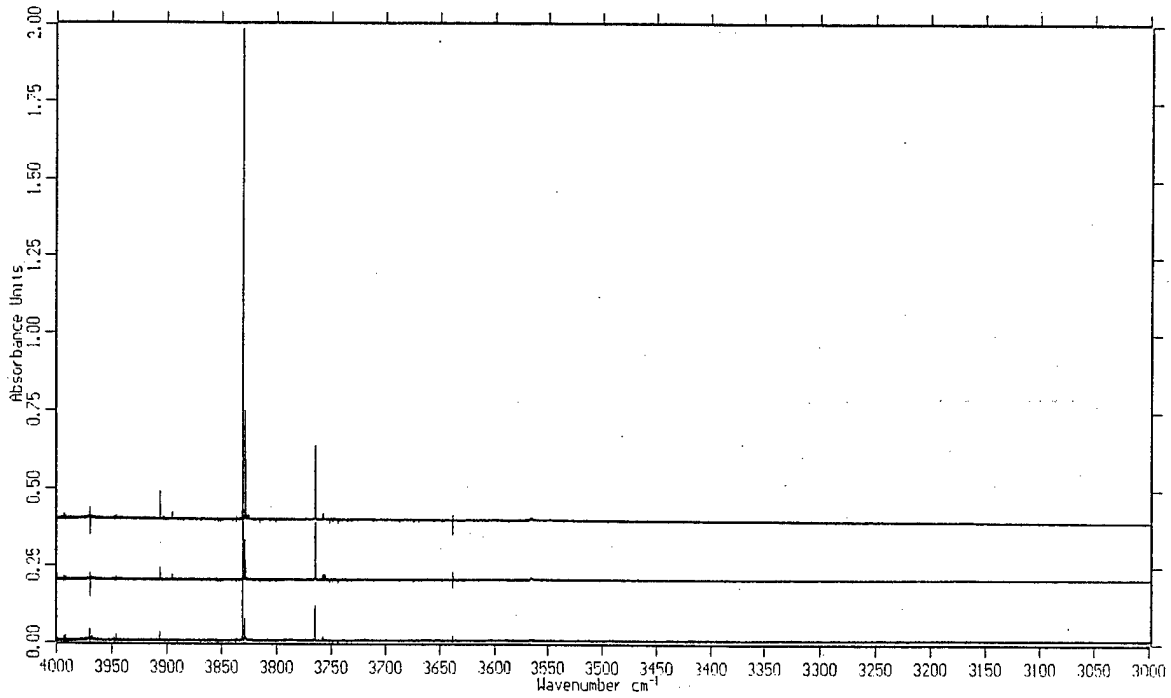


st27140.9      annealed    T=2.4K  
st27140.7      annealing    T=4.8K  
st27140.5      as deposited T=2.4K

resolution = 0.005 cm<sup>-1</sup>

st27140.5

# HF-(HF, HCl, HBr)/pH<sub>2</sub>



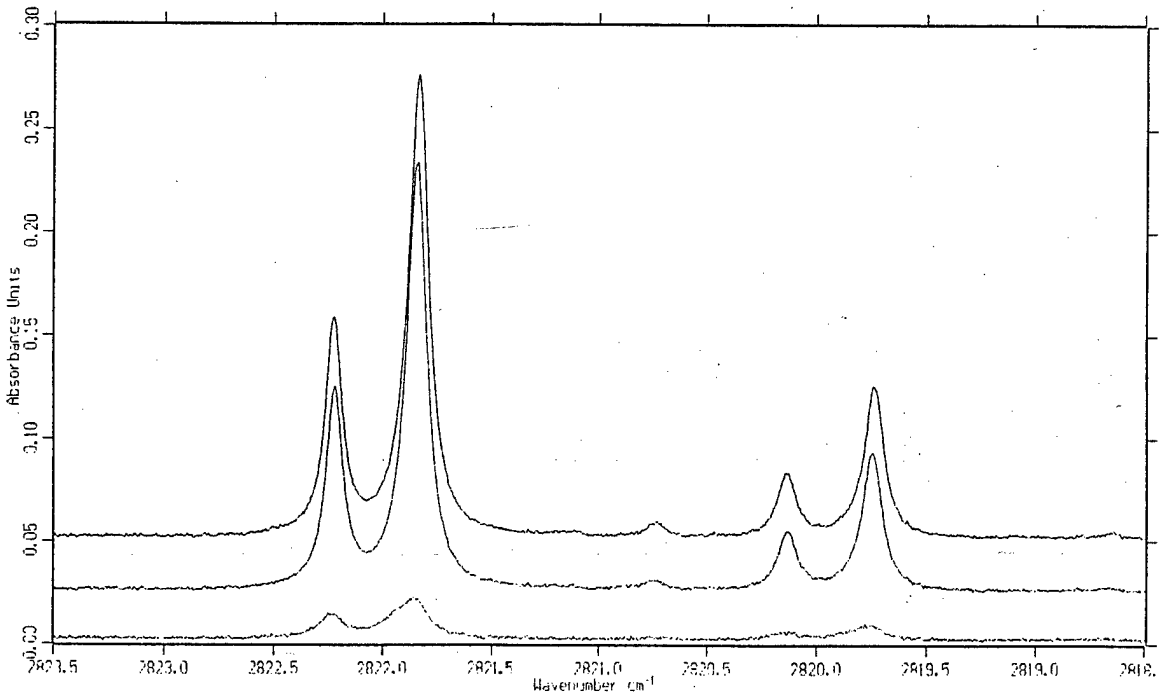
st27140.9      annealed    T=2.4K  
st27140.7      annealing   T=4.8K  
st27140.5      as deposited T=2.4K

80 PPM HBr/pH<sub>2</sub> d≈3mm

resolution = 0.005 cm<sup>-1</sup>

ST27140.5

# HCl-HBr/pH<sub>2</sub>



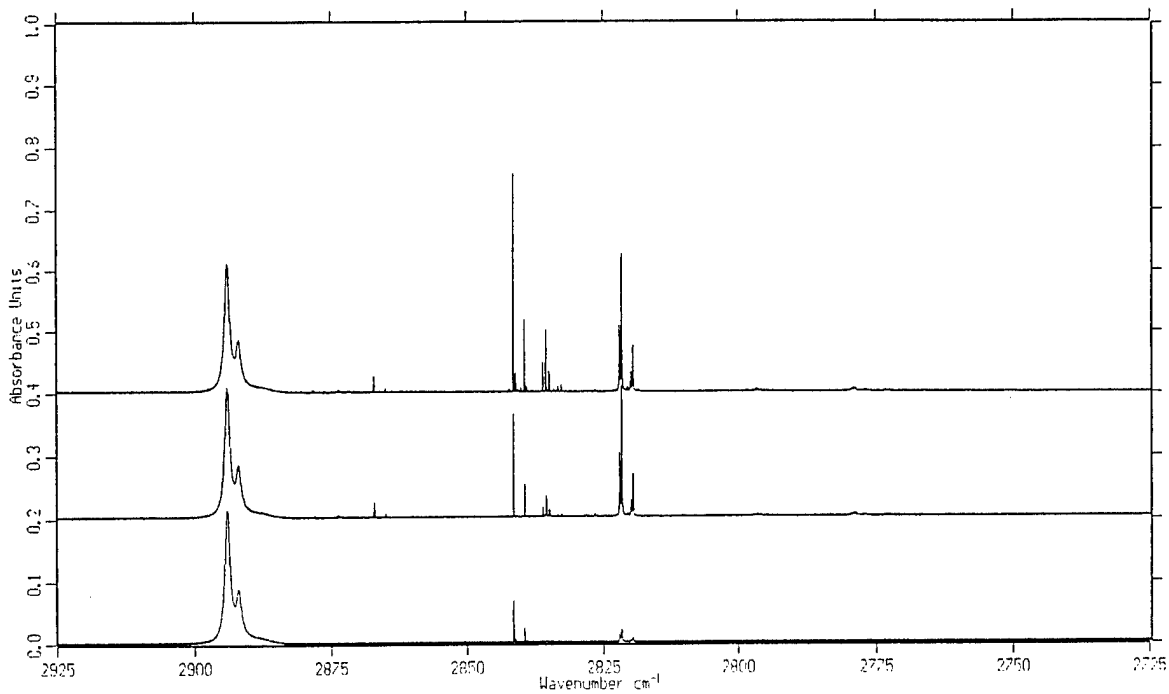
st27140.9      annealed    T=2.4K  
st27140.7      annealing   T=4.8K  
st27140.5      as deposited T=2.4K

80 PPM HBr/pH<sub>2</sub> d≈3mm

resolution = 0.005 cm<sup>-1</sup>

ST27140.5

# HCl-(HF, HCl, HBr)/pH<sub>2</sub>



st27140.9  
st27140.7  
st27140.5

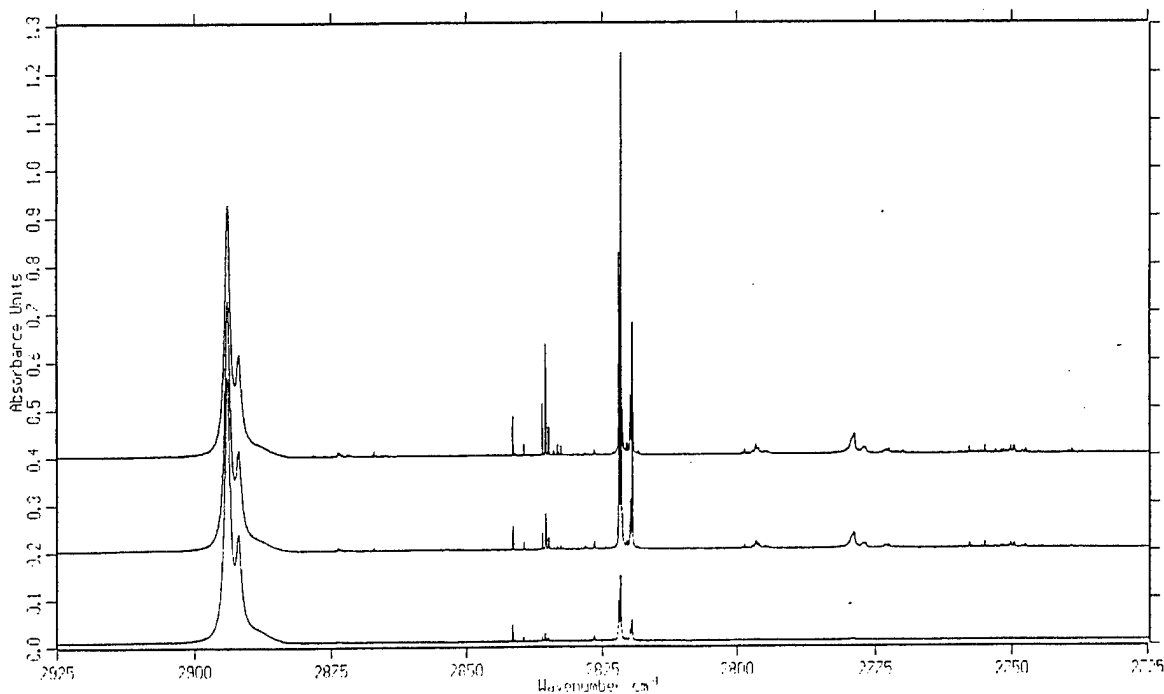
annealed T=2.4K  
annealing T=4.8K  
as deposited T=2.4K

80 PPM HBr/pH<sub>2</sub> d≈3mm

resolution = 0.005 cm<sup>-1</sup>

st27140.5

# HCl-(HF, HCl, HBr)/pH<sub>2</sub>



st27145.9  
st27145.7  
st27145.5

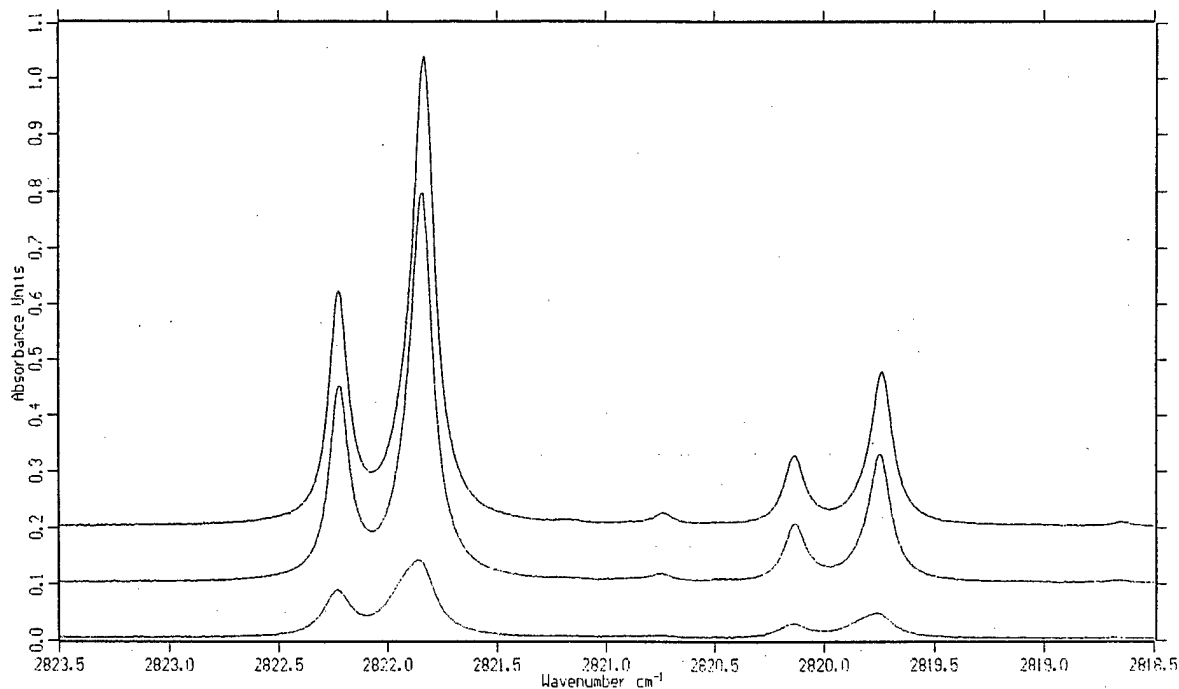
annealed T=2.4K  
annealing T=4.8K  
as deposited T=2.4K

260 PPM HBr/pH<sub>2</sub> d≈3mm

resolution = 0.005 cm<sup>-1</sup>

st27145.5

# HCl-HBr/pH<sub>2</sub>



st27145.9  
st27145.7  
st27145.5

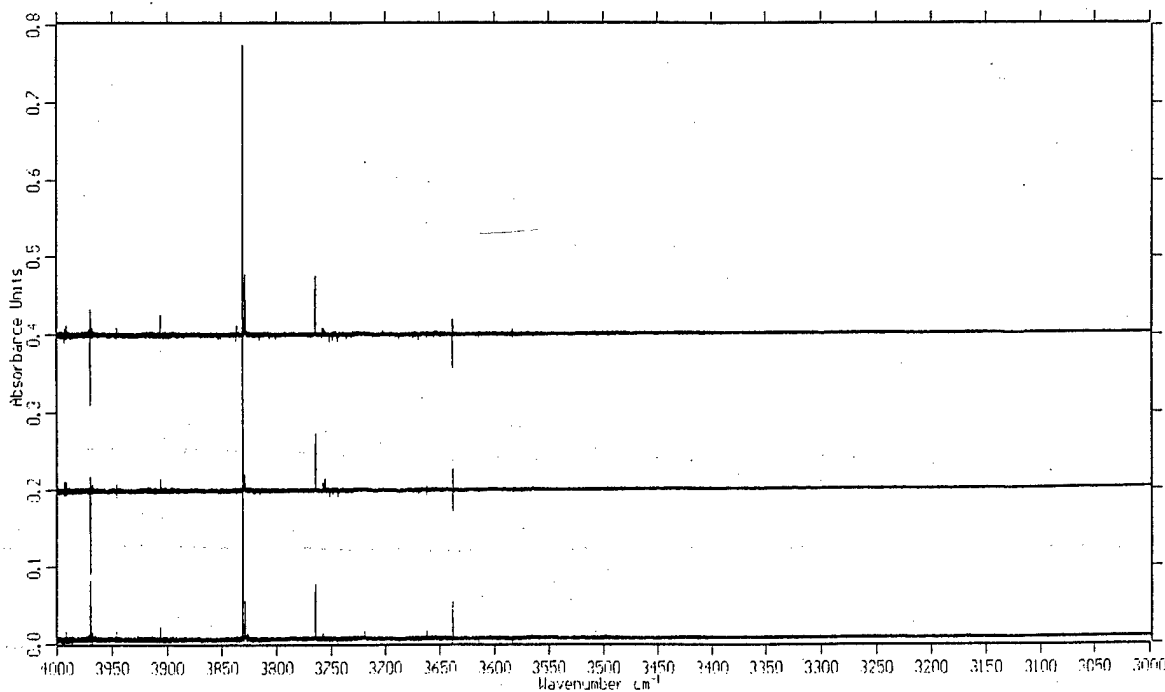
annealed T=2.4K  
annealing T=4.8K  
as deposited T=2.4K

260 PPM HBr/pH<sub>2</sub> d≈3mm

resolution = 0.005 cm<sup>-1</sup>

ST27145.5

# HF-(HF, HCl, HBr)/pH<sub>2</sub>



st27145.9  
st27145.7  
st27145.5

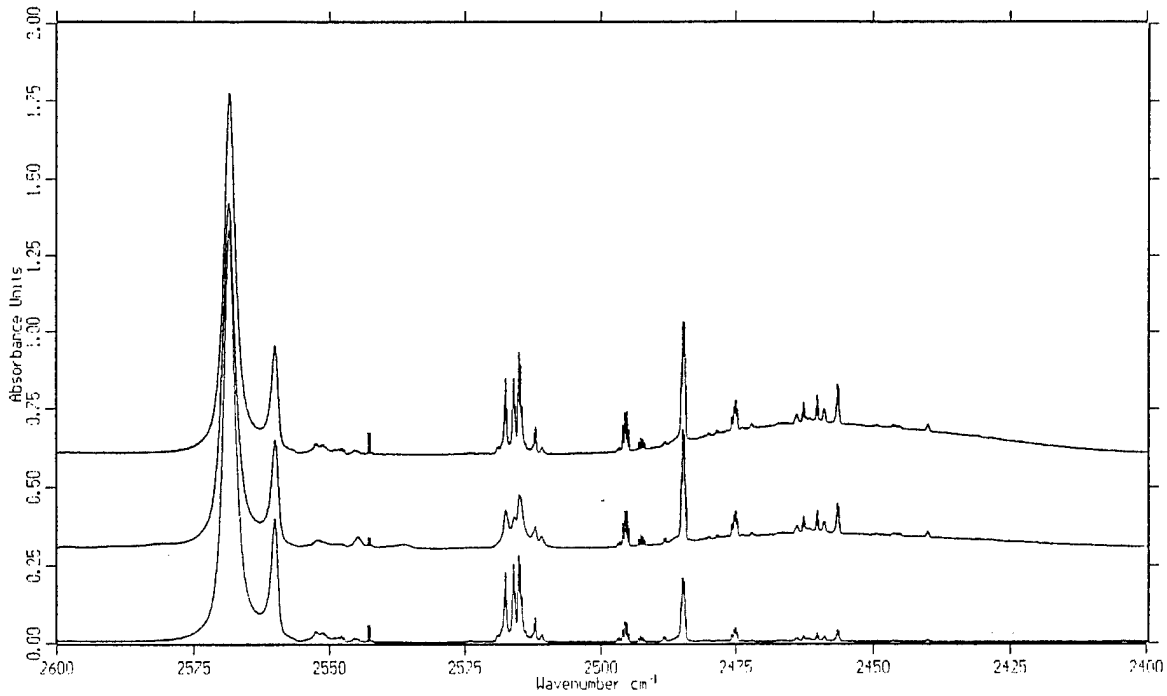
annealed T=2.4K  
annealing T=4.8K  
as deposited T=2.4K

260 PPM HBr/pH<sub>2</sub> d≈3mm

resolution = 0.005 cm<sup>-1</sup>

ST27145.5

# 645 HBr/pH<sub>2</sub> d≈3mm

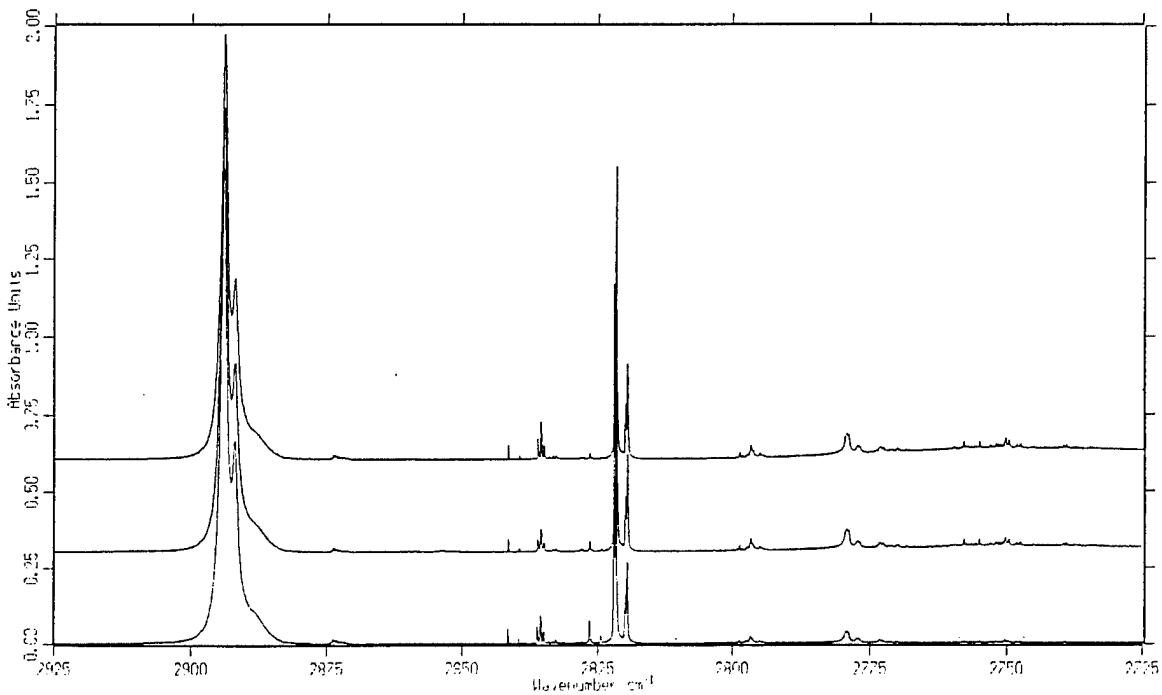


st28003.9     annealed     T=2.4K  
st28003.7     annealing     T=4.8K  
st28003.5     as deposited     T=2.4K

resolution = 0.005 cm<sup>-1</sup>

ST28003.5

# HCl(HBr)<sub>n</sub>/pH<sub>2</sub>



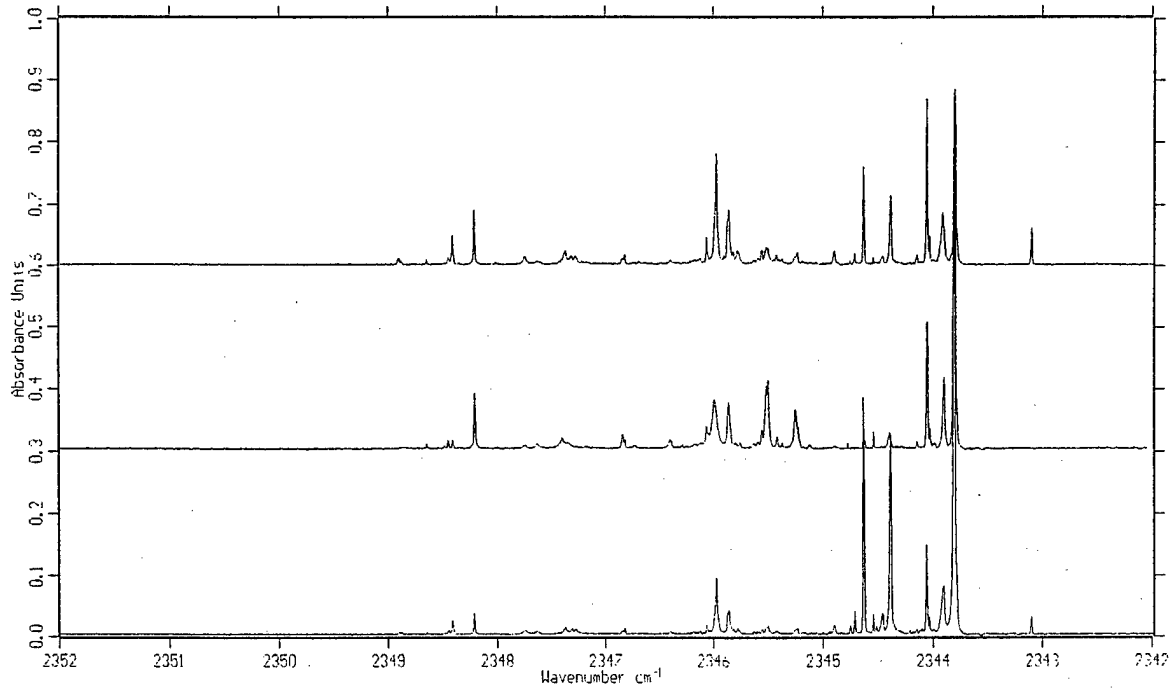
st28003.9     annealed     T=2.4K  
st28003.7     annealing     T=4.8K  
st28003.5     as deposited     T=2.4K

645 HBr/pH<sub>2</sub> d≈3mm

resolution = 0.005 cm<sup>-1</sup>

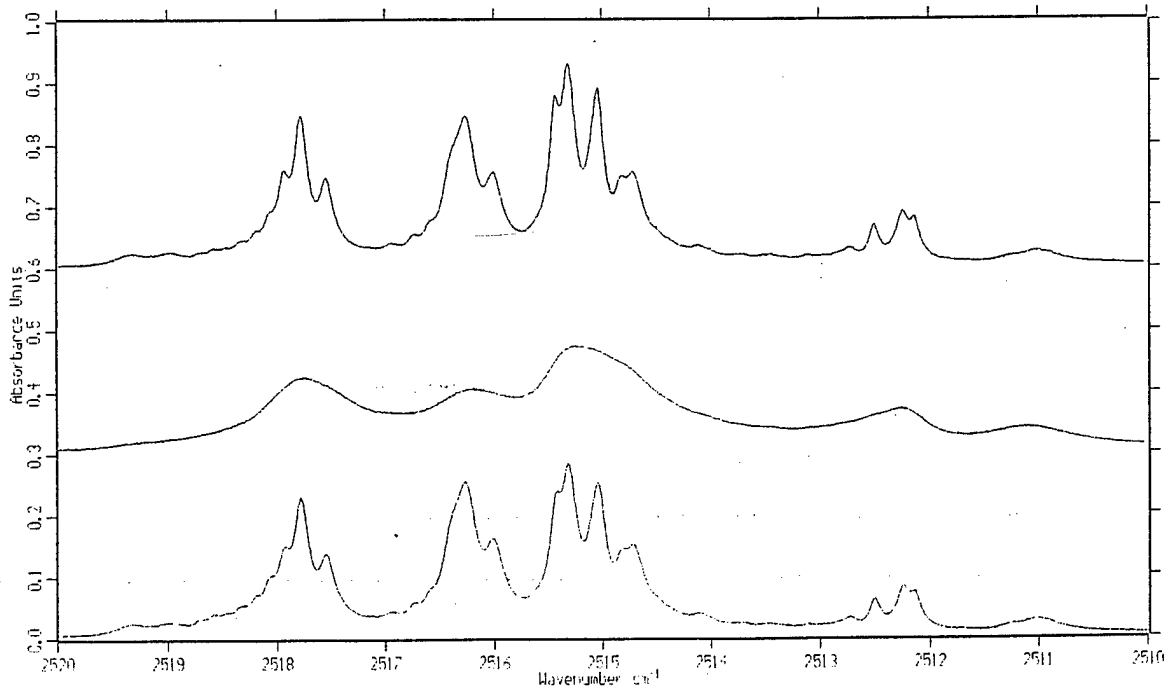
ST28003.5

# $\text{CO}_2(\text{HBr})_n/\text{pH}_2$



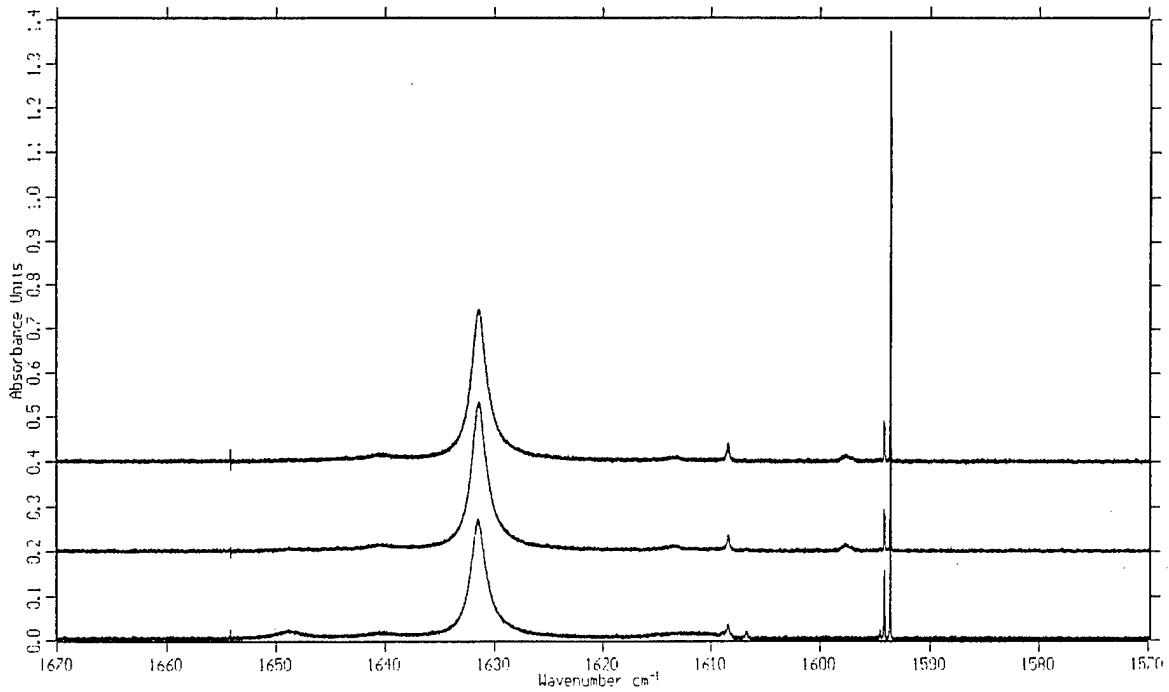
st28003.9      annealed    T=2.4K  
st28003.7      annealing    T=4.8K  
st28003.5      as deposited T=2.4K      645 HBr/ $\text{pH}_2$   $d \approx 3\text{mm}$       resolution =  $0.005 \text{ cm}^{-1}$       ST28003.5

# $(\text{HBr})_2/\text{pH}_2$



st28003.9      annealed    T=2.4K  
st28003.7      annealing    T=4.8K  
st28003.5      as deposited T=2.4K      645 HBr/ $\text{pH}_2$   $d \approx 3\text{mm}$       resolution =  $0.005 \text{ cm}^{-1}$       ST28003.5

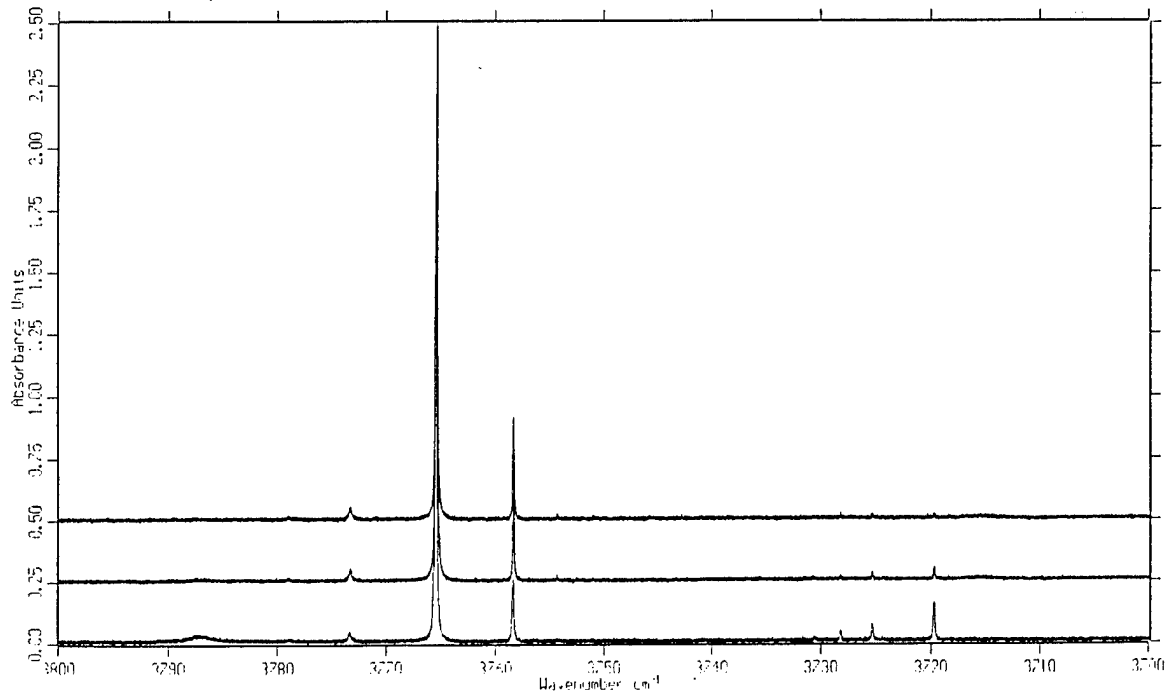
<sup>ppm</sup>  
15 ~~PPM~~ H<sub>2</sub>O/pH<sub>2</sub> d $\approx$ 3mm



st28010.6      annealed    T=2.4K  
st28010.4      annealing   T=4.8K  
st28010.2      as deposited T=2.4K      resolution = 0.005 cm<sup>-1</sup>

ST28010.2

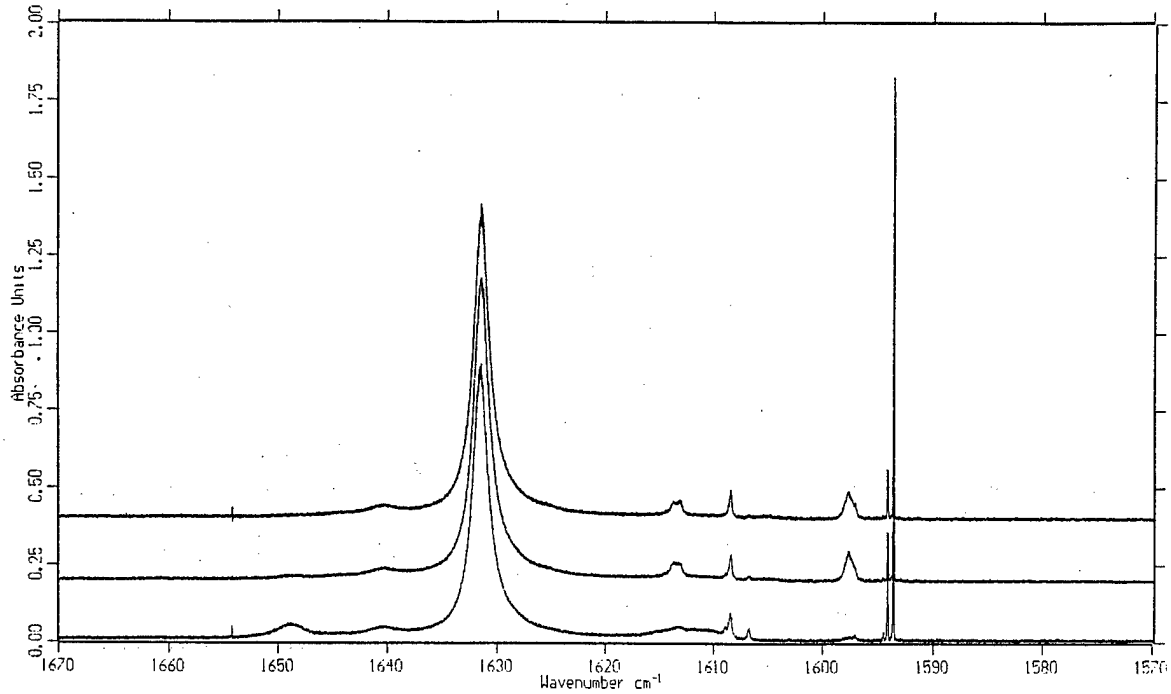
<sup>ppm</sup>  
15 ~~PPM~~ H<sub>2</sub>O/pH<sub>2</sub> d $\approx$ 3mm



st28010.6      annealed    T=2.4K  
st28010.4      annealing   T=4.8K  
st28010.2      as deposited T=2.4K      resolution = 0.005 cm<sup>-1</sup>

ST28010.2

45 PPM H<sub>2</sub>O/pH<sub>2</sub> d≈3mm

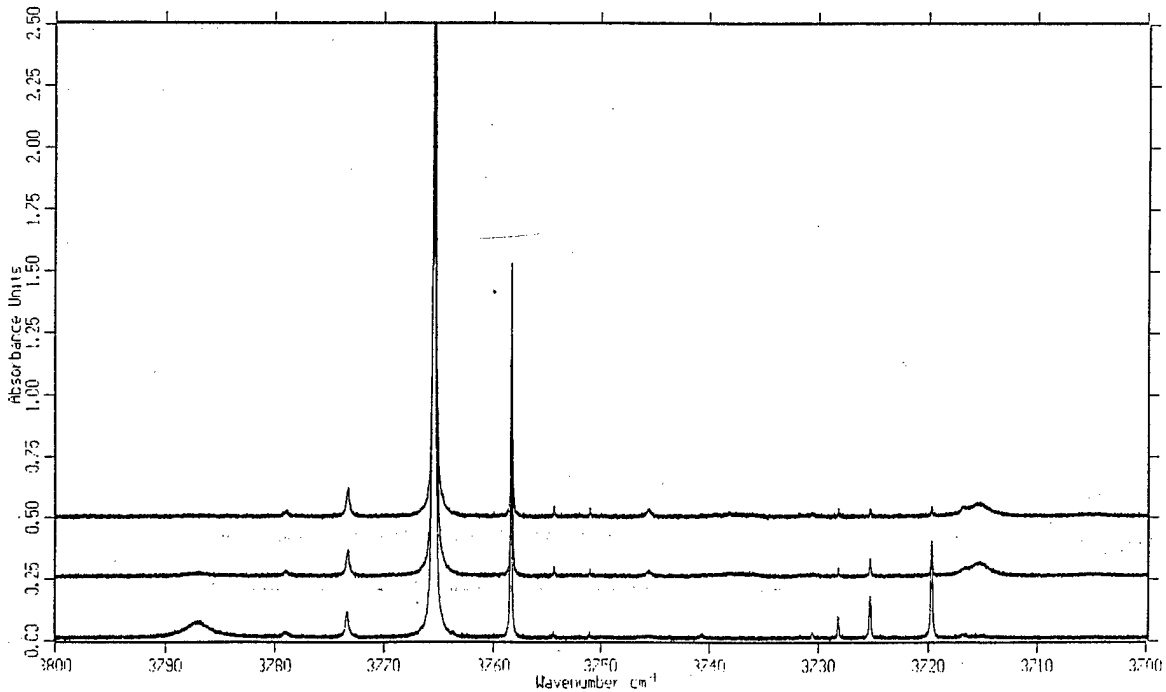


st28014.6      annealed    T=2.4K  
st28014.4      annealing   T=4.8K  
st28014.2      as deposited T=2.4K

resolution = 0.005 cm<sup>-1</sup>

ST28014.2

45 PPM H<sub>2</sub>O/pH<sub>2</sub> d≈3mm

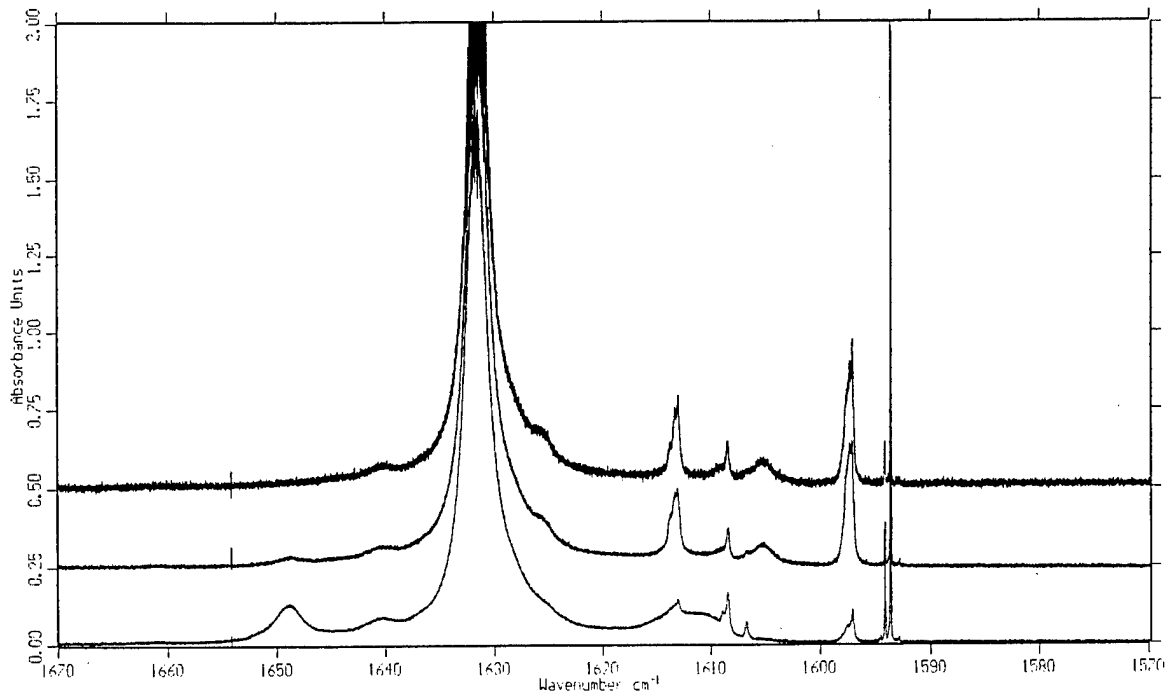


st28014.6      annealed    T=2.4K  
st28014.4      annealing   T=4.8K  
st28014.2      as deposited T=2.4K

resolution = 0.005 cm<sup>-1</sup>

ST28014.2

ppm  
138 PPM H<sub>2</sub>O/pH<sub>2</sub> d≈3mm

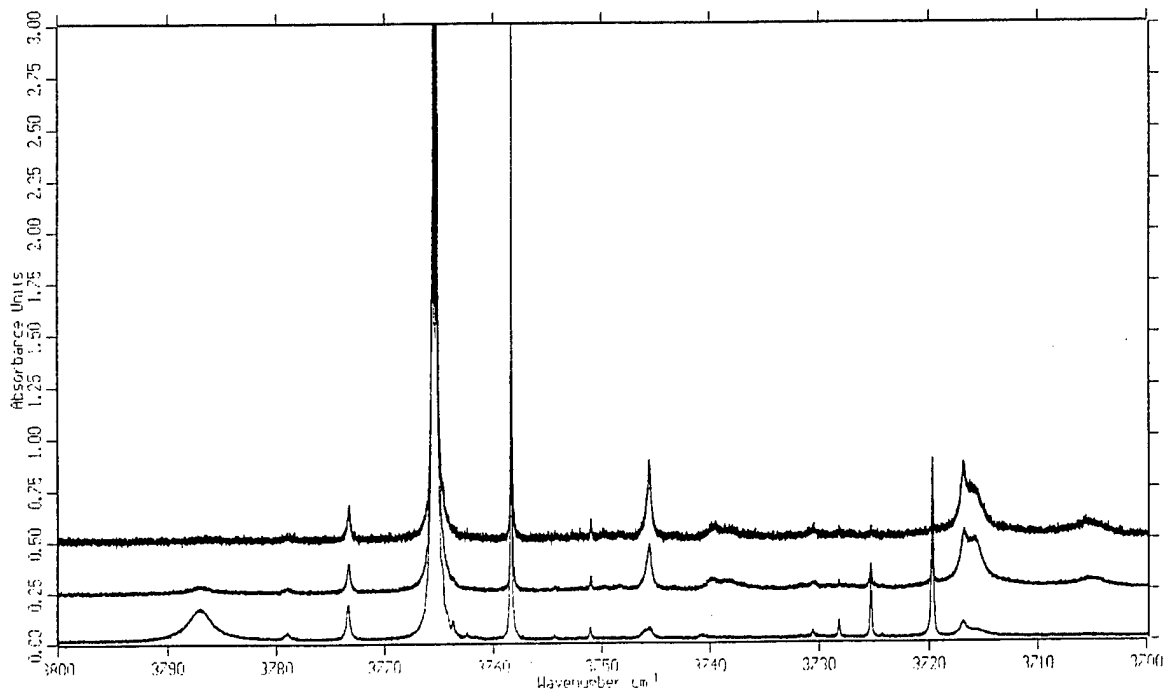


st28018.6      annealed    T=2.4K  
st28018.4      annealing   T=4.8K  
st28018.2      as deposited T=2.4K

resolution = 0.005 cm<sup>-1</sup>

ST28018.2

ppm  
138 PPM H<sub>2</sub>O/pH<sub>2</sub> d≈3mm

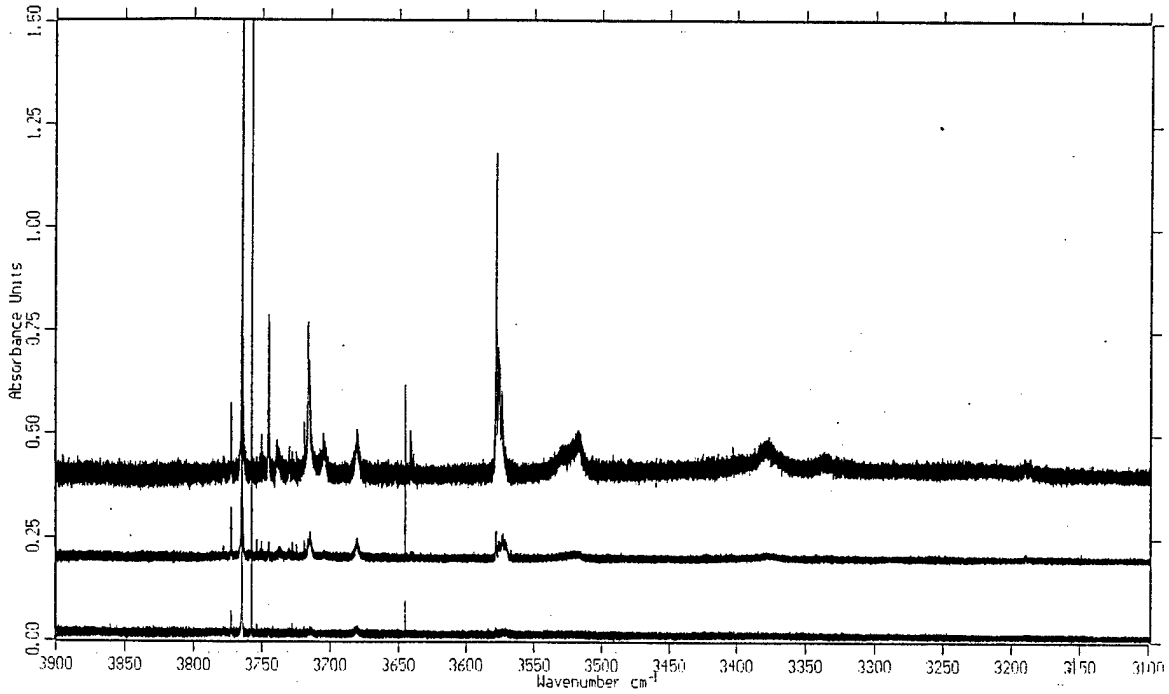


st28018.6      annealed    T=2.4K  
st28018.4      annealing   T=4.8K  
st28018.2      as deposited T=2.4K

resolution = 0.005 cm<sup>-1</sup>

ST28018.2

# H<sub>2</sub>O clusters in pH<sub>2</sub>

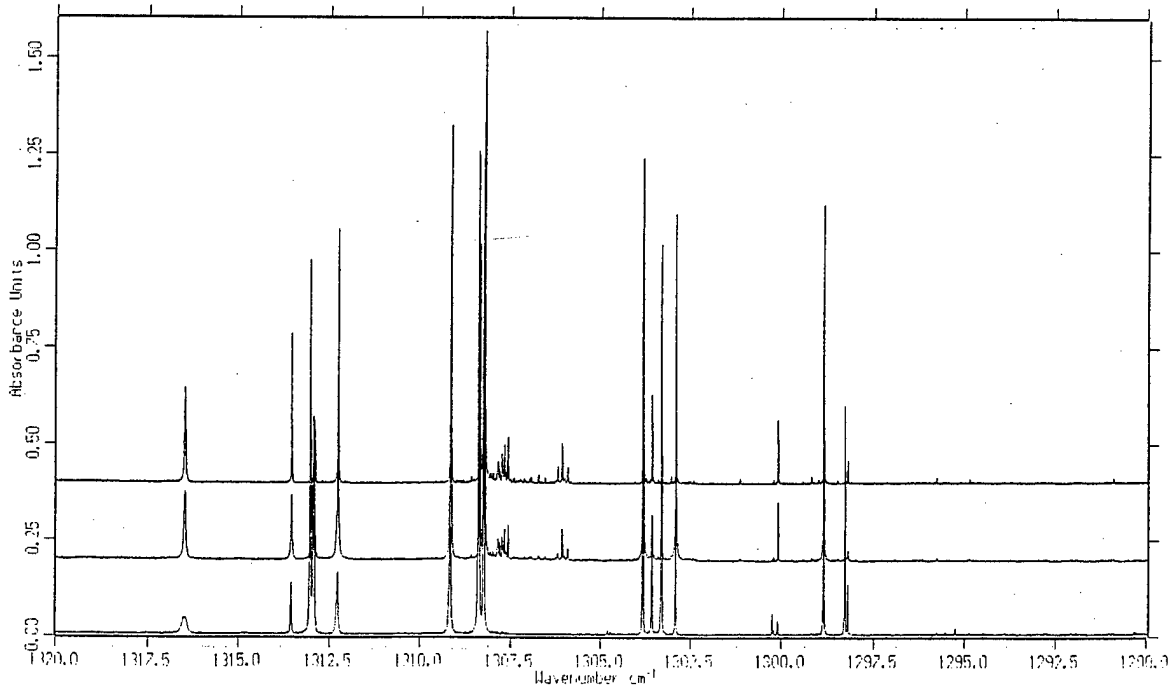


st28018.6      annealed    T=2.4K    138 PPM H<sub>2</sub>O/pH<sub>2</sub>  
 st28014.6      annealed    T=2.4K    45 PPM H<sub>2</sub>O/pH<sub>2</sub>  
 st28010.6      annealed    T=2.4K    15 PPM H<sub>2</sub>O/pH<sub>2</sub>

resolution = 0.005 cm<sup>-1</sup>

ST28010.6

# 56 <sup>ppm</sup> PPM CH<sub>4</sub>/pH<sub>2</sub> <sup>0.7mm</sup> d ≈ 0.7mm

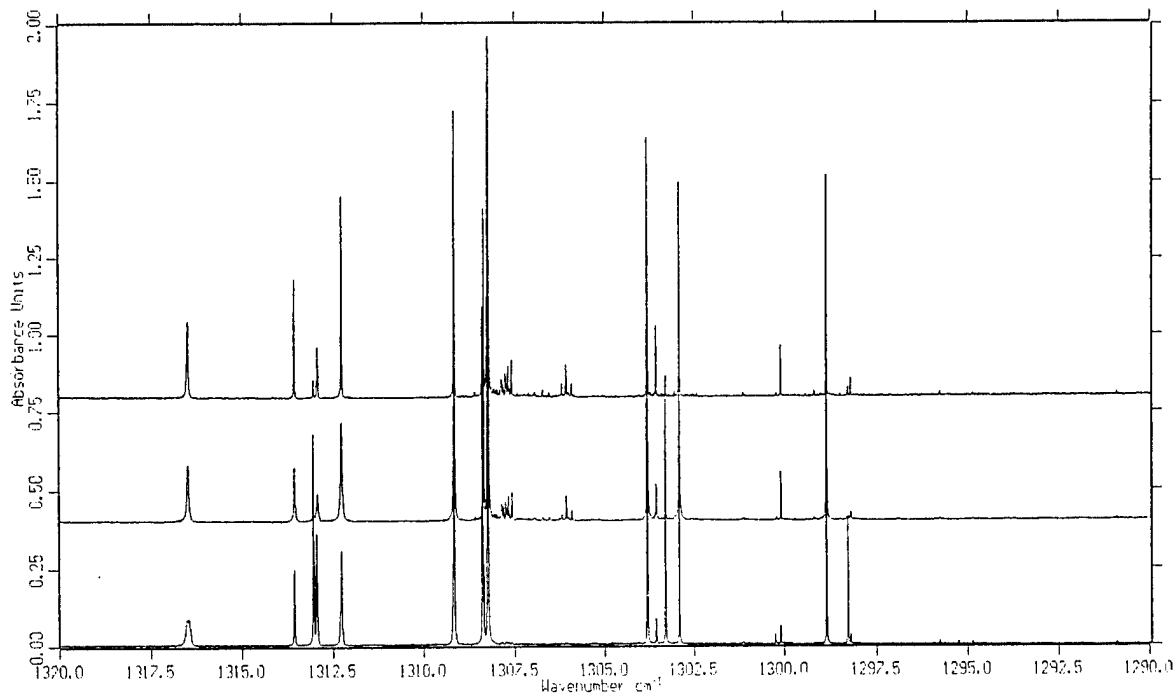


st28022.20      annealed    T=2.4K  
 st28022.19      annealing    T=4.8K  
 st28022.18      as deposited T=2.4K

resolution = 0.005 cm<sup>-1</sup>

ST28022.18

ppm  
200 PPM CH<sub>4</sub>/pH<sub>2</sub> d≈0.2mm

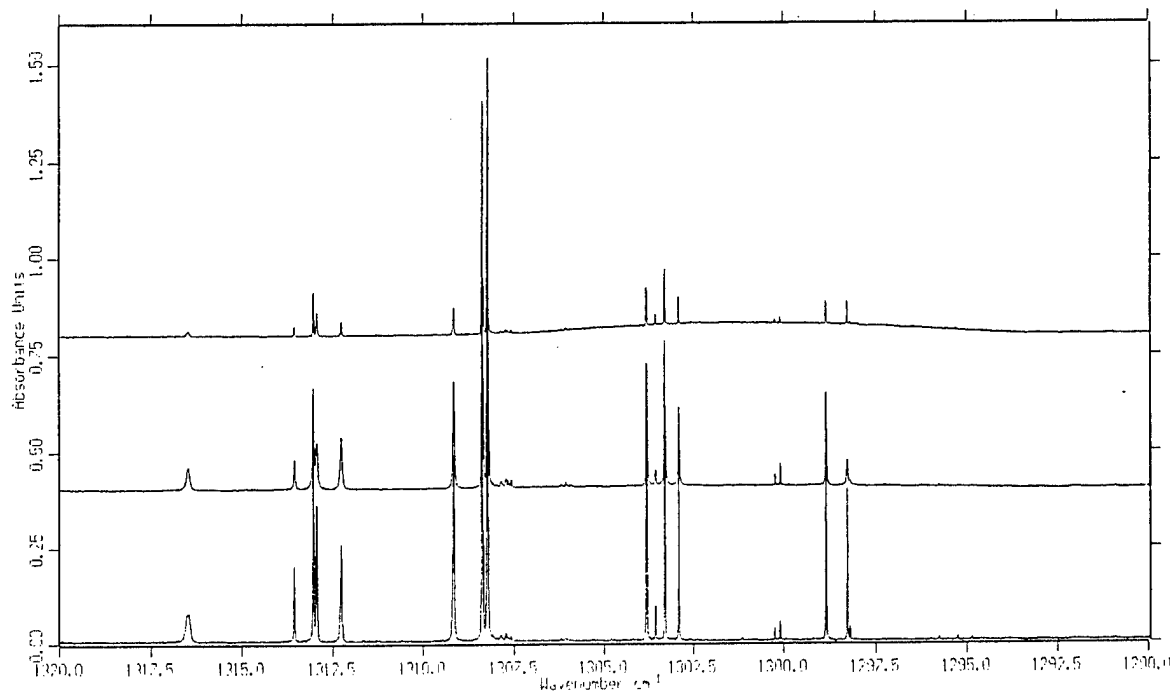


st28026.21      annealed      T=2.4K  
st28026.20      annealing      T=4.8K  
st28026.19      as deposited      T=2.4K

resolution = 0.005 cm<sup>-1</sup>

ST28026.19

ppm  
550 PPM CH<sub>4</sub>/pH<sub>2</sub> d≈0.05mm

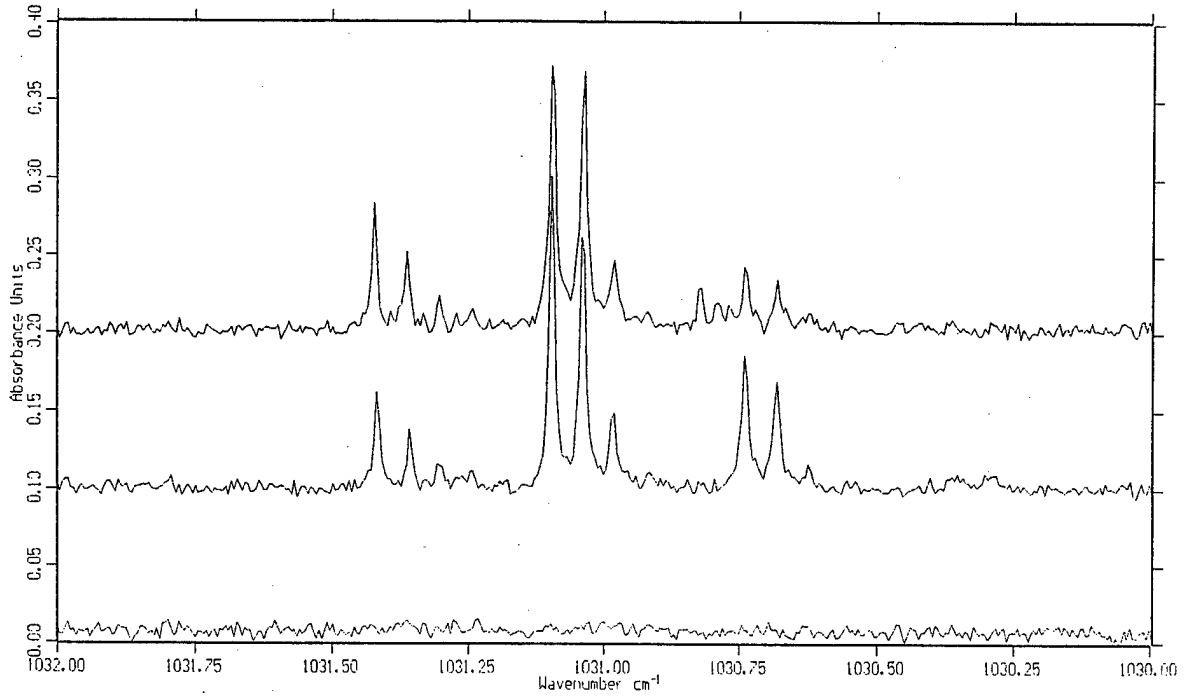


st28030.14      annealed      T=2.4K  
st28030.13      annealing      T=4.8K  
st28030.12      as deposited      T=2.4K

resolution = 0.005 cm<sup>-1</sup>

ST28030.1

# $(\text{CH}_3\text{F})_2/\text{pH}_2$

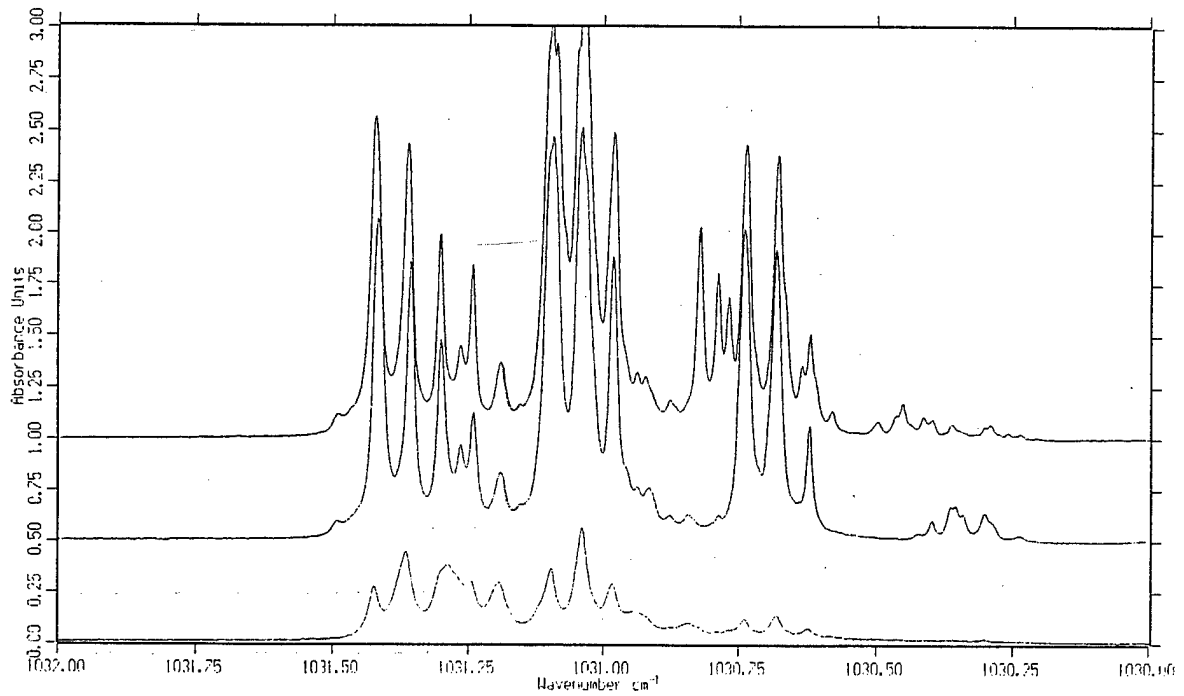


st28039.11      annealed    T=2.4K  
st28039.9        annealing    T=4.8K  
st28039.5        as deposited T=2.4K

10 PPM  $\text{CH}_3\text{F}/\text{pH}_2$       resolution =  $0.005 \text{ cm}^{-1}$

ST28039.5

# $(\text{CH}_3\text{F})_2/\text{pH}_2$

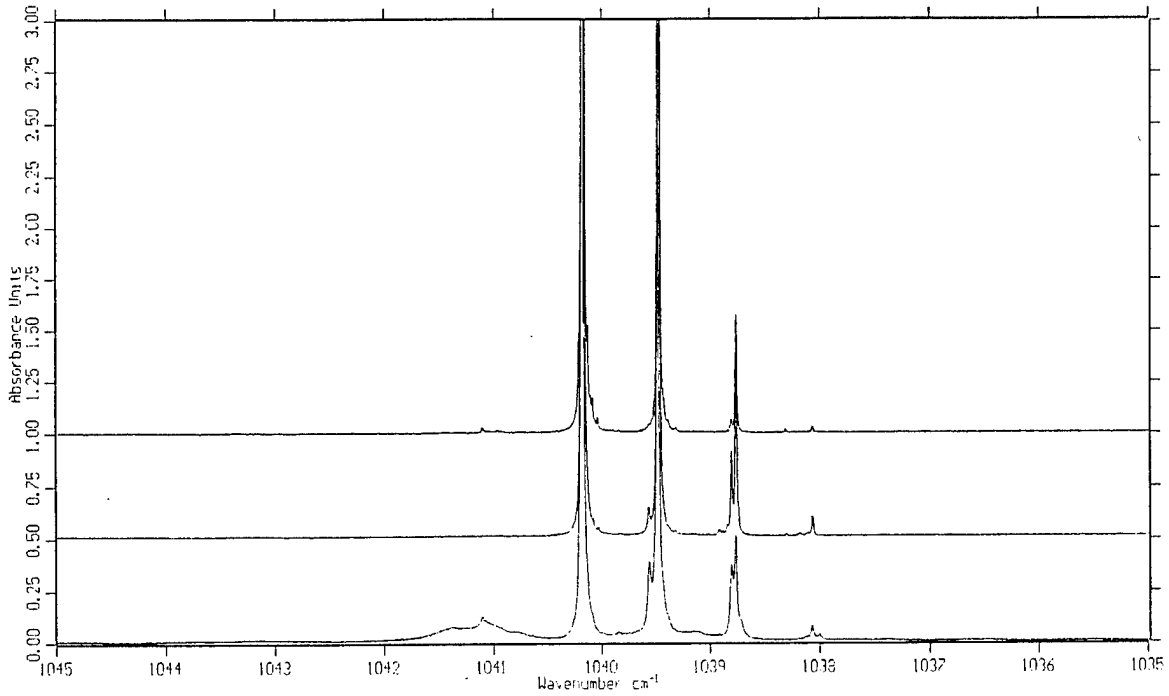


st28048.11      annealed    T=2.4K  
st28048.7        annealing    T=4.8K  
st28048.3        as deposited T=2.4K

91 PPM  $\text{CH}_3\text{F}/\text{pH}_2$       resolution =  $0.005 \text{ cm}^{-1}$

ST28048.3

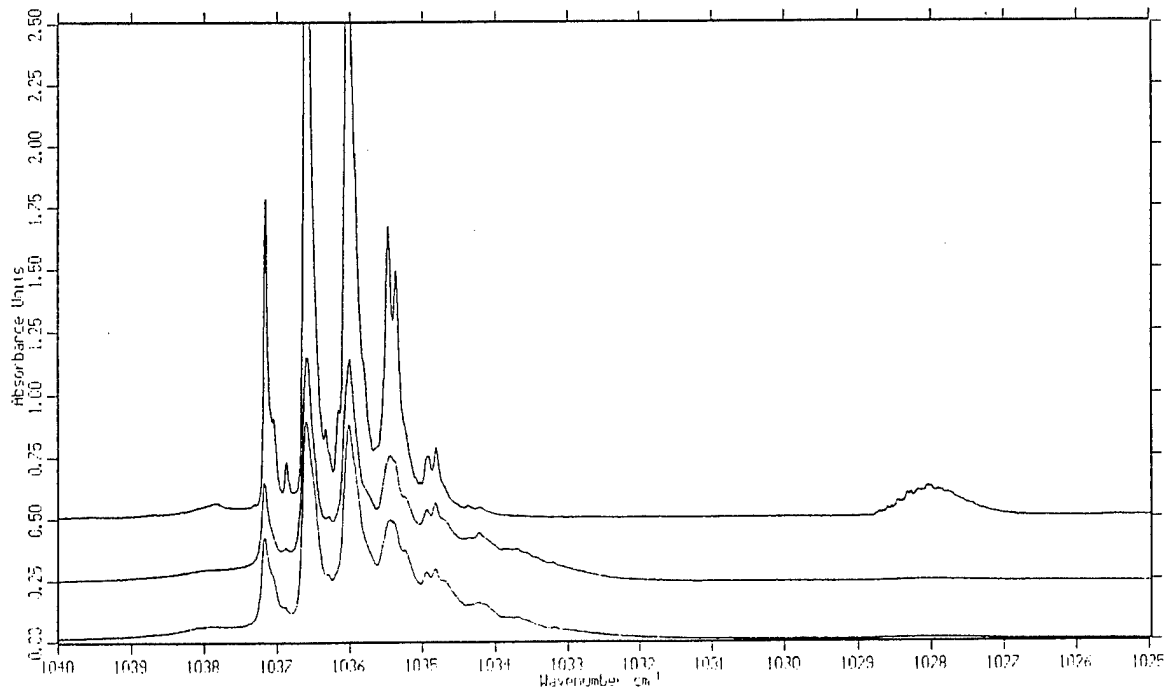
<sup>ppm</sup>  
6 PPM CH<sub>3</sub>F/pH<sub>2</sub> d≈3mm



st28052.10 annealed T=2.4K  
st28052.6 annealing T=4.8K  
st28052.2 as deposited T=2.4K resolution = 0.005 cm<sup>-1</sup>

ST28052.2

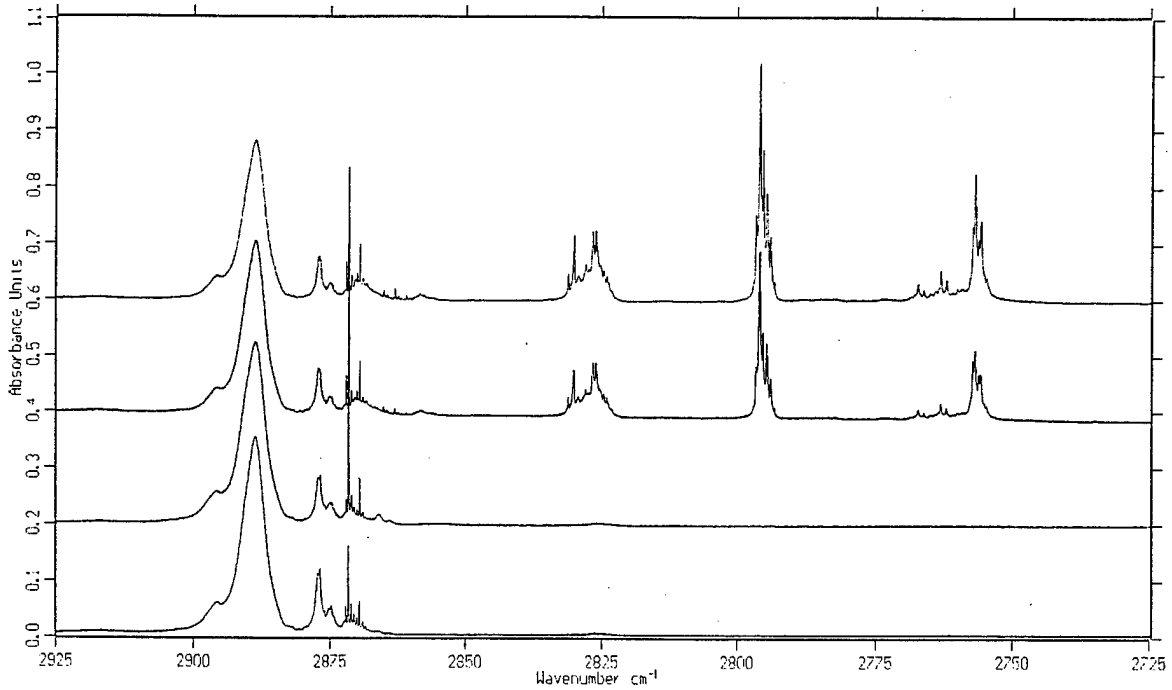
<sup>ppm</sup>  
33 PPM CH<sub>3</sub>F/oD<sub>2</sub> d≈2mm



st28073.11 flash annealed to 10K T=2.4K  
st28073.7 annealing T=4.8K  
st28073.3 as deposited T=2.4K resolution = 0.005 cm<sup>-1</sup>

ST28073.3

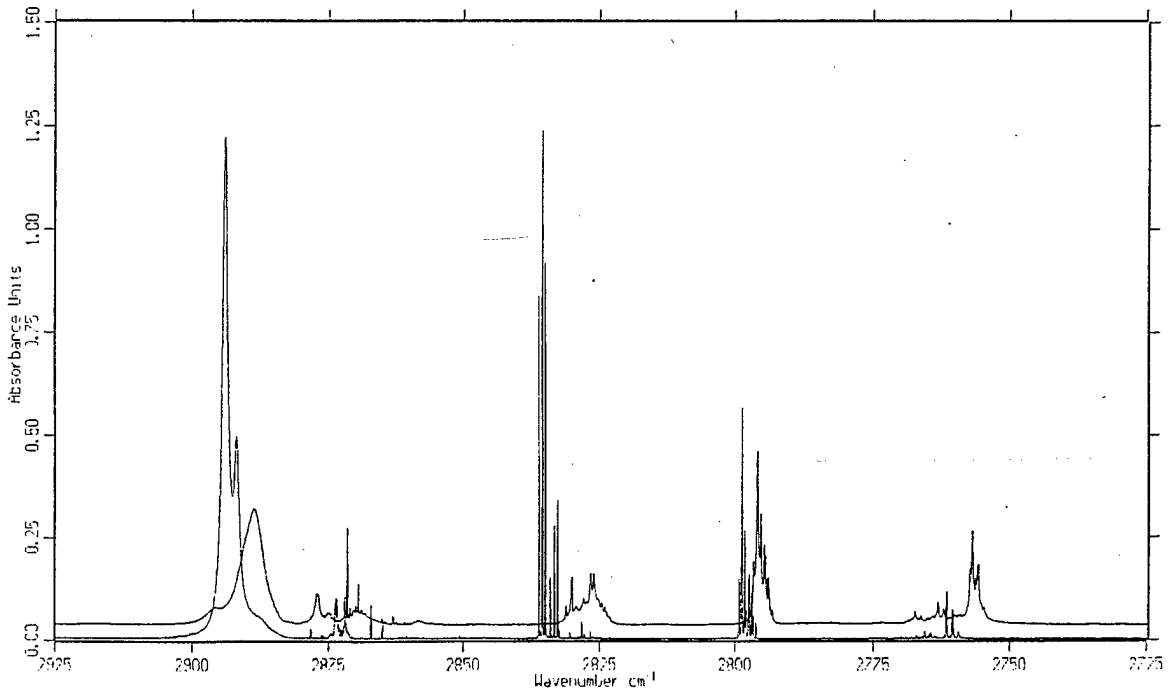
ppm  
 93 PPM HCl/oD<sub>2</sub> d≈2mm



st28079.7 2nd flash annealing T=2.4K st28079.3 annealing T=4.8K  
 st28079.5 flash annealed to 10K T=2.4K st28079.1 as deposited T=2.4K resolution = 0.005 cm<sup>-1</sup>

st28079.1

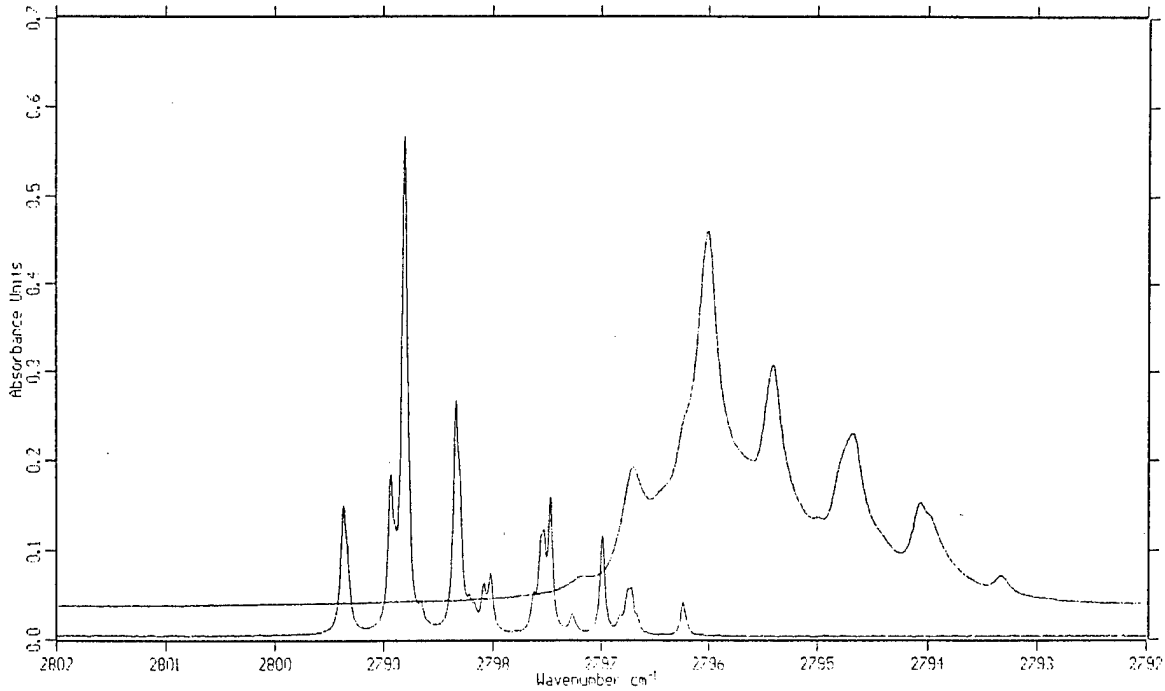
## HCl/pH<sub>2</sub> vs. HCl/oD<sub>2</sub>



st28079.7 annealed T=2.4K 93 PPM HCl/oD<sub>2</sub> (≈98%)  
 st27061.11 annealed T=2.4K 88 PPM HCl/pH<sub>2</sub> (99.99+%)

st27061.11

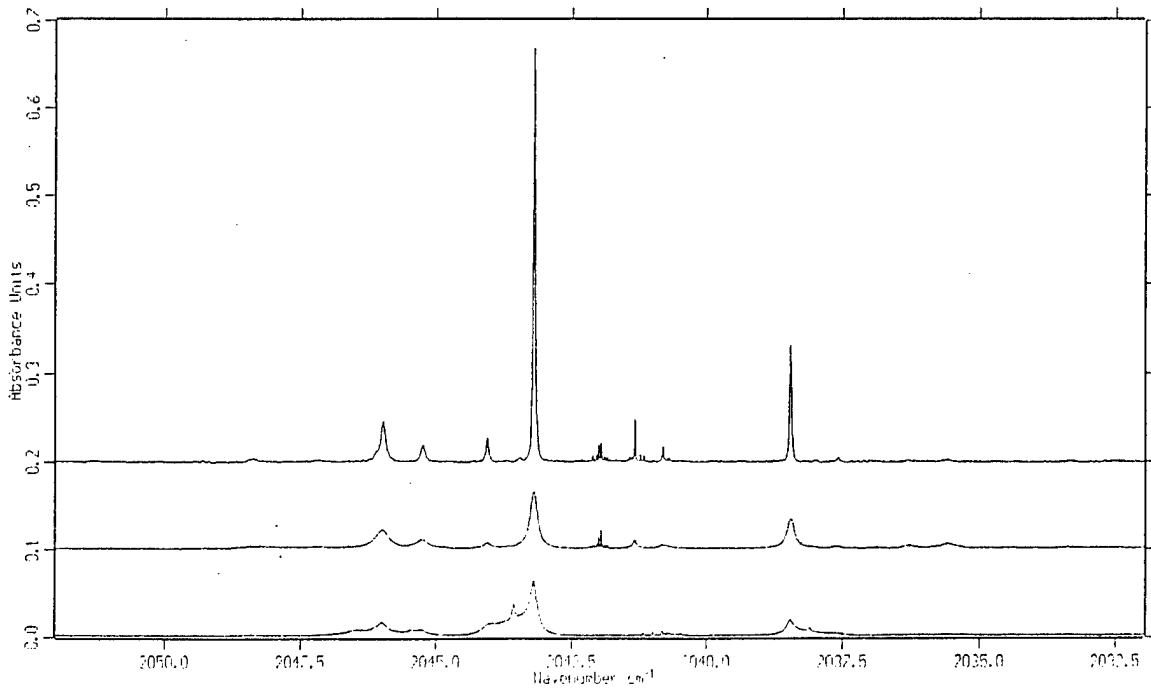
# $(\text{HCl})_3/\text{pH}_2$ & $(\text{HCl})_3/\text{oD}_2$



st28079.7 annealed T=2.4K 93 PPM HCl/oD<sub>2</sub> (≈98%)  
 st27061.11 annealed T=2.4K 88 PPM HCl/pH<sub>2</sub> (99.99+%)

ST27061.11

# $^{13}\text{C}^{18}\text{O}/\text{pH}_2$ $d \approx 3\text{mm}$



st28082.6 annealed T=2.4K  
 st28082.4 annealing T=4.8K  
 st28082.2 as deposited T=2.4K

11 PPM  $^{13}\text{C}/\text{pH}_2$  resolution = 0.005  $\text{cm}^{-1}$

ST28082.2