Precision spectroscopy of hydrogen

- Laboratory spectroscopy
- Spectroscopic Observations of quasars
- Detecting a variation of the proton-electron mass ratio

Wim Ubachs

TULIP Summer School IV 2009
Noordwijk, April 15-18

Empirical search for a change in μ

- Spectroscopy
- Compare H_2 spectra in different epochs:

Composition
of the universe:
80 % hydrogen H/H_2
20 % helium
<0.1% other elements

Lab
today

QSO
12 Gyr ago

90-112 nm

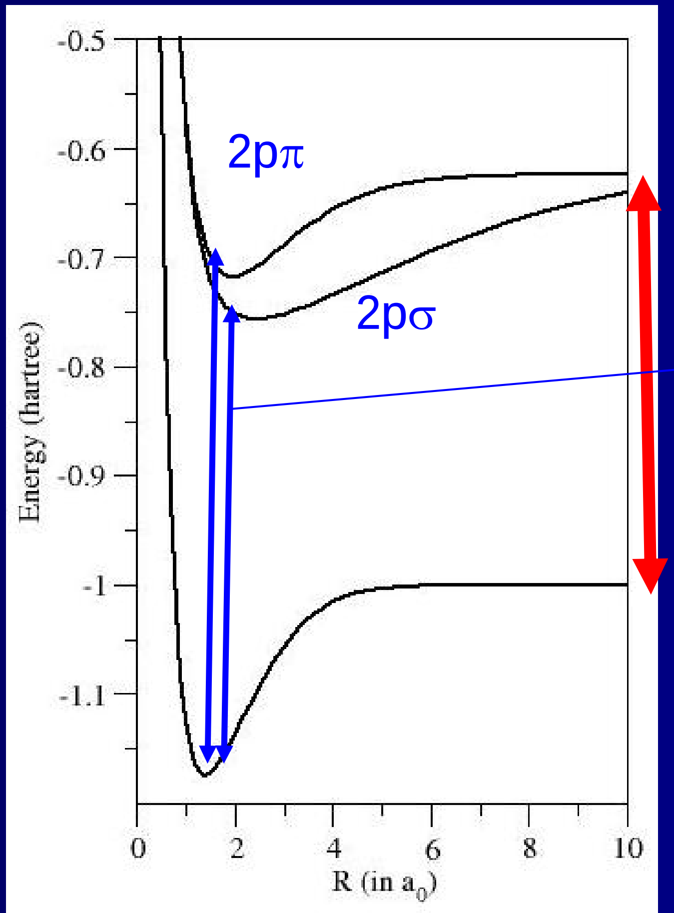
~275-350 nm

$$\frac{\lambda_i}{\lambda_i^0} \equiv 1 + z_i$$ Cosmological redshift


Edwin Hubble

Laboratory measurements: spectra of H_2

H_2



H (Lyman-α) ~ 121 nm

H_2, Lyman en Werner Lines
~90 - 110 nm
Extreme Ultraviolet Wavelengths

Note : Band structure

Partition function

Only a few states populated in H_2

Vibration: v=0

$$P(\mathrm{v}) = \frac{e^{-E(\mathrm{v})/kT}}{Z} = \frac{e^{-\omega_e(\mathrm{v}+1/2)/kT}}{Z}$$

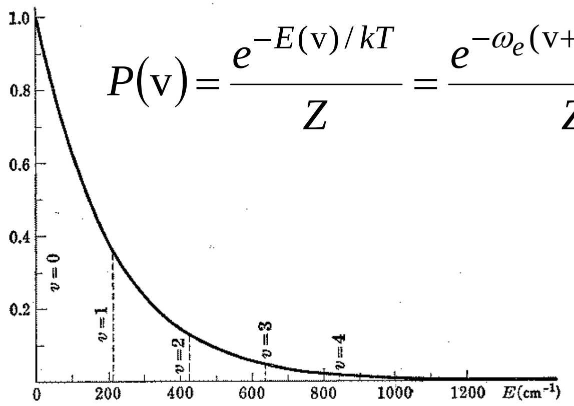


FIG. 58. **Boltzmann Factor and Thermal Distribution of the Vibrational Levels.** The curve gives the function $e^{-E/kT}$ for $T = 300°$ K. with E in cm^{-1}. The broken-line ordinates correspond to the vibrational levels of the I_2 molecule.

TABLE 14. RATIO OF THE NUMBER OF MOLECULES IN THE FIRST TO THAT IN THE ZEROTH VIBRATIONAL LEVEL FOR 300° K. AND 1000° K.

Gas	$\Delta G_{1/2}$ (cm^{-1})	$e^{-\Delta G_{1/2} hc/kT}$ For 300° K.	$e^{-\Delta G_{1/2} hc/kT}$ For 1000° K.
H_2	4160.2	2.16×10^{-9}	2.51×10^{-3}
HCl	2885.9	9.77×10^{-7}	1.57×10^{-2}
N_2	2330.7	1.40×10^{-5}	3.50×10^{-2}
CO	2143.2	3.43×10^{-5}	4.58×10^{-2}
O_2	1556.4	5.74×10^{-4}	1.07×10^{-1}
S_2	721.6	3.14×10^{-2}	3.54×10^{-1}
Cl_2	556.9	6.92×10^{-2}	4.49×10^{-1}
I_2	213.2	3.60×10^{-1}	7.36×10^{-1}

Rotation: J=0-5

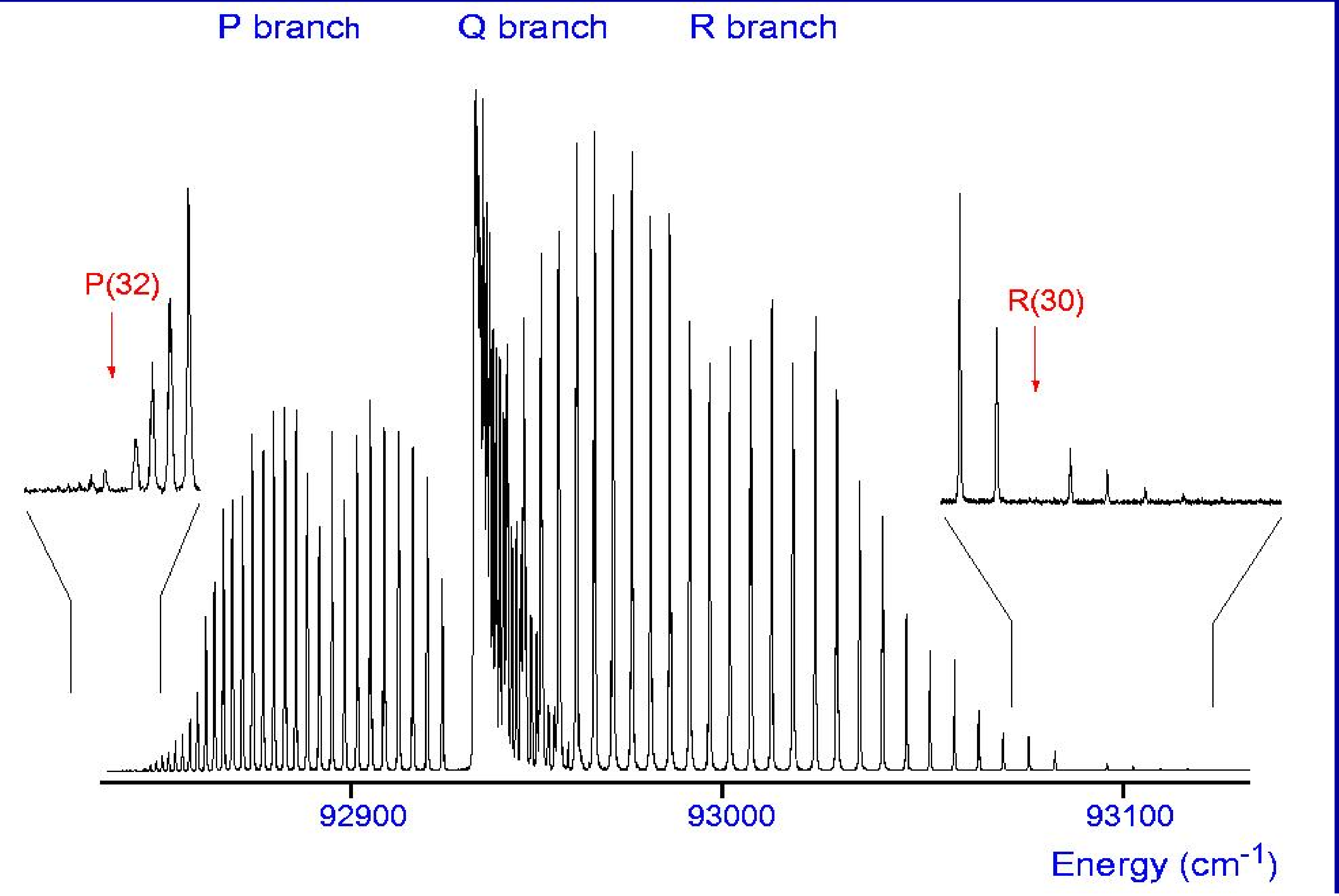
$$P(J) = \frac{(2J+1)e^{-BJ(J+1)}}{Z}$$

Ortho-Para 3:1   J=1 most populated

“Complexity” of the H_2 electronic spectrum

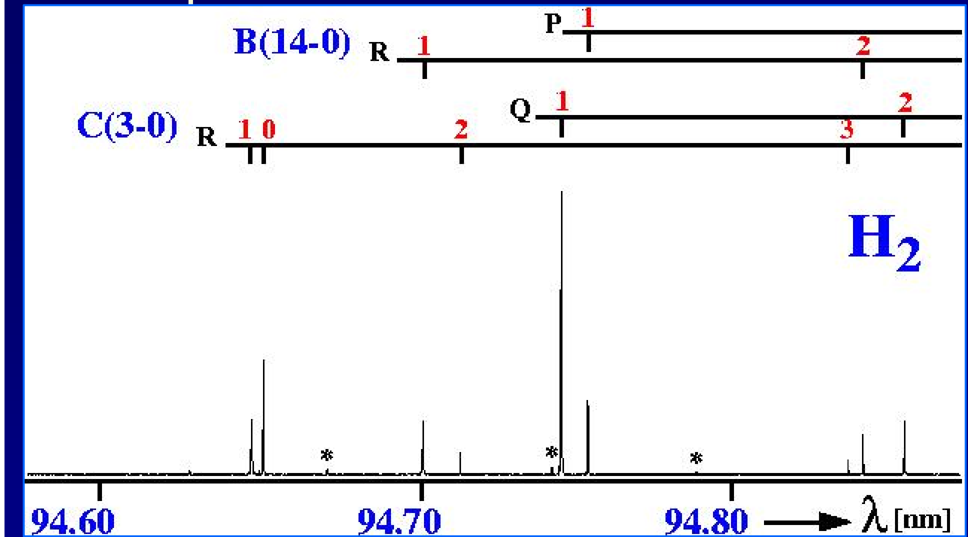
“Molecules have a band spectrum”

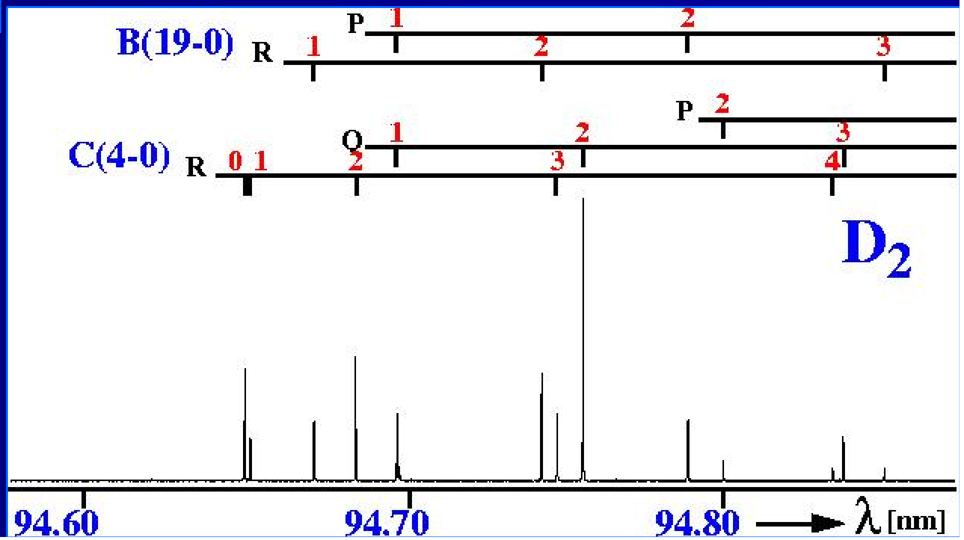
CO (VUV)



"Complexity" of the H_2 electronic spectrum

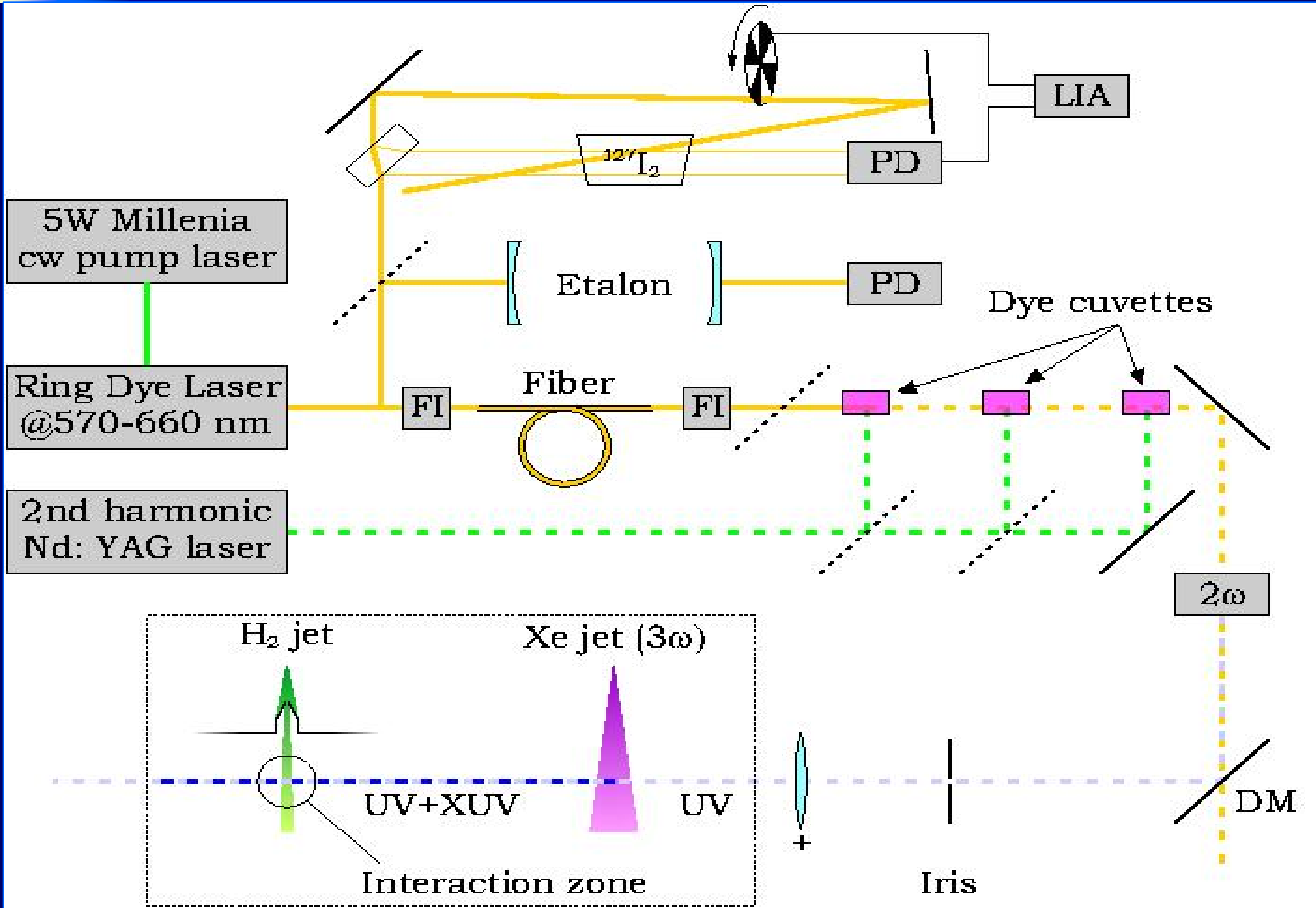
"H_2 does not have a band spectrum"





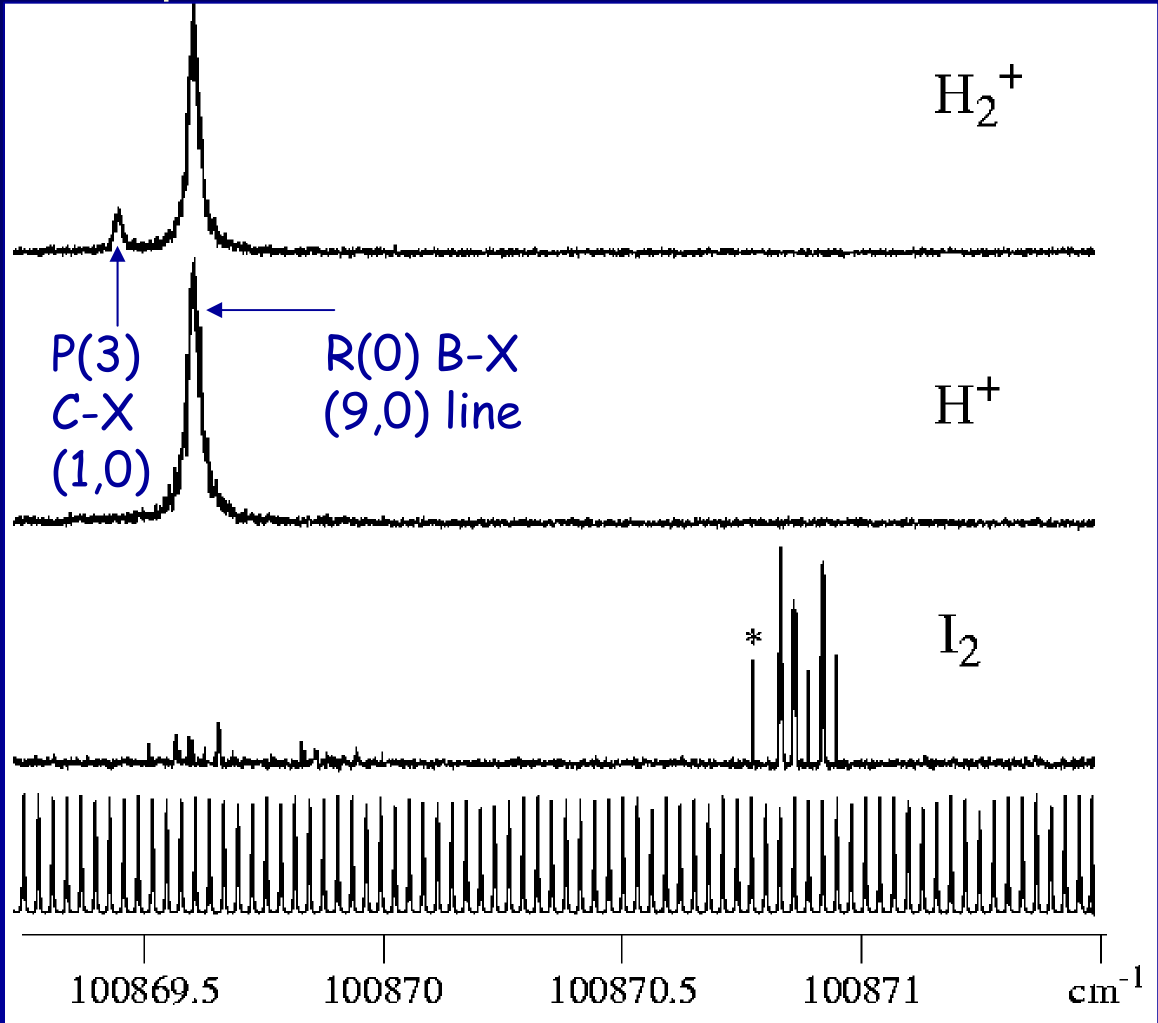
XUV-laser spectroscopy

Laser Centre
vrije Universiteit amsterdam



XUV-spectroscopy of H_2

The $B^1\Sigma_u^+$ - $X^1\Sigma_g^+$ Lyman and $C^1\Pi_u$ – $X^1\Sigma_g^+$ Werner bands



Evaluation of uncertainties:
Error budget

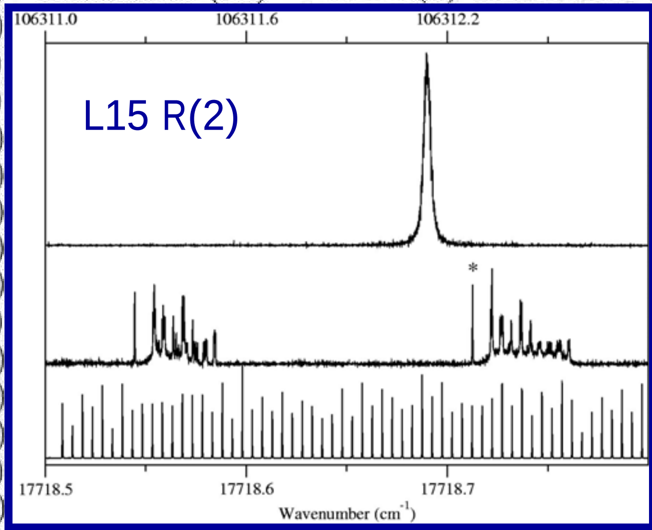
Residual Doppler	40 MHz
AC Stark	30 MHz
Freq chirp (PDA)	100 MHz
I_2 calibration	10 MHz
Statistical	30 MHz

Total (best lines): 0.004 cm^{-1}
0.000004 nm

$\Delta\lambda/\lambda$=4-6 x 10^{-8}

TABLE I: Comprehensive list of measured transition wavelengths of the Lyman (L) and Werner (W) lines using the ultr narrowband XUV laser source in Amsterdam. Values in nm.

Line	λ_0	Line	λ_0	Line	λ_0	Line	λ_0
L0 P(1)	111.006 251 (6)	L8 P(3)	100.838 615 (6)	L13 R(3)	95.894 665 (6)	W1 P(3)	99.138 046 (8)
L0 R(0)	110.812 733 (7)	L8 R(0)	100.182 387 (5)	L13 R(4)	96.215 297 (6)	W1 Q(1)	98.679 800 (5)
L0 R(1)	110.863 326 (7)	L8 R(1)	100.245 210 (5)	L14 P(1)	94.751 403 (10)	W1 Q(2)	98.797 445 (6)
L1 P(1)	109.405 198 (6)	L8 R(2)	100.398 545 (5)	L14 R(0)	94.616 931 (10)	W1 Q(3)	98.972 929 (8)
L1 P(2)	109.643 894 (6)	L8 R(3)	100.641 416 (6)	L14 R(1)	94.698 040 (10)	W1 R(0)	98.563 371 (5)
L1 P(3)	109.978 718 (7)	L9 P(1)	99.280 968 (5)	L14 R(2)	[illegible]	[illegible]	[illegible] 5)
L1 R(0)	109.219 523 (6)	L9 R(0)	99.137 891 (5)	L15 P(1)	[illegible]	[illegible]	[illegible] 6)
L1 R(1)	109.273 243 (6)	L9 R(1)	99.201 637 (5)	L15 P(3)	[illegible]	[illegible]	[illegible] 9)
L1 R(2)	109.424 460 (6)	L9 R(2)	99.355 061 (9)	L15 R(0)	[illegible]	[illegible]	[illegible] 6)
L1 R(3)	109.672 534 (6)	L9 R(3)	99.597 278 (20)	L15 R(1)	[illegible]	[illegible]	[illegible] 7)
L2 P(1)	107.892 547 (5)	L10 P(1)	98.283 533 (5)	L15 R(2)	[illegible]	[illegible]	[illegible] 7)
L2 R(0)	107.713 874 (5)	L10 P(2)	98.486 398 (5)	L15 R(3)	[illegible]	[illegible]	[illegible] 5)
L2 R(1)	107.769 894 (5)	L10 P(3)	98.776 882 (6)	L15 R(4)	[illegible]	[illegible]	[illegible] 5)
L2 R(2)	107.922 542 (6)	L10 R(0)	98.143 871 (5)	L16 P(1)	[illegible]	[illegible]	[illegible] 7)
L2 R(3)	108.171 124 (7)	L10 R(1)	98.207 427 (5)	L16 R(0)	[illegible]	[illegible]	[illegible] 7)
L2 R(4)	108.514 554 (6)	L10 R(2)	98.359 107 (5)	L16 R(1)	[illegible]	[illegible]	[illegible] 8)
L3 P(1)	106.460 539 (5)	L10 R(3)	98.596 279 (6)	L16 R(2)	[illegible]	[illegible]	[illegible] 5)
L3 P(2)	106.690 068 (5)	L11 P(1)	97.334 458 (5)	L17 P(1)	[illegible]	[illegible]	[illegible] 5)
L3 R(0)	106.288 214 (5)	L11 P(2)	97.534 576 (5)	L17 R(0)	[illegible]	[illegible]	[illegible] 6)
L3 R(1)	106.346 014 (5)	L11 P(3)	97.821 804 (6)	L17 R(1)	92.464 326 (9)	W2 R(3)	96.678 035 (7)
L3 R(2)	106.499 481 (5)	L11 R(0)	97.198 623 (5)	L18 P(1)	91.841 331 (9)	W3 P(2)	94.961 045 (5)
L3 R(3)	106.747 855 (5)	L11 R(1)	97.263 275 (5)	L18 R(0)	[illegible]	[illegible]	95.167 186 (5)
L4 P(1)	105.103 253 (4)	L11 R(2)	97.415 791 (5)	L18 R(1)	[illegible]	[illegible]	[illegible]742 188 (5)
L4 R(0)	104.936 744 (4)	L11 R(3)	97.655 283 (6)	L18 R(2)	[illegible]	[illegible]	[illegible]861 583 (5)
L4 R(1)	104.995 976 (4)	L11 R(4)	97.980 512 (7)	L19 P(1)	[illegible]	[illegible]	[illegible]039 773 (5)
L4 R(2)	105.149 857 (5)	L11 R(5)	98.389 896 (7)	L19 P(2)	[illegible]	[illegible]	94.642 557 (4)
L4 R(3)	105.397 610 (4)	L12 P(1)	96.431 064 (5)	L19 P(3)	91.638 293 (34)	W3 R(1)	94.638 475 (4)
L5 P(1)	103.815 713 (4)	L12 P(2)	96.627 550 (5)	L19 R(0)	91.082 073 (17)	W3 R(2)	94.711 169 (4)
L5 R(0)	103.654 581 (4)	L12 P(3)	96.908 984 (6)	L19 R(1)	91.147 950 (17)	W3 R(3)	94.841 967 (5)
L5 R(1)	103.714 992 (4)	L12 R(0)	96.297 800 (5)	L19 R(2)	91.295 107 (17)	W3 R(4)	95.031 536 (5)
L5 R(2)	103.869 027 (4)	L12 R(1)	96.360 800 (5)	L19 R(3)	91.521 225 (17)	W4 P(2)	93.260 468 (10)
L5 R(3)	104.115 892 (4)	L12 R(2)	96.504 574 (5)	W0 P(2)	101.216 942 (6)	W4 P(3)	93.479 006 (10)
L6 P(1)	102.593 517 (8)	L12 R(3)	96.767 695 (6)	W0 P(3)	101.450 423 (6)	W4 Q(1)	93.057 708 (10)
L6 R(0)	102.437 395 (8)	L12 R(4)	97.083 820 (8)	W0 Q(1)	100.977 088 (5)	W4 Q(2)	93.178 086 (10)
L6 R(1)	102.498 790 (8)	L12 R(5)	97.488 649 (9)	W0 Q(2)	101.093 845 (6)	W4 Q(3)	93.357 794 (10)



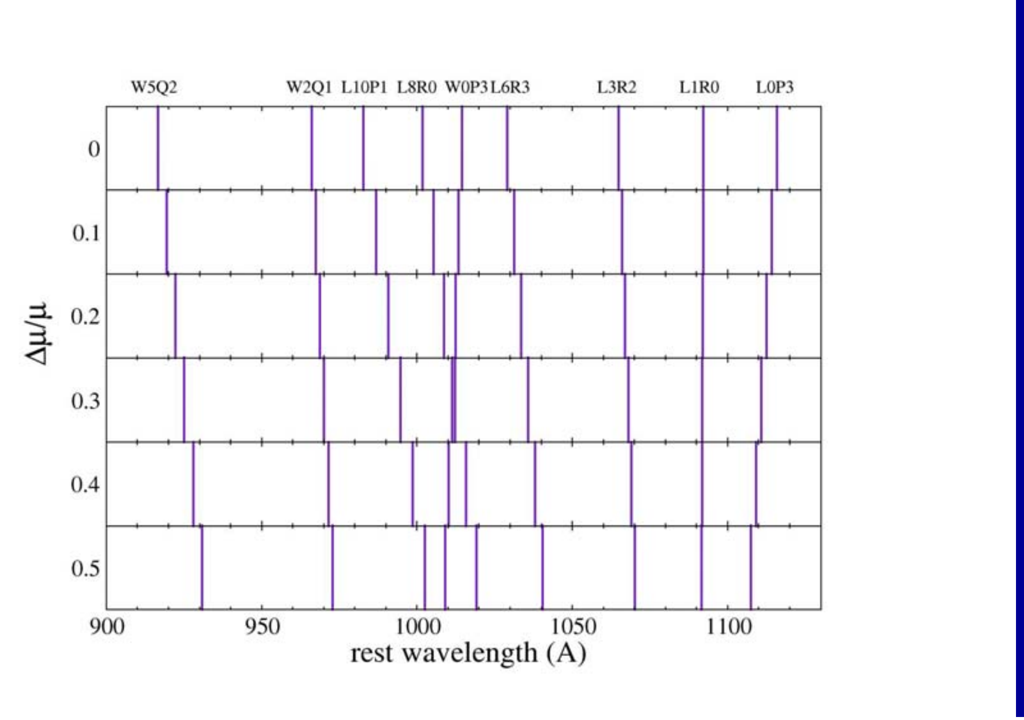
162 lines measured at ~ 5 x 10^{-8}

$\Delta\mu/\mu$ and spectrum H_2

QSO: (2-10) x 10^{-7}

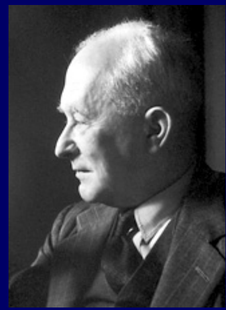
Accurately calculated

$$\frac{\lambda_i}{\lambda_i^0} \equiv 1 + z_i = (1 + z_{abs})\left(1 + \frac{\Delta\mu}{\mu} K_i\right)$$

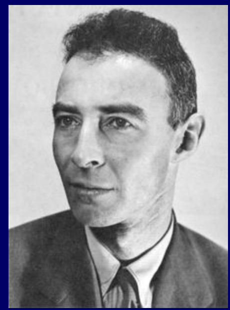


Explanation on K-coefficients

How do spectral lines depend on μ ?



Max Born



Robert Oppenheimer

First order

$$E_{molecule} = E_{electr} + E_{vibr} + E_{rot}$$

$$E_{elec} \propto Const$$

$$E_{vib} \propto \sqrt{\frac{m_e}{M_p}} \propto \frac{1}{\sqrt{\mu}}$$ (Harmonic oscillator)

$$E_{rot} \propto \left(\frac{m_e}{M_p}\right) \propto \frac{1}{\mu}$$ (Rigid rotor)

$$\mu = \frac{m_p}{m_e}$$

Dunham representation
includes rovibrational couplings

$$E_{vJ} = \sum_{kl} Y_{kl} (v + \tfrac{1}{2})^k J^l (J+1)^l$$

- Energies fit to the accurate laser measurements
- These parameters have a *known* mass-dependence

$$Y_{kl} \propto \mu^{-\frac{k}{2}-l}$$

- Evaluate sensitivity to mass

$$K_i = \frac{\mu}{\lambda_i}\frac{d\lambda_i}{d\mu} = \frac{-\mu}{E_{e,i} - E_{g,i}} \frac{d(E_{e,i} - E_{g,i})}{d\mu}$$

- Can be expressed in Dunham coefficients

$$K_i = \frac{1}{E_{e,i} - E_{g,i}} \left(\sum_{kl} (\tfrac{-k}{2} - l) Y_{kl,g} (v + \tfrac{1}{2})^k J^l (J+1)^l - \sum_{kl} \ldots Y_{kl,e} \ldots \right)$$

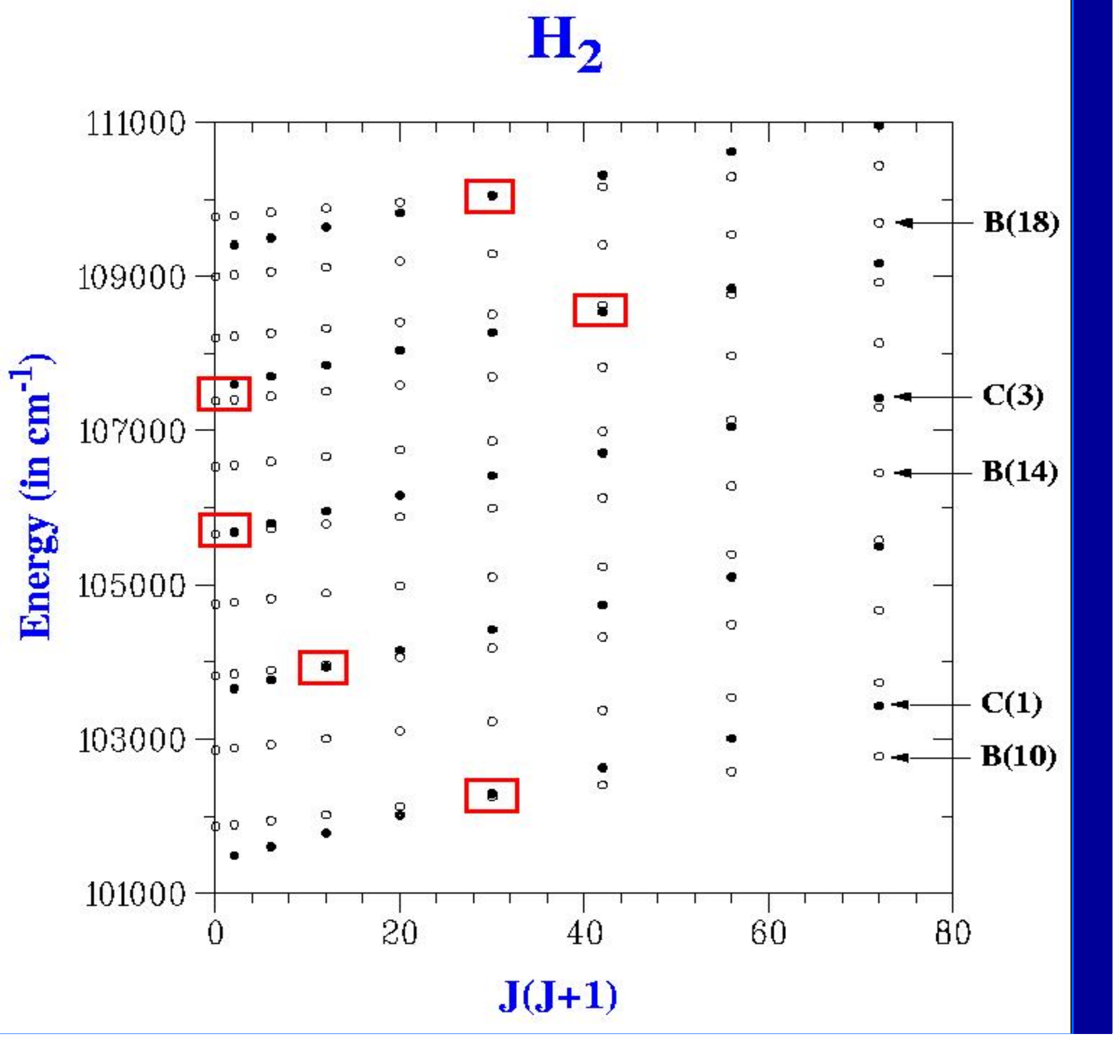
Correction: non-adiabatic interactions in H_2

and adiabatic effects (mass dependent electronic energies)

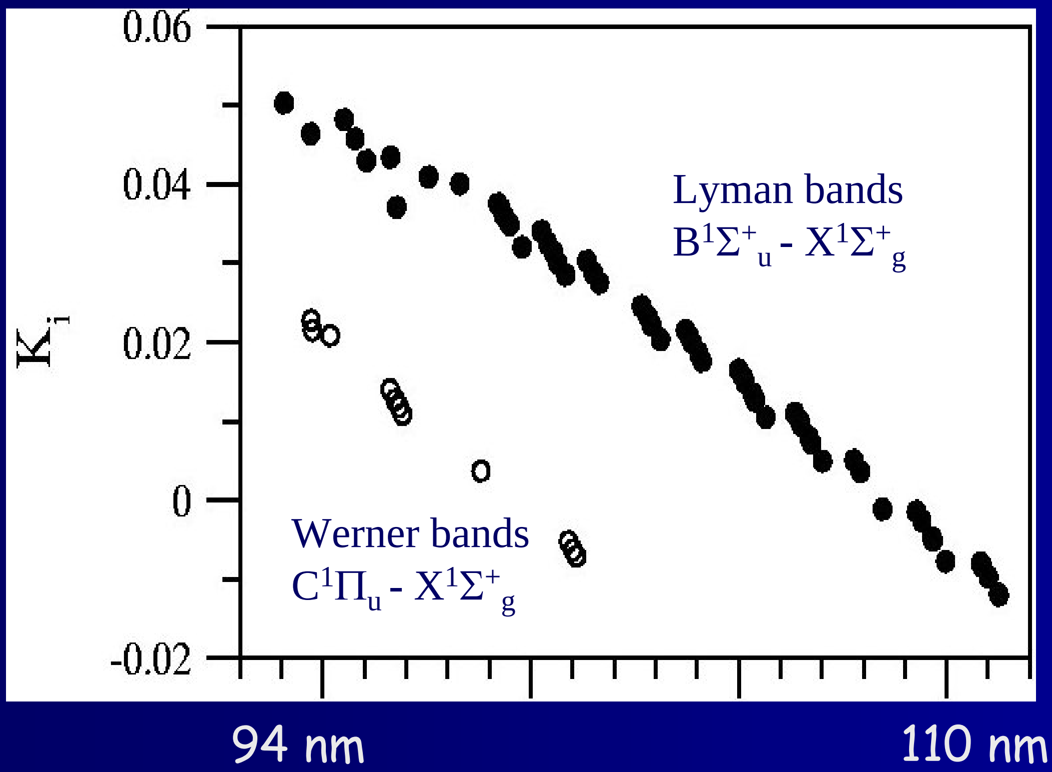
Mixing of wave functions
of low **v** and high **v**
In **B** and **C** states

Semi-empirical
treatment

$$\begin{pmatrix} E_{C4}(J) & H_{CB17}\sqrt{J(J+1)} \\ H_{CB17}\sqrt{J(J+1)} & E_{B17}(J) \end{pmatrix}$$



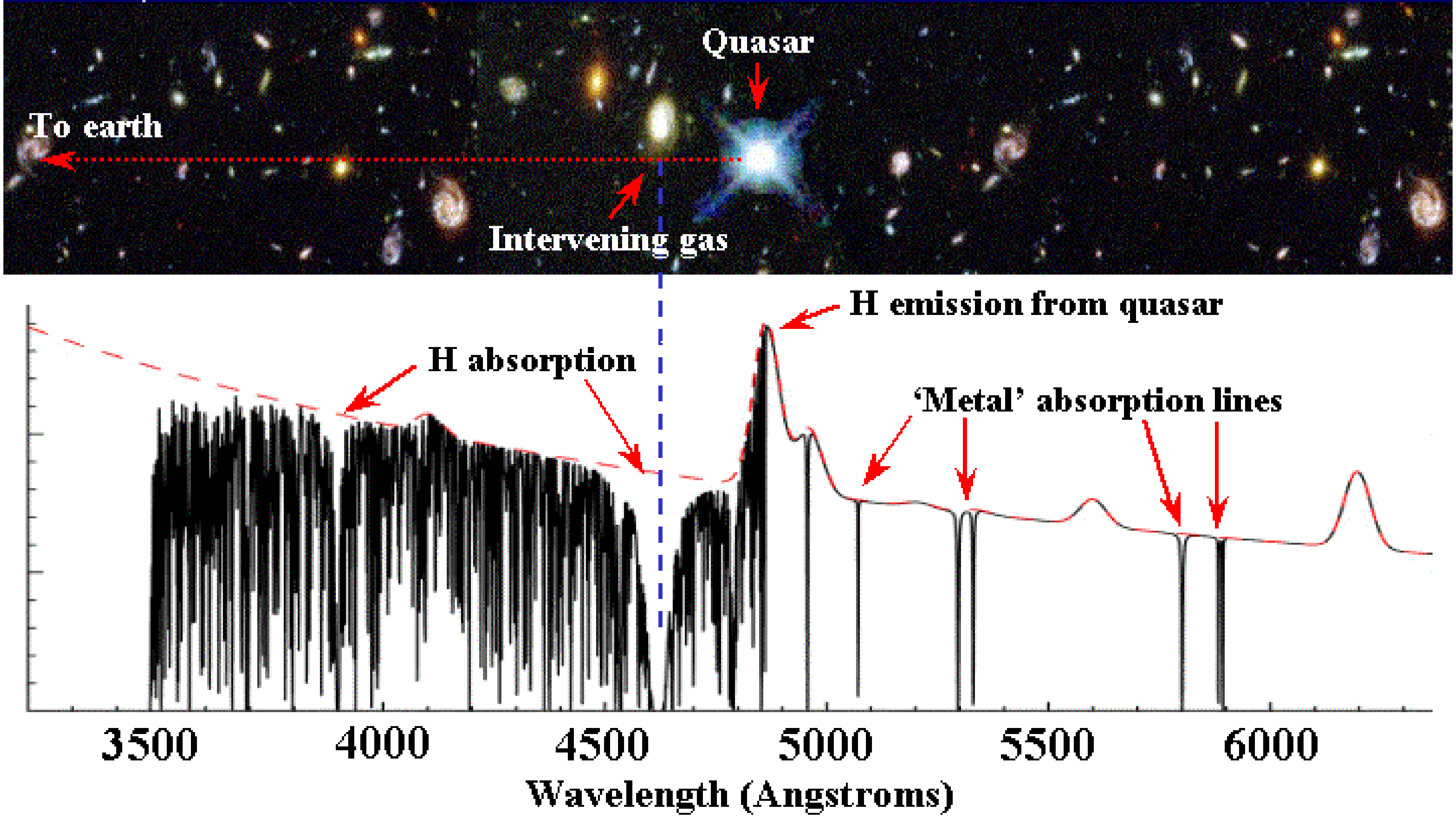
K_i different for H_2 lines



for 76 data in Q 0405 and Q 0347

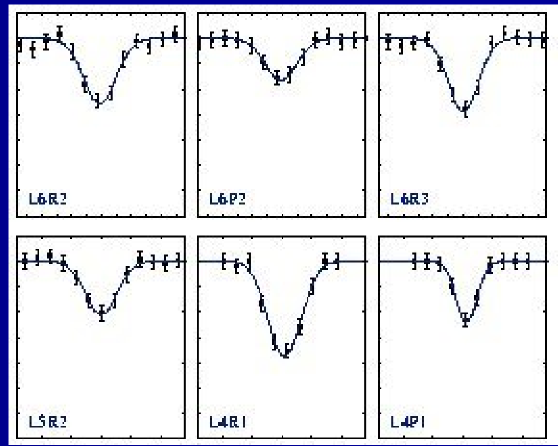
$$K_i = \frac{d \ln \lambda_i}{d \ln \mu}$$

Empirical search for a change in μ: quasars



Quasars or QSO's

- >2300 HI absorption systems
- ~600 DLA's
- 14 H_2 absorption systems
- 6 useful
- 4 high-quality spectra
  - Q0347: 39 lines at z_{abs}=3.02
  - Q0405: 37 lines at z_{abs}=2.59



Data from:
Ivanchik, Petitjean et al, A&A 440, 45 (2005)
Uncertainty: 2 x 10^{-7} – 1 x 10^{-6}

$$T = T_0\left[1 - \frac{1}{(1+z)^{3/2}}\right]$$

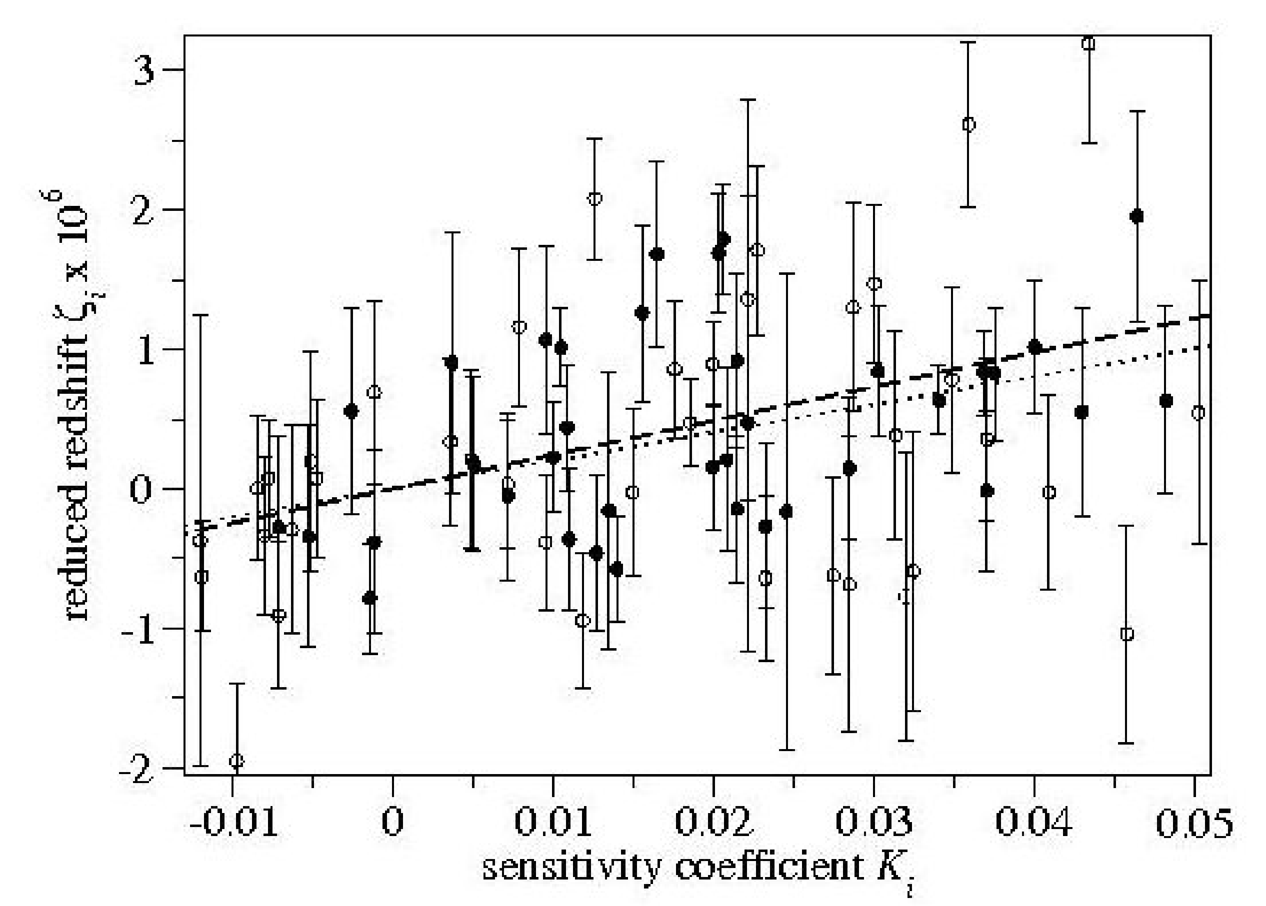
T_0=13.7 Gyrs

T=11.7-12.0 Gyrs

Δμ/μ determination

"reduced redshift"

$$\zeta_i = \frac{z_i - \bar{z}_Q}{1 + \bar{z}_Q} = \frac{\Delta\mu}{\mu} K_i$$



Data Q0405 and Q0347

$$\frac{\Delta\mu}{\mu} = (2.5 \pm 0.6) \times 10^{-5}$$

Indication: μ has decreased by 0.002% in past 12 billion years

Improvement of H_2 laboratory data

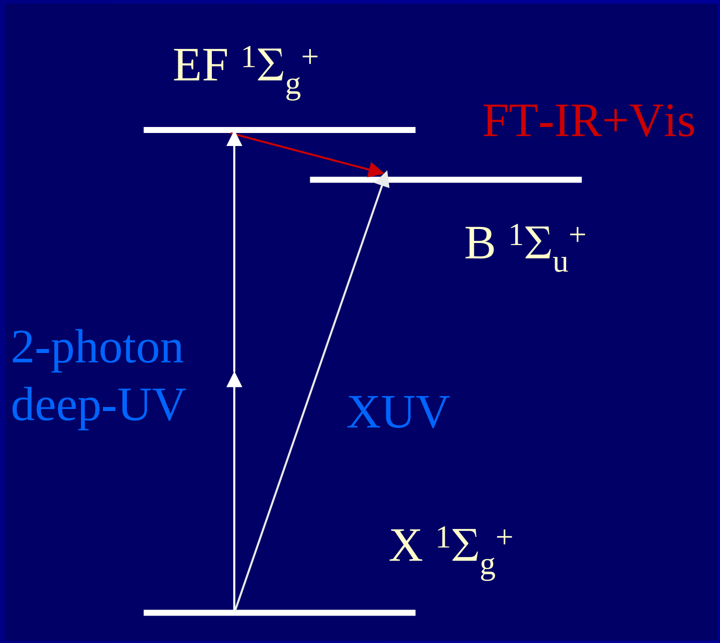
XUV experiments

Total (best lines): 0.005 cm^{-1}

0.000005 nm

$\Delta\lambda/\lambda = 5 \times 10^{-8}$

Novel combination scheme
Two different experiments
- 2 photon UV excitation
- FTIR



Improvement accuracy on Lyman bands

→ $\Delta\lambda/\lambda \sim 1\text{-}5 \times 10^{-9}$

PHYSICAL REVIEW A 74, 062514 (2006)

Frequency metrology on the $EF\,^1\Sigma_g^+ \leftarrow X\,^1\Sigma_g^+(0,0)$ transition in H_2, HD, and D_2

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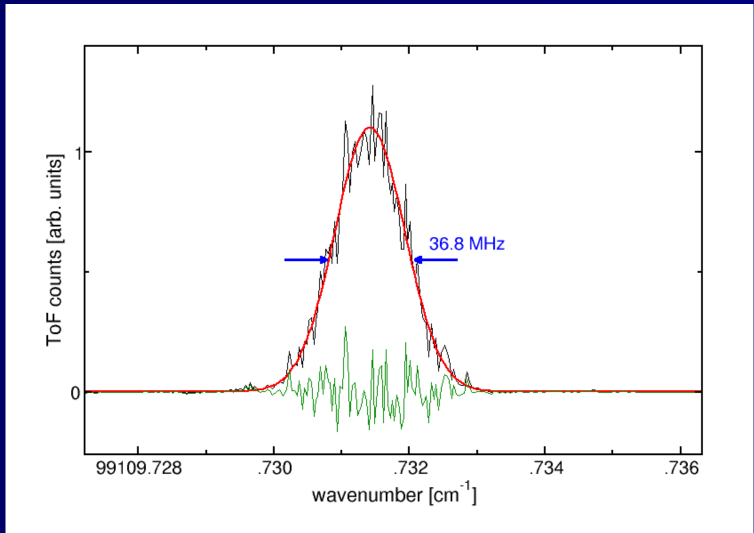
(Received 11 October 2006; published 28 December 2006)



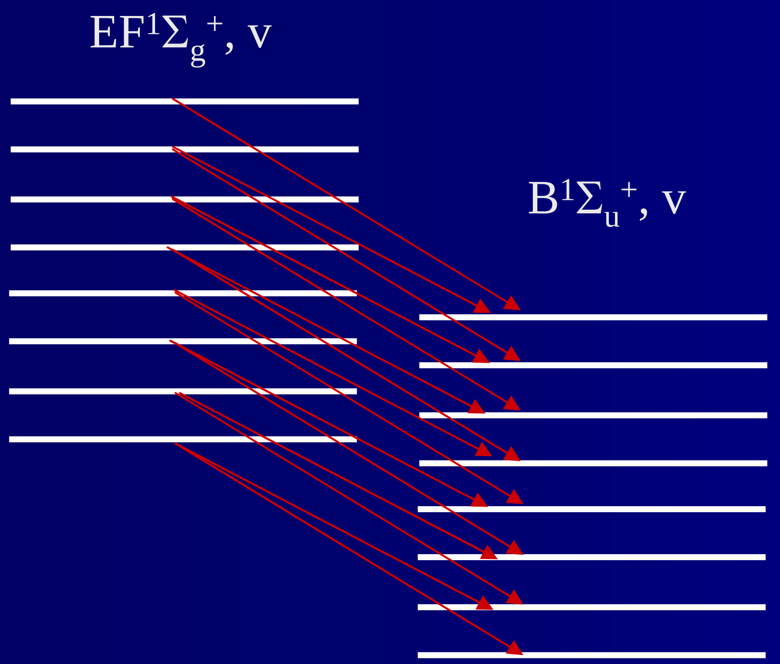
Species	Line	This work (cm^{-1})	Ref. [19] (cm^{-1})	Δ (cm^{-1})
H_2	Q(0)	99 164.786 91(11)	99 164.7871(8)	−0.0002
	Q(1)	99 109.731 39(18)	99 109.7316(8)	−0.0002
	Q(2)	99 000.183 01(11)		
HD	Q(0)	99 301.346 62(20)	99 301.3461(8)	+0.0005
	Q(1)	99 259.917 93(20)	99 259.9184(8)	−0.0005
D_2	Q(0)	99 461.449 08(11)	99 461.4490(8)	+0.0001
	Q(1)	99 433.716 38(11)	99 433.7166(8)	−0.0002
	Q(2)	99 378.393 52(11)	99 378.3937(8)	−0.0002

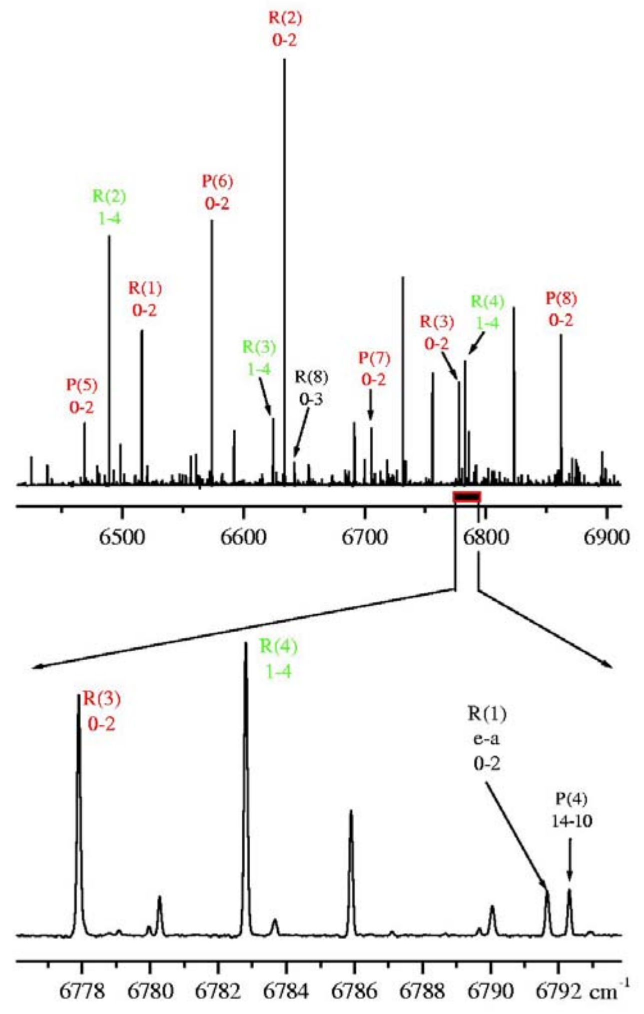
All the tricks of precision metrology;
-Doppler-free
-Counter-propagating in Sagnac Interf.
-Frequency comb calibration
-AC Stark assessment

$\Delta\lambda/\lambda \sim 1 \times 10^{-9}$

FT-IR data on $EF^1\Sigma_g^+$ - $B^1\Sigma_u^+$

with M. Vervloet & Denis Bailly (Orsay)





Statistical averaging

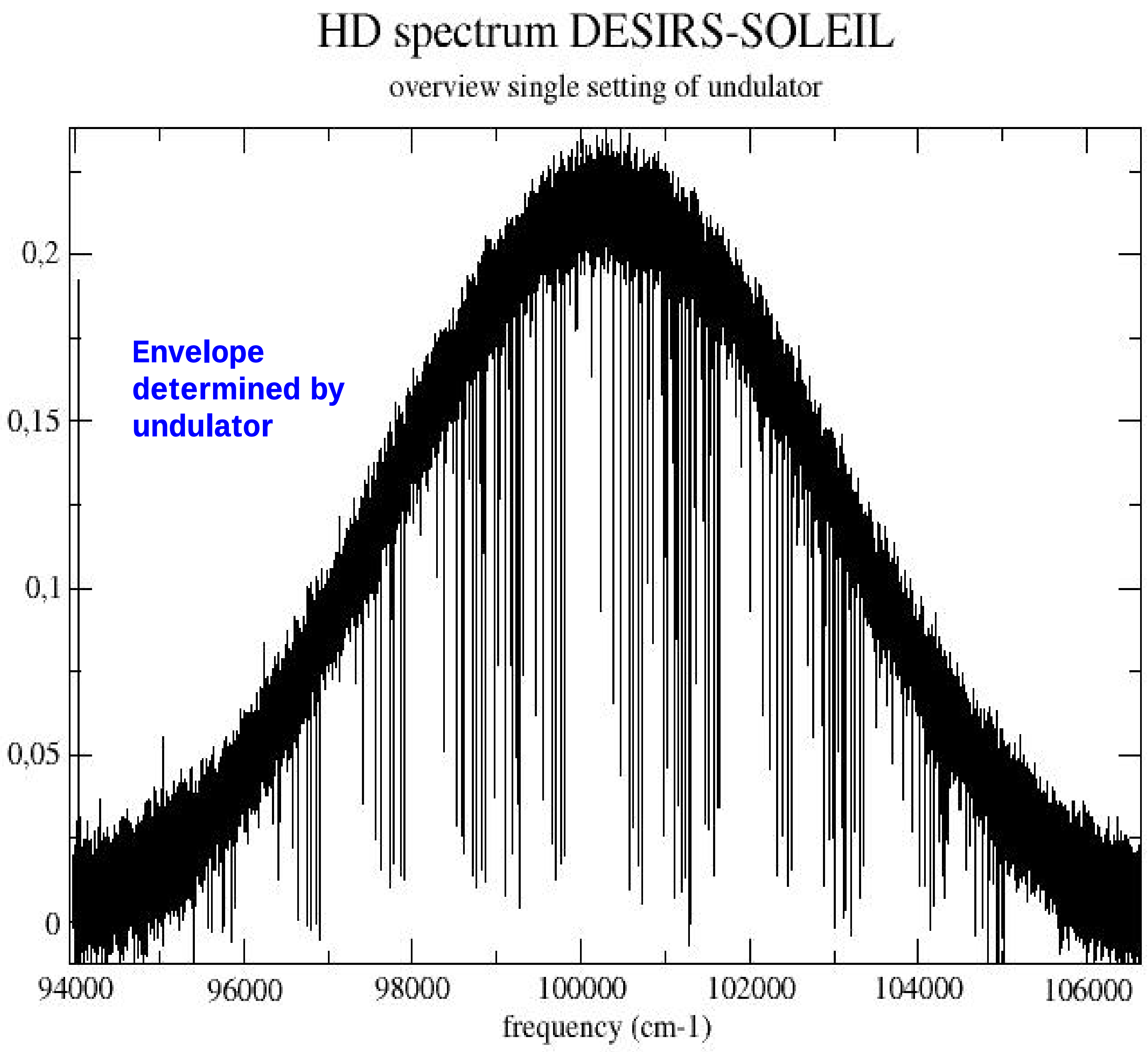
Level energies

Accuracy

$\Delta\nu \sim 10^{-4}$ cm^{-1}

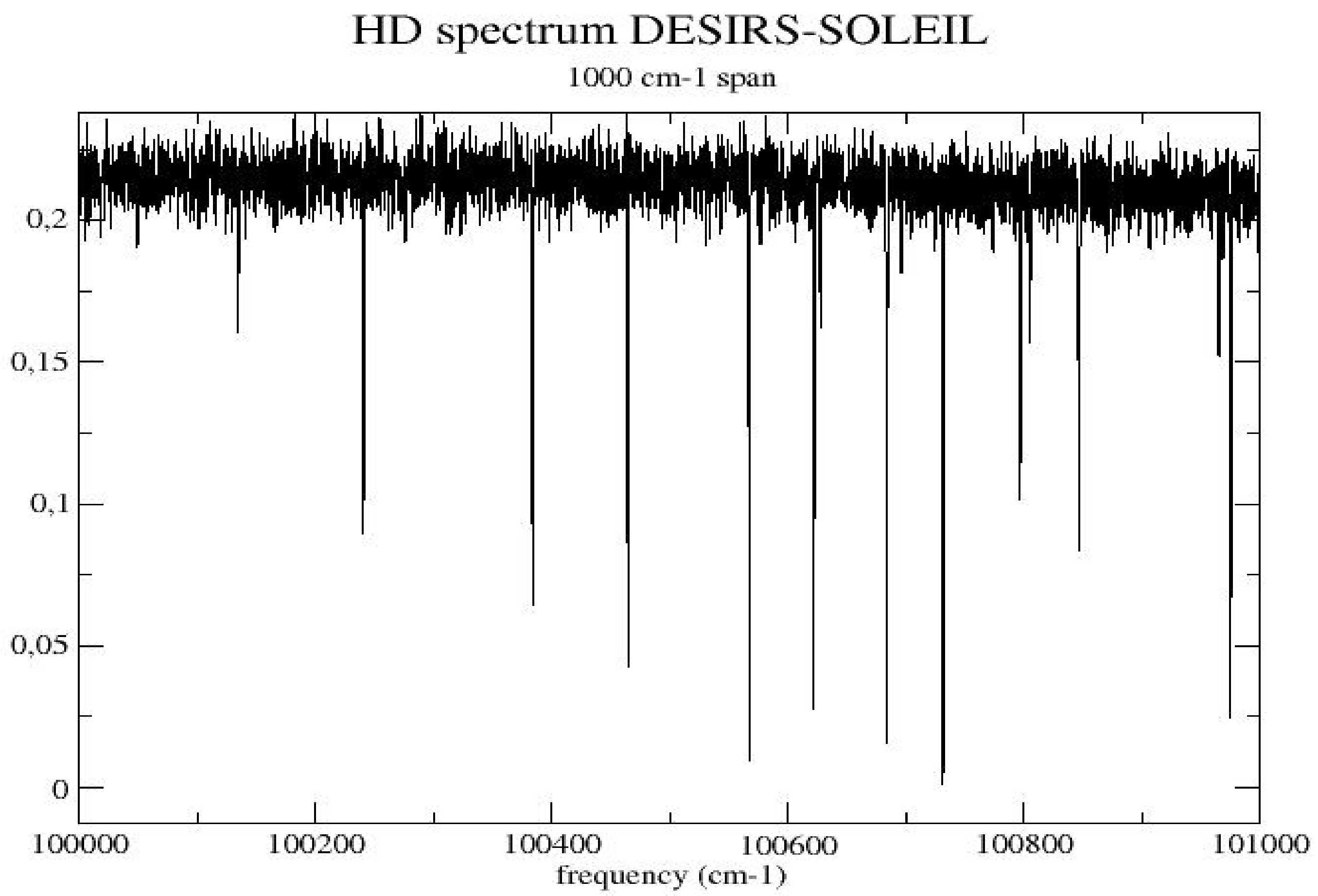
And a novel tool:
The DESIRS XUV-FT-spectrometer at SOLEIL

→ Direct absorption



Spectrum
2 h
data
collection

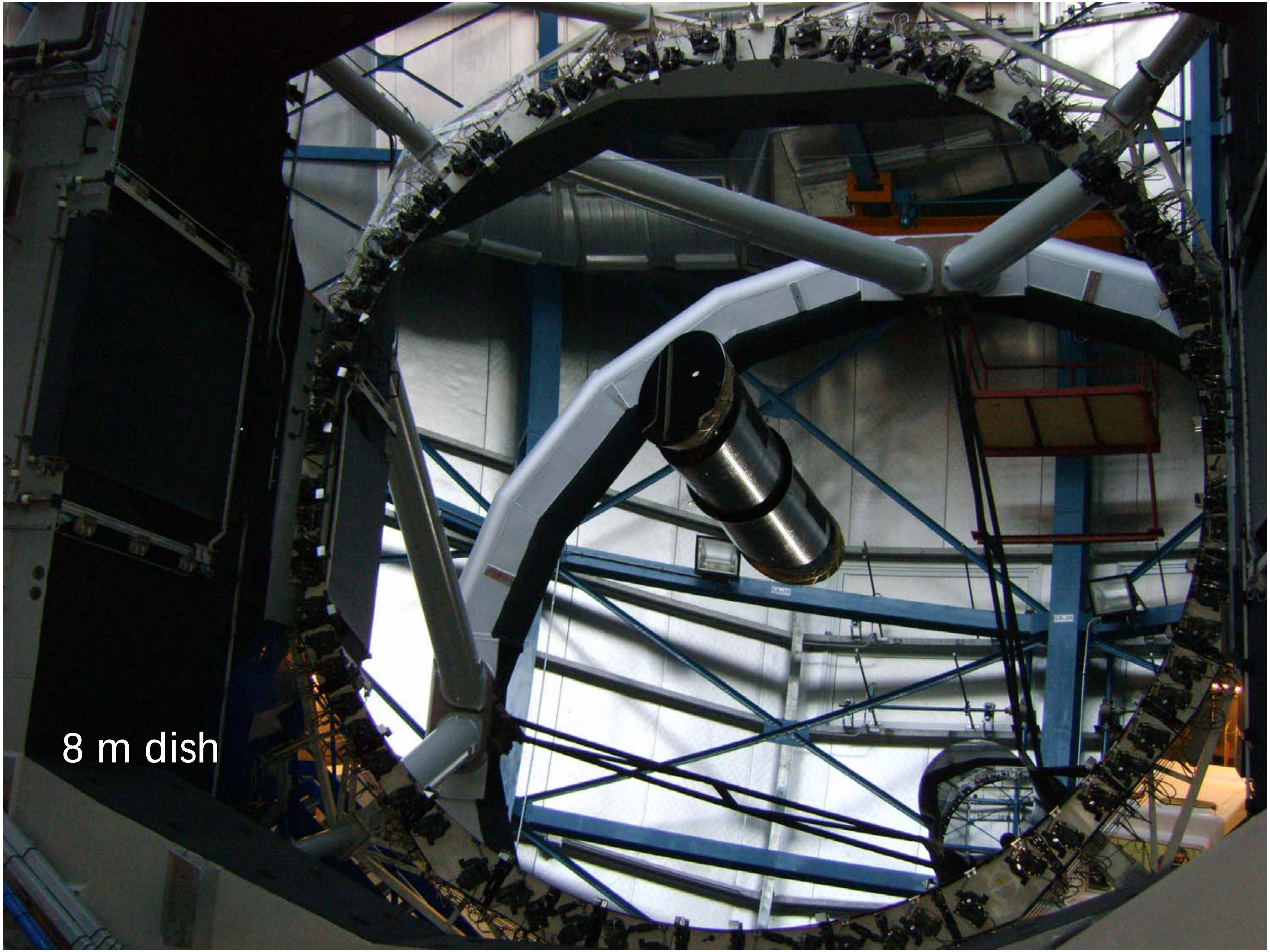
Goal: determine line intensities of H_2/HD



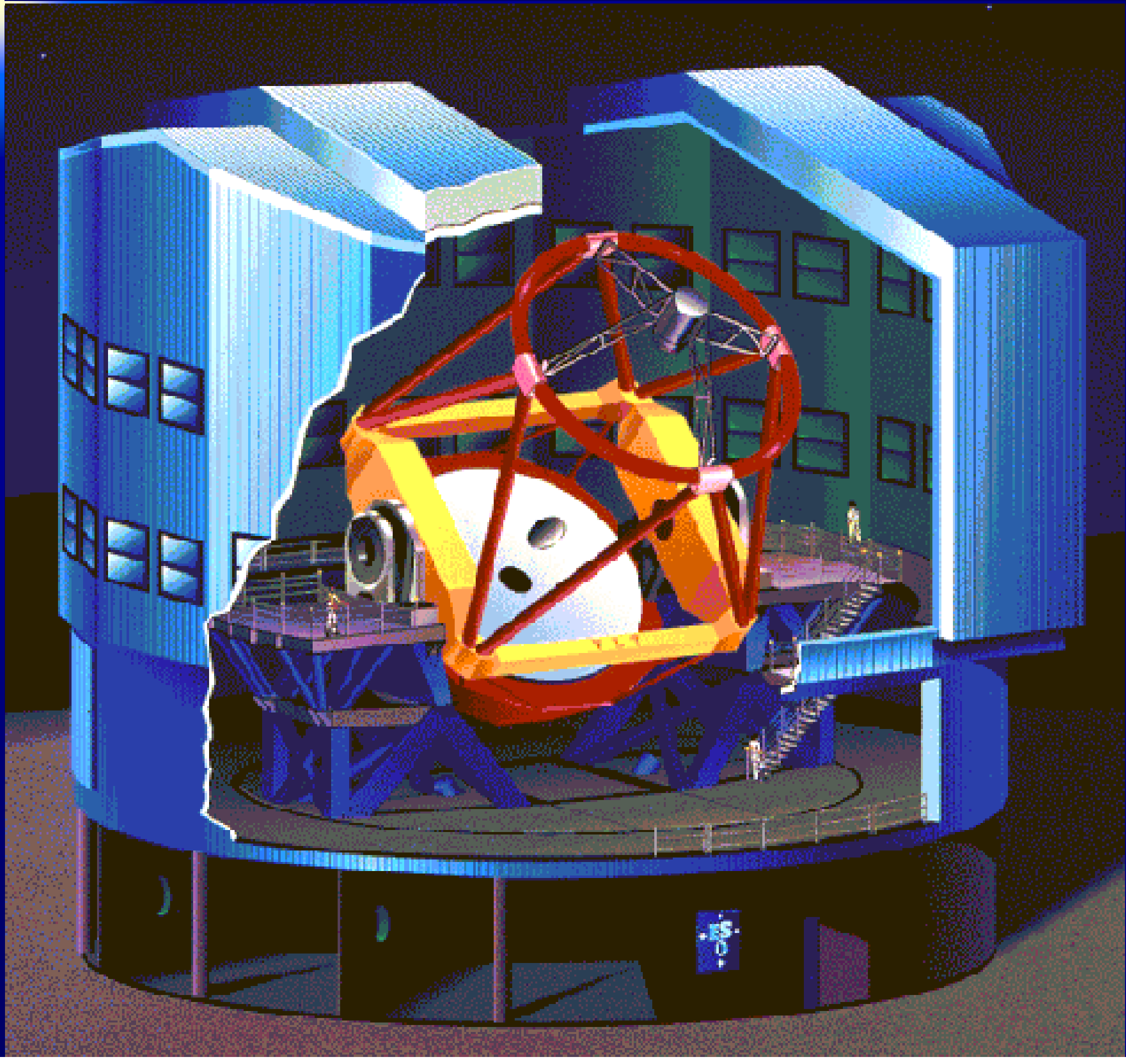

Progress on the astrophysical side

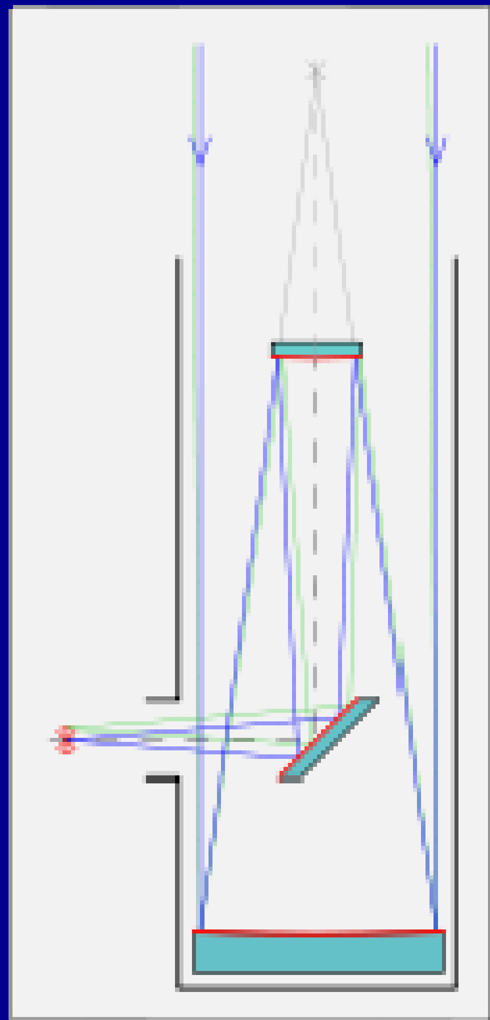
VLT at Paranal

ESO PR Photo 43a/99 (8 December 1999)

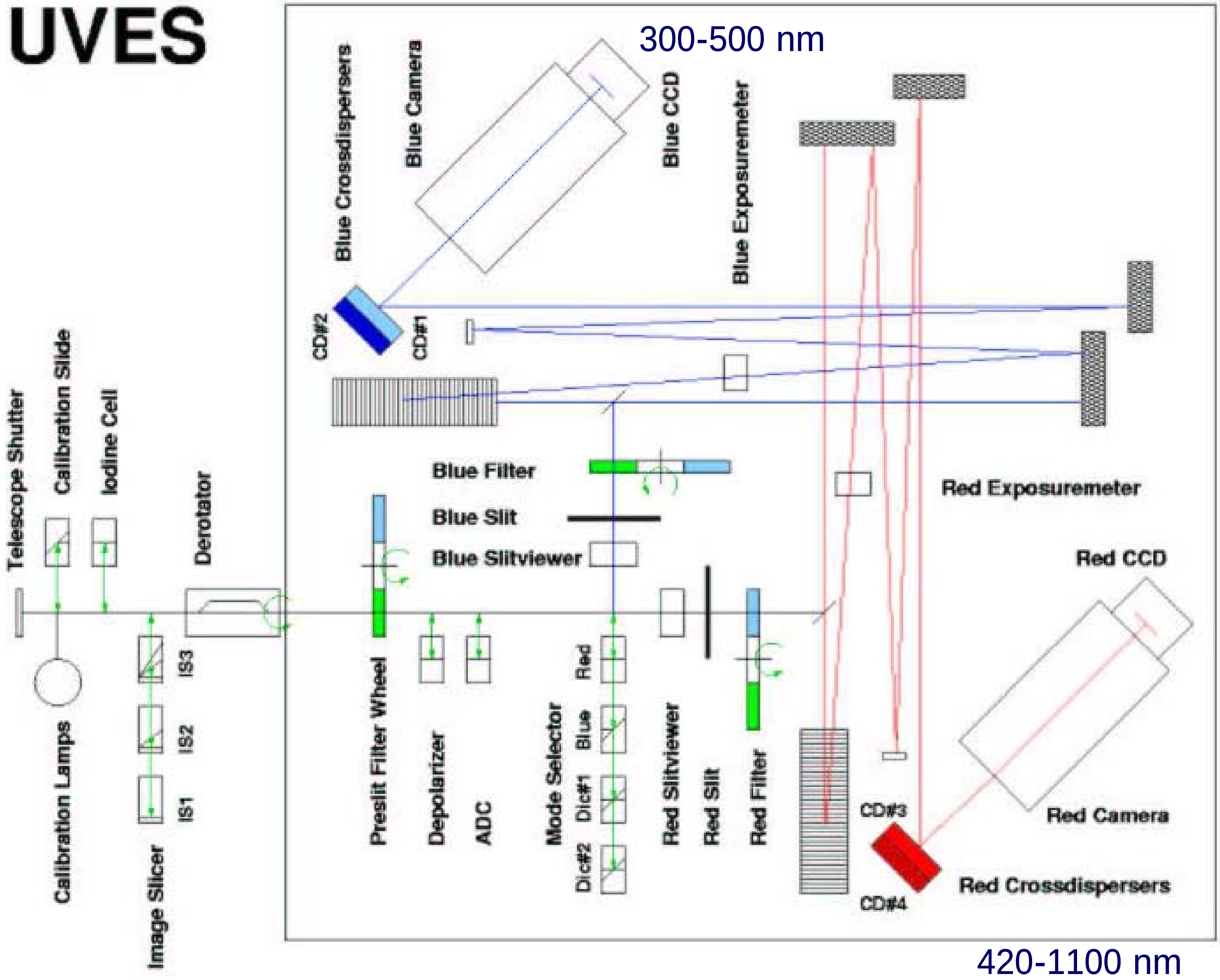

8 m dish

The telescope and the instrument





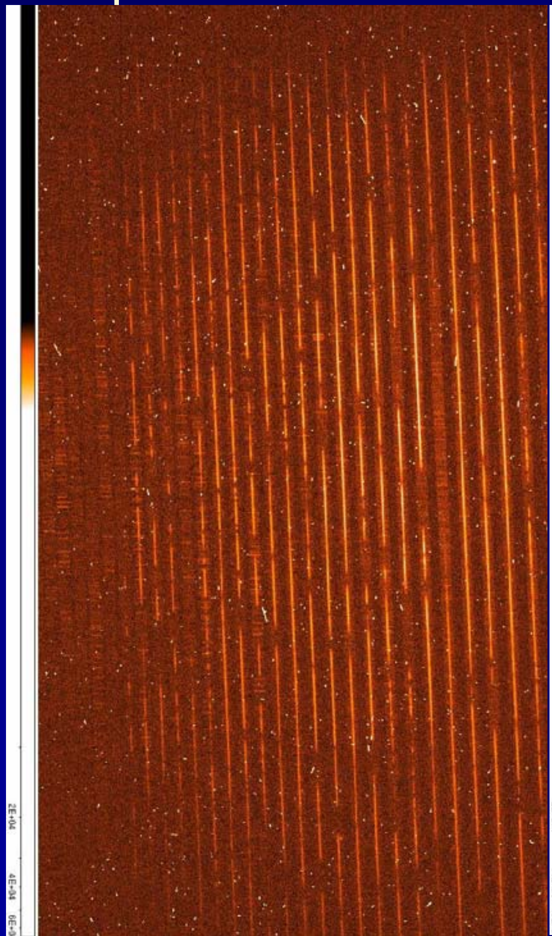
UVES



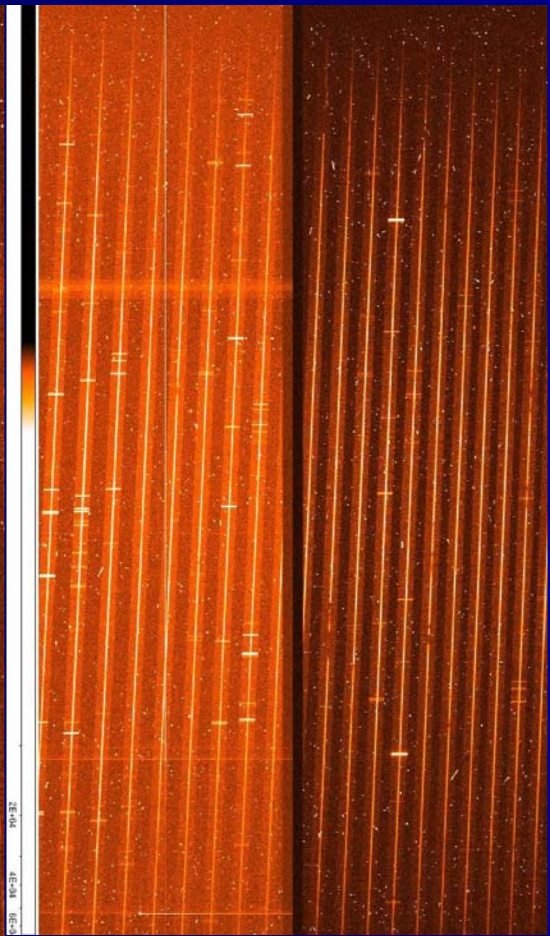
300-500 nm
Blue Crossdispersers
Blue Camera
Blue CCD
Blue Exposuremeter
CD#2
CD#1
Blue Filter
Blue Slit
Blue Slitviewer
Red Exposuremeter
Red CCD
Telescope Shutter
Calibration Slide
Iodine Cell
Derotator
Calibration Lamps
Image Slicer
IS3
IS2
IS1
Presilt Filter Wheel
Depolarizer
ADC
Mode Selector
Red
Blue
Dic#1
Dic#2
Red Slitviewer
Red Slit
Red Filter
CD#3
CD#4
Red Camera
Red Crossdispersers
420-1100 nm

Data acquisition on CCD's after "cross-dispersion"

Science data: at once
entire spectrum (315 – 800 nm)

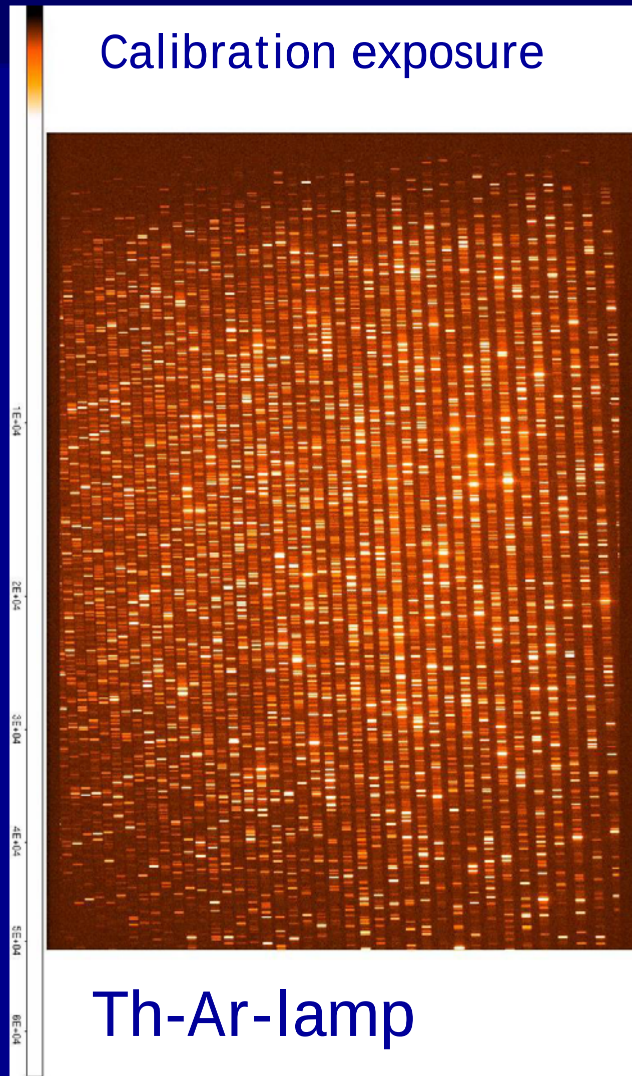


"Blue chip"



"Red chip"

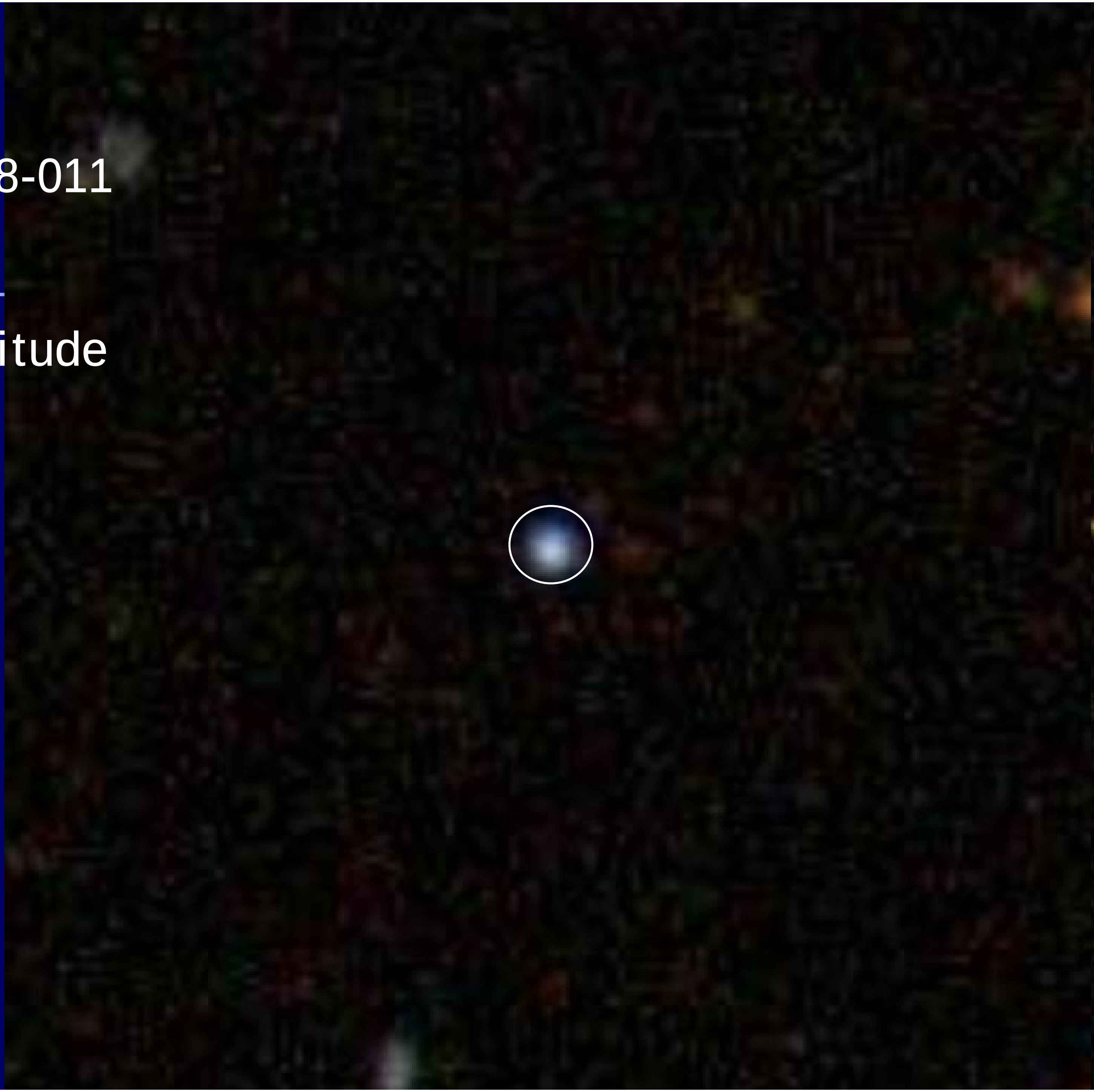
Calibration exposure



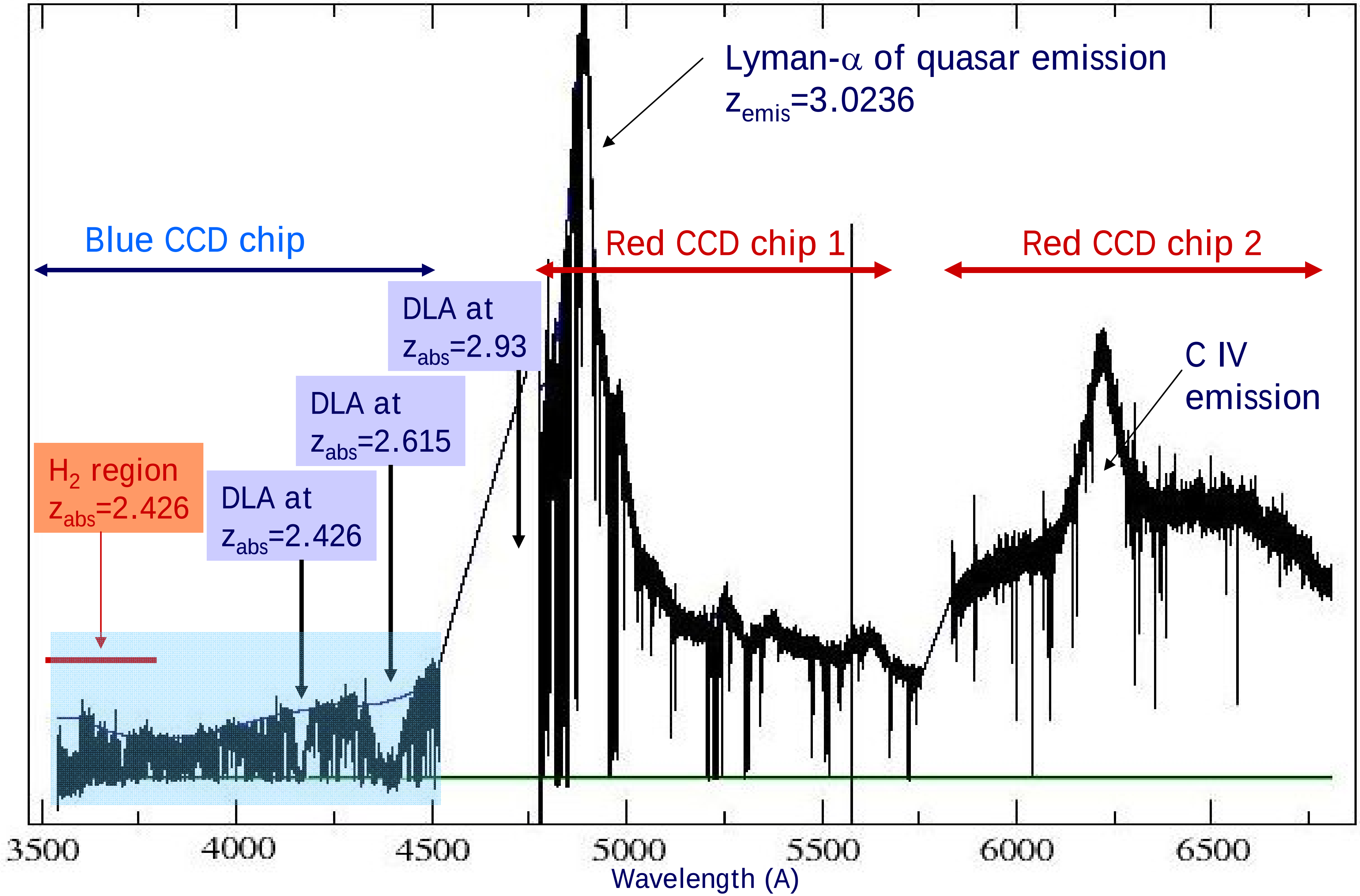
Th-Ar-lamp

Q2348-011

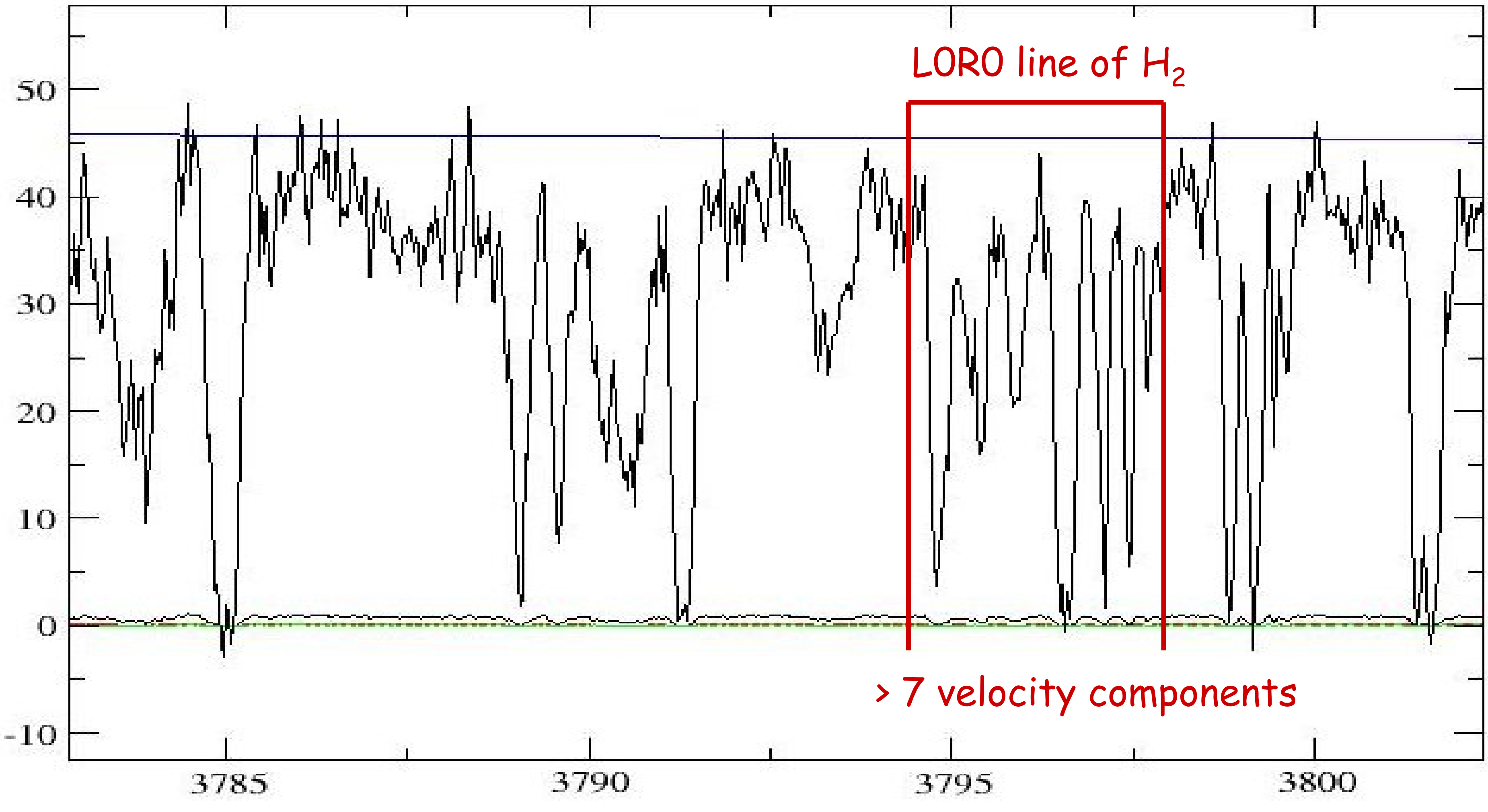
Magnitude 18.4



QSO 1: Q2348 (VLT) Ubachs-Buning observations 2007



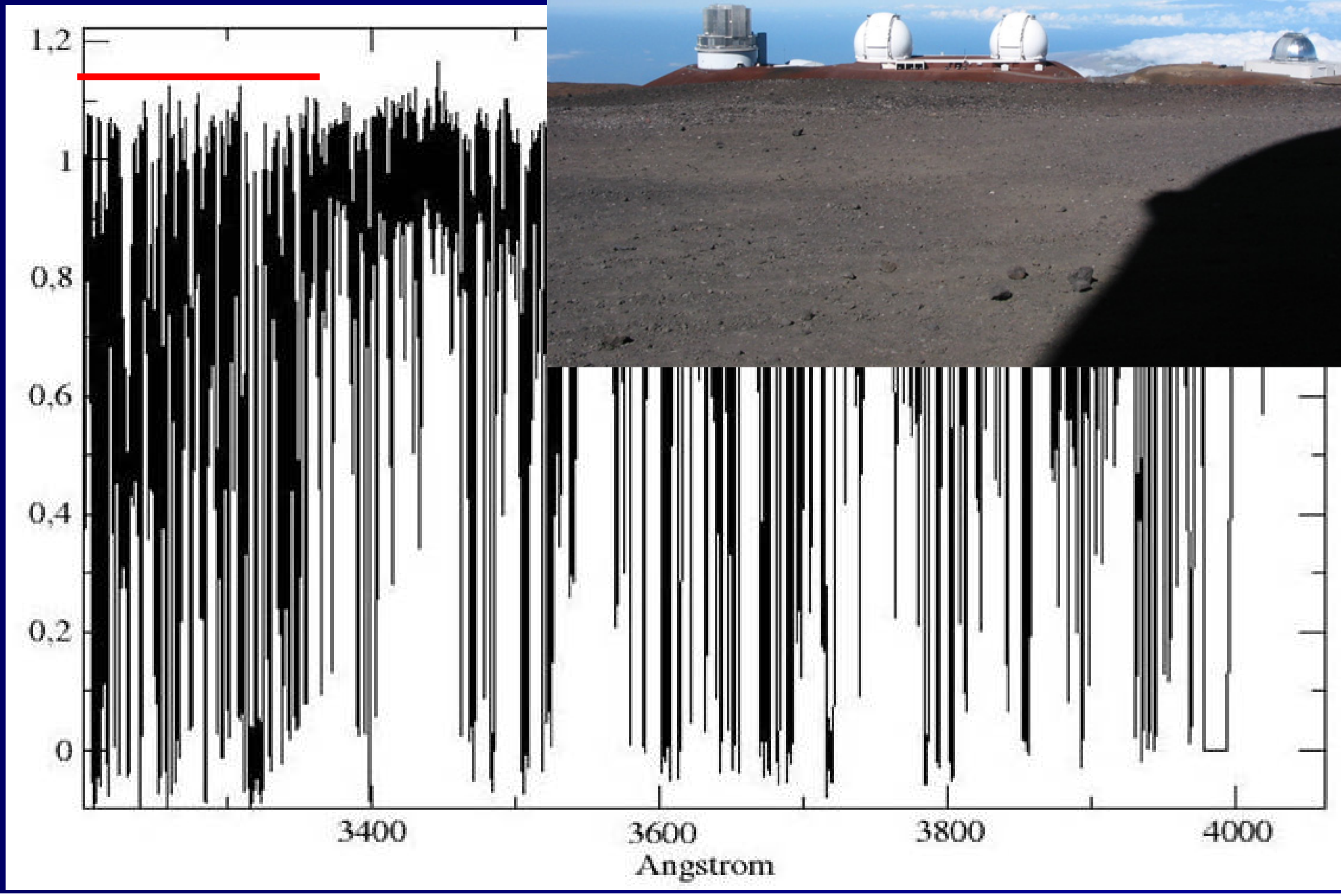
H_2 in Q2348-011; velocity components

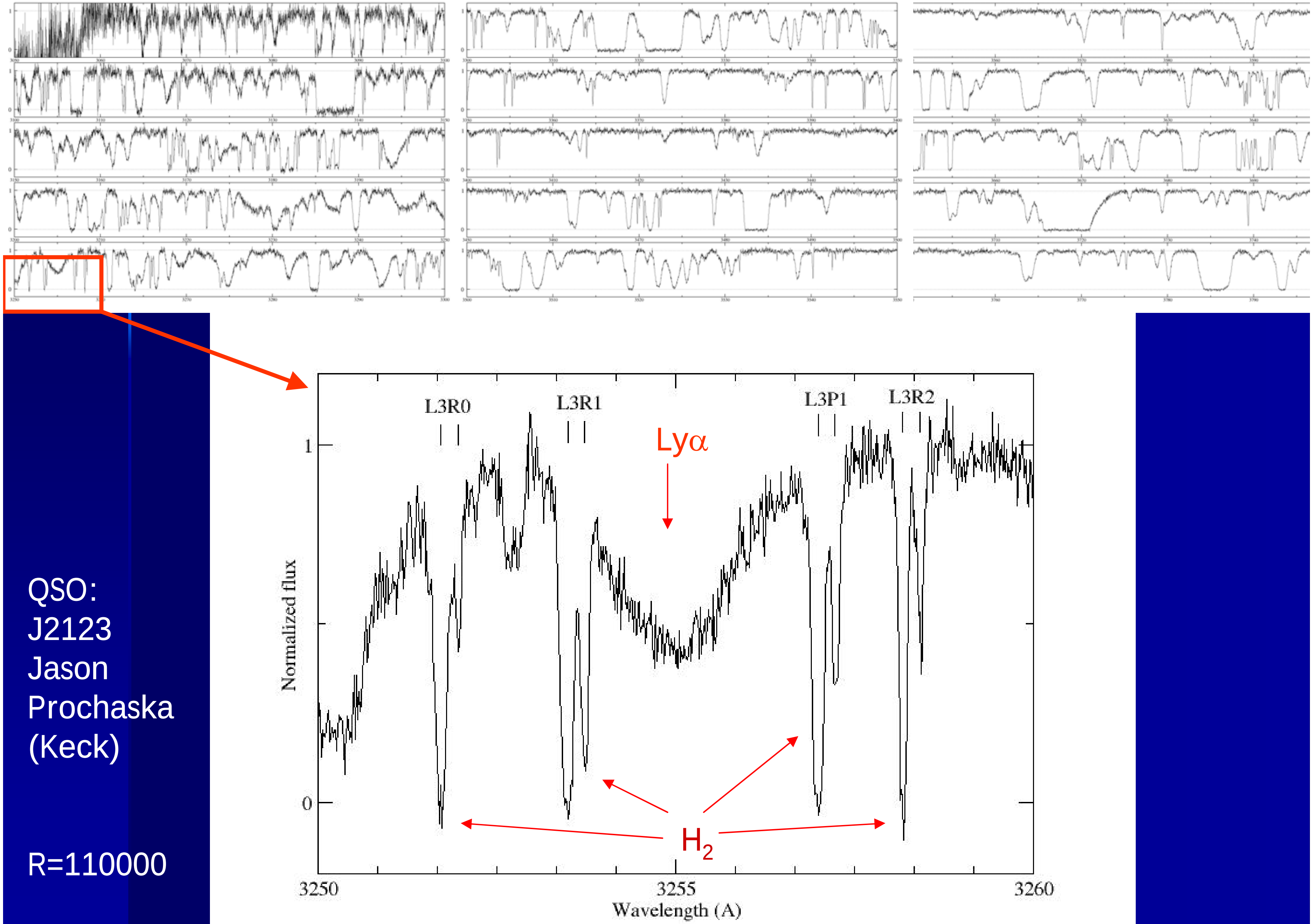


J2123 from HIRES-Kec

(Jason Prochaska)

H_2

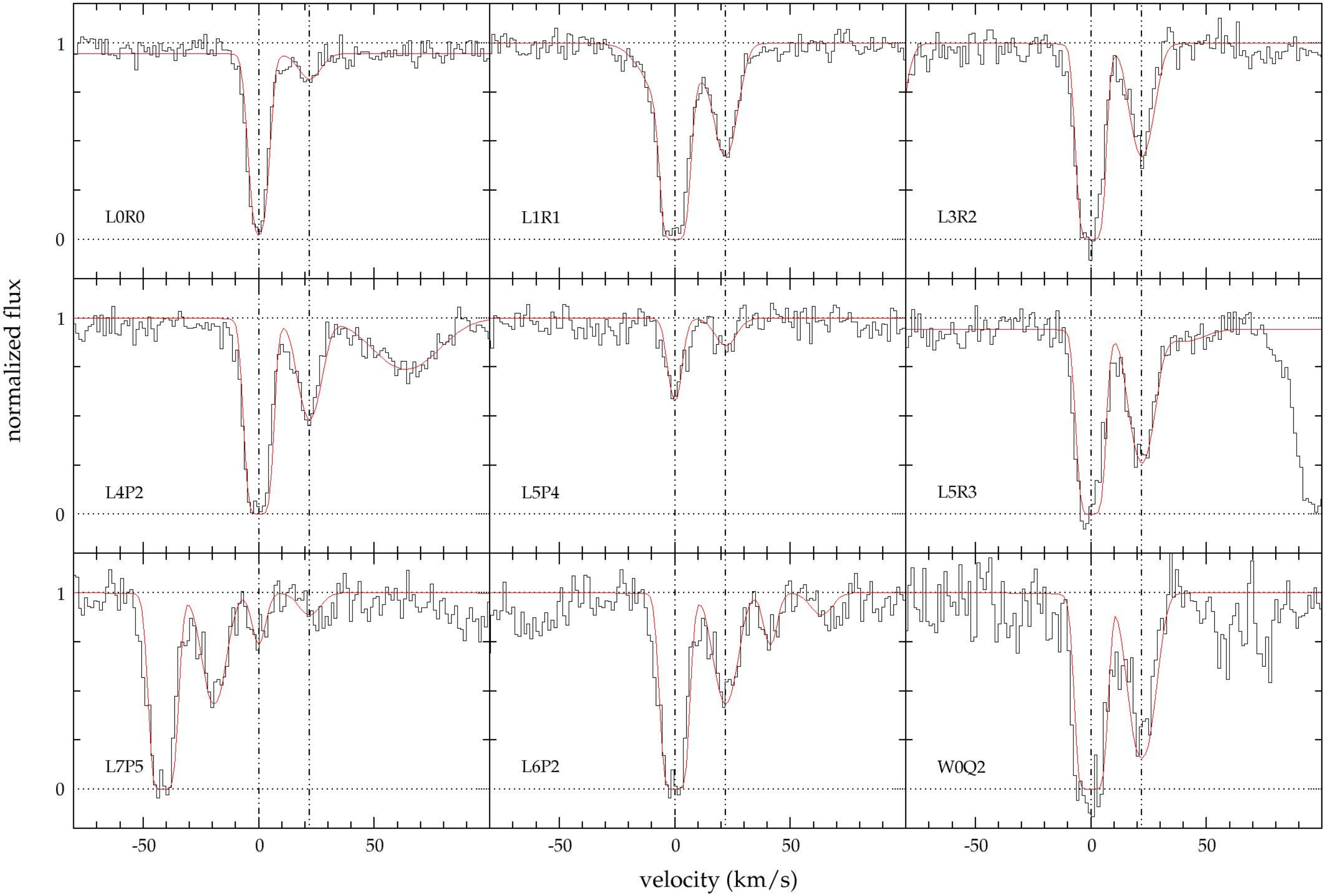




QSO:
J2123
Jason
Prochaska
(Keck)

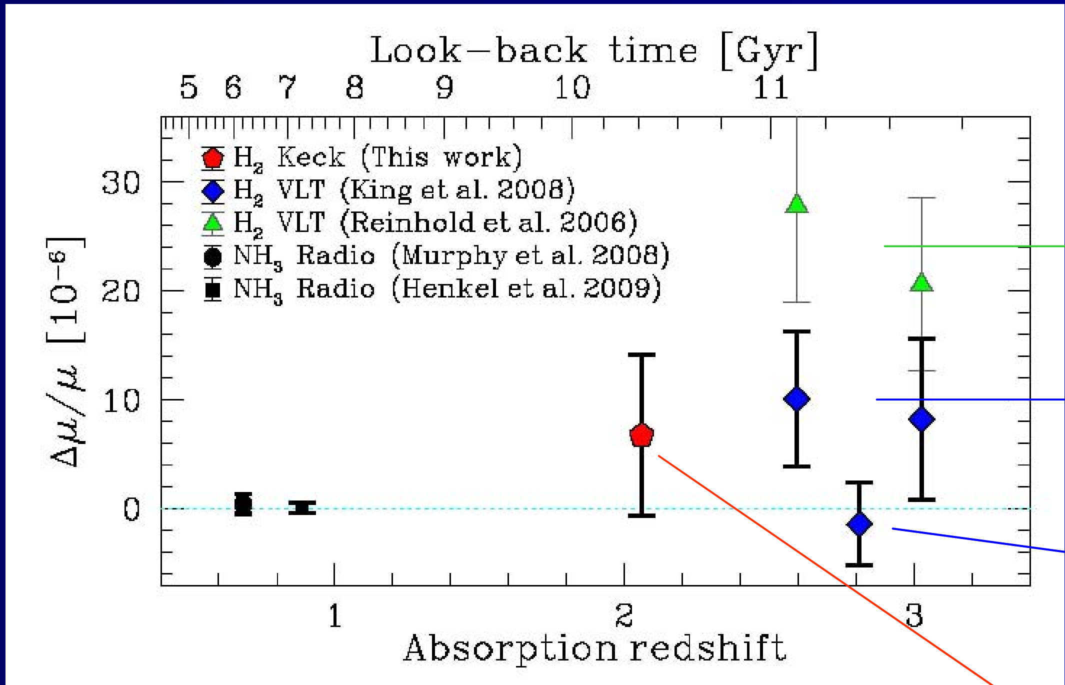
R=110000

J2123, z_{abs} = 2.0593426, H2 lines



Conclusion:

- QSO H_2 and NH_3 spectra for $\Delta\mu/\mu$ determination



1st analysis
Q0347 / Q0405

reanalysis
Q0347 / Q0405
King, Webb

analysis
Q0528 old data
King, Webb

analysis
J2123 Keck
Ubachs, Murphy, Buning, Malec, Prochaska

+ data pending (Ubachs, Murphy, Kaper)
Q2348 (VLT-2007)
J2123 (VLT-2008)
Q0528 (VLT-2009)