Focus exp. :
Naines brunes et bandes moléculaires de FeH et CrH

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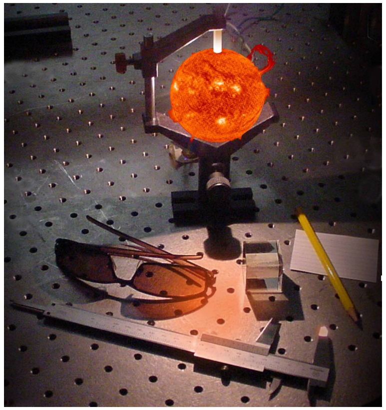
PLAN



1. **Présentation**	équipe et thématiques
2. **Problématique**	étoiles froides et MH
3. **Etat de l'Art au labo**	FeH et CrH.
4. **Projet en cours**	spectromètre Vernier (CrH)
5. **Conclusion**	perspectives

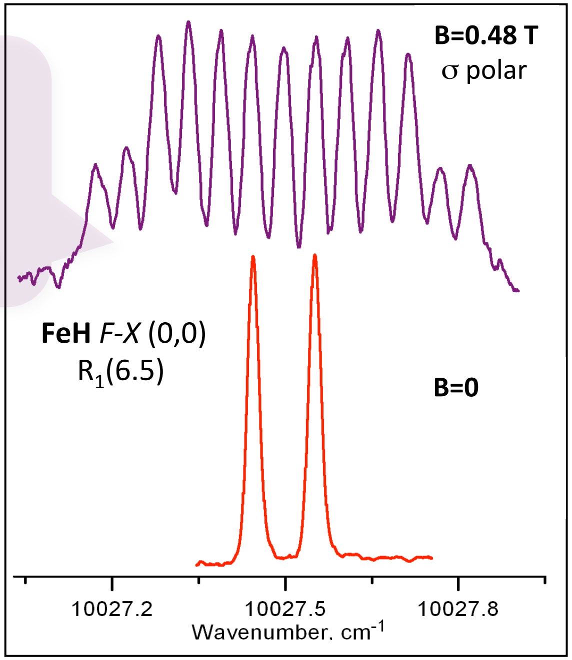
1. Présentation / **Equipe et thématique**

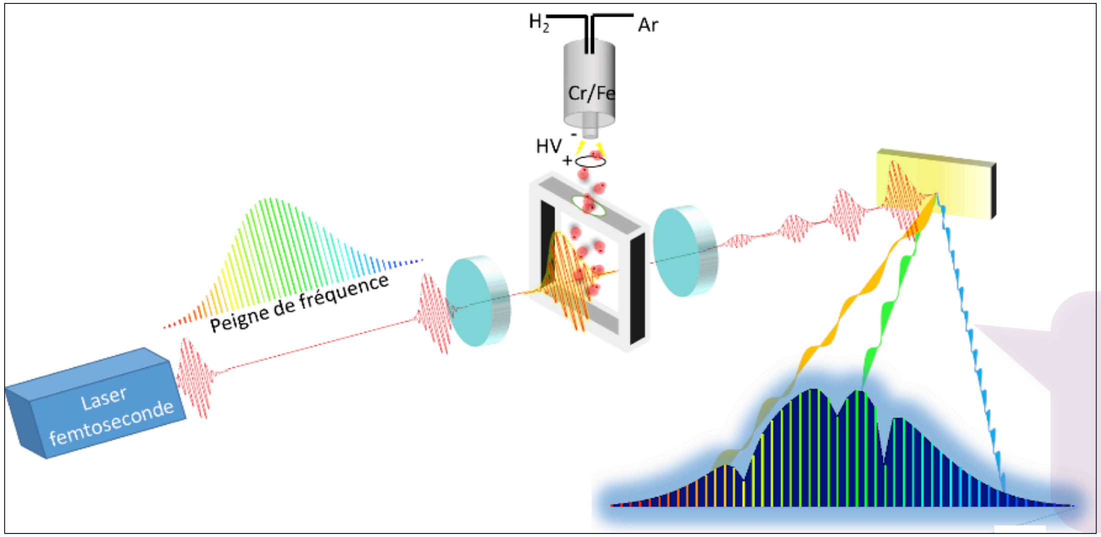
Spectrométrie Moléculaire, *Institut Lumière Matière*

Amanda ROSS , Heather HARKER , Jérôme MORVILLE , Patrick CROZET
Georgi DOBREV (doctorant), Cassandre MIRALLEI (M2 Lyon1), Ella WYLLIE (M2 U. Strathclyde/Lyon1).

Spectroscopie Laser de radicaux MH (M=Ni,Fe,Cr)

- Source à décharge (T<500K) : FTS/LIF, CRDS
- Analyse de spectres champ nul et Zeeman : B=0, B<0.6 T.

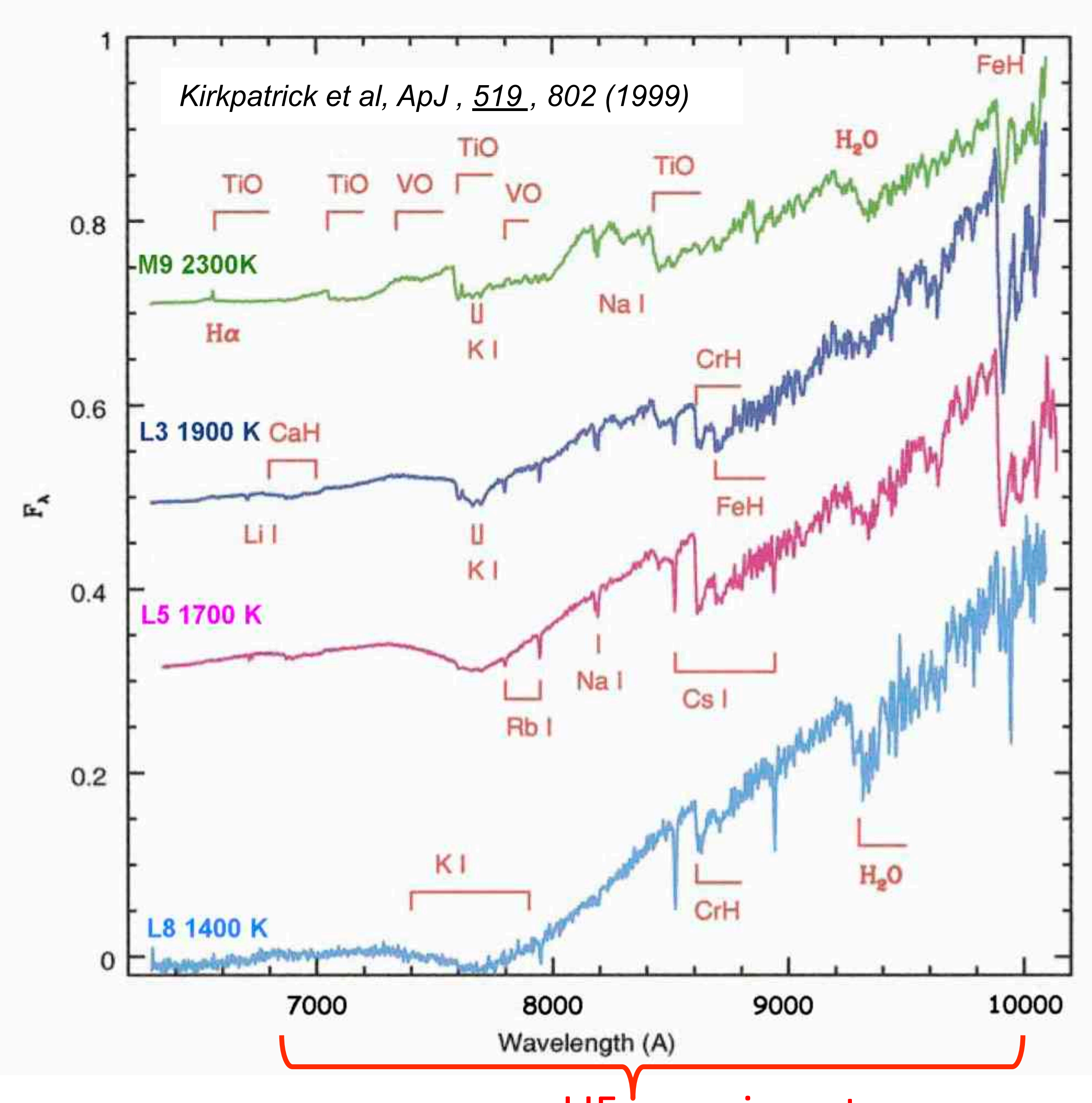




Spectromètre Vernier

Couplage Vernier d'un peigne de fréquences aux résonances multiples d'une cavité optique.

2. Problématique / FeH & CrH in late-M and L dwarfs



Kirkpatrick et al, ApJ , 519 , 802 (1999)

our LIF experiments

Ldwarfs : $T_{eff} \approx 1400 - 2000$ K

Observed bands 640-1020 nm

High Res.(R=33k) Atlas L0 - -> T1
Reiners et al, A&A 473, 245–255 (2007).

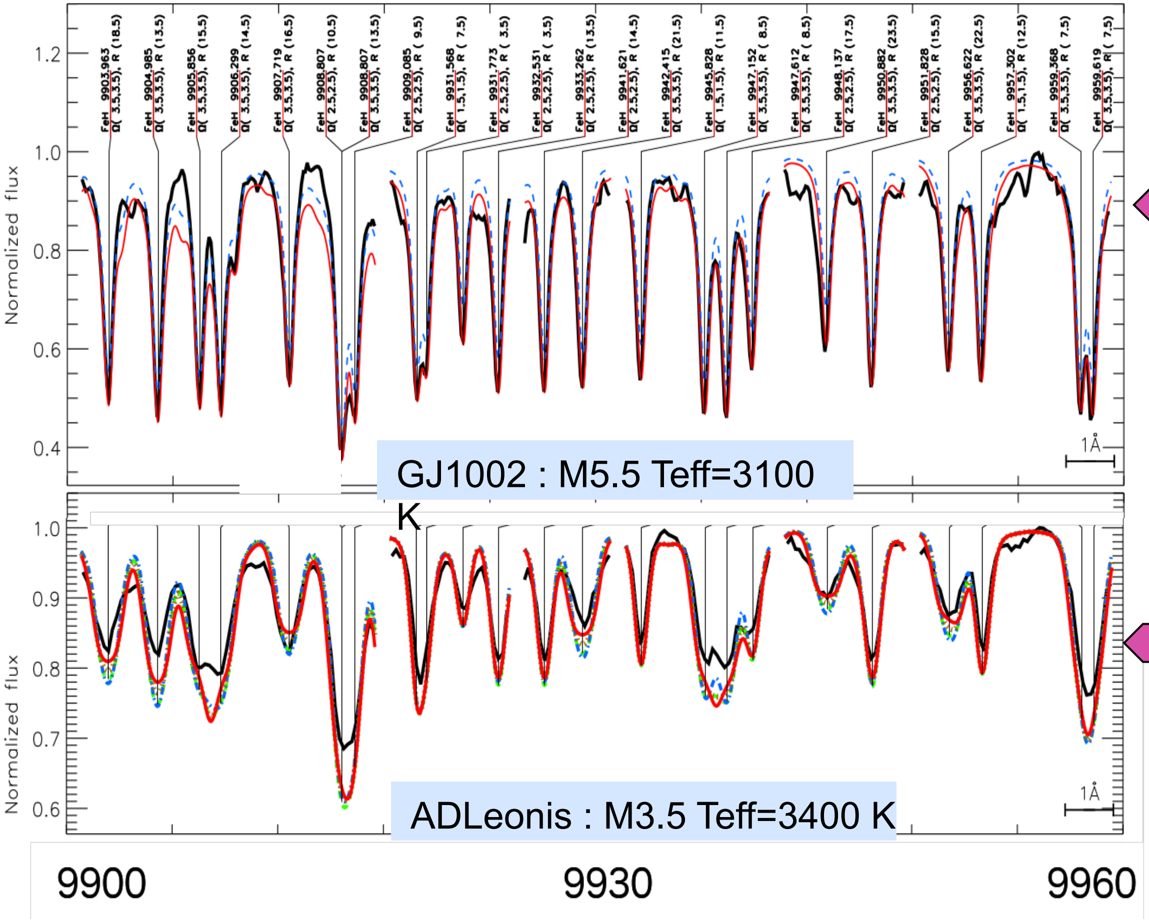
FeH : *F-X* 0-0 @ 989.6 nm *Wing-Ford*
F-X 1-0 @ 869.2 nm
CrH : *A-X* 0-0 @ 861.1 nm
? 1-0 @ 764.0 nm, blend O_2
? 0-1 @ 996.9.0 nm, blend FeH

" the 1-0 (764 nm) and 0-0 (861 nm) bands of the $A\ ^6\Sigma^+ - X\ ^6\Sigma^+$ transition of CrH are primary markers for L-type brown dwarfs"
Bauschlicher, J. Chem. Phys., 115(3), 1312 (2001).

J- band : Spirou ?

FeH *F-X* 0-1, 1-2 ≈ 1.2 μm
FeH *E-A* ≈ 1.6 μm
Low Res (R=2000) Atlas 0.8-5.0 μm
J.T. Rayner et al, ApJS, 185:289 (2009)

2. Problématique / **High Res. FeH in red dwarfs**



GJ1002 : M5.5 Teff=3100 K

ADLeonis : M3.5 Teff=3400 K

Strong features near 1 micron in a non-magnetic star are assigned to FeH, based on the <u>FeH atlas</u>

Dulick *et al*, ApJ, <u>594</u> 651 (2003)

Zeeman-broadened profiles on AD Leonis interpreted via <u>Landé factors from telescope spectra</u>.

Shulyak *et al,* Proceedings Astr.Soc. Pacific. Conf.<u>*448*</u> 1263S (2011)

Difficult to find a unique solution :

B (uniform?) 2.5 - 3 kG

Shulyak *et al,* A& A <u>563</u>, A35 (2014)

g_J Landé Factors : what uncertainty?

3. Etat de l'Art au labo / **FeH (S=3/2)**

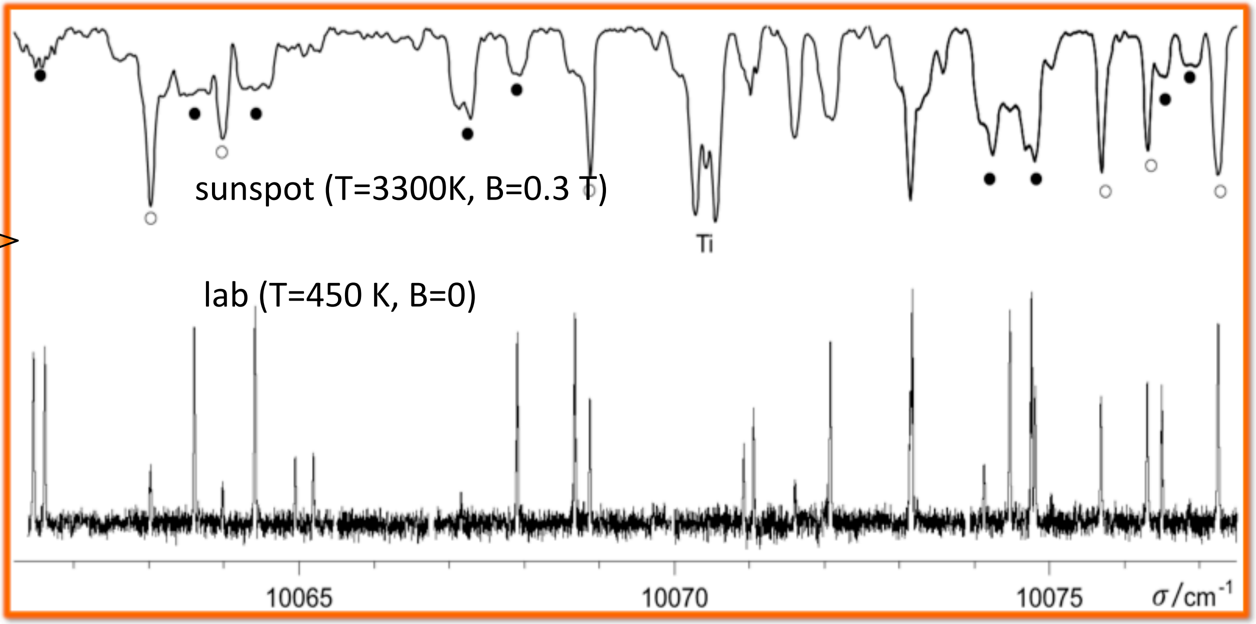
Zero field data

- FTS/King furnace : J<32, v' and v"= 0,1,2 : J.G. Phillips et al, ApJS, 65 (1975)721.
- Bernath's Atlas : line list of experimental and extrapolated to high J transitions from ab-initio calculations. M. Dulick et al, ApJ, 594:651(2003) ; *http://bernath.uwaterloo.ca/FeH*

Magnetic response

- LMR /discharge : ground state $X\,^4\Delta$, v''=0, J"<8 : Brown et al, JCP, 124, 234309(2006)
- LIF / molecular beam *F-X,* J"=3.5 v'=1-0 : Harrison et al. ApJ, 679,854 (2008)
- LIF /discharge *F-X,* J"<10 v'=1,0 : Crozet et al, J. Mol. Spec, 303, 46 (2014)

Magnetic sensitivity of FeH
Wing-Ford band
$F\,^4\Delta - X\,^4\Delta$ (0,0)



3. Etat de l'Art au labo / **CrH (S=5/2)**

Zero field data

- FTS/discharge : A $^6\Sigma^+$ - *X* $^6\Sigma^+$ (0-0) @ 861 nm
  Ram et al, J. Mol. Spectrosc.,161, 445(1993)
  --> quantum mechanical *Heff* model
- Bernath Atlas *:*
  Burrows et al, ApJ, 57, 986 (2002).

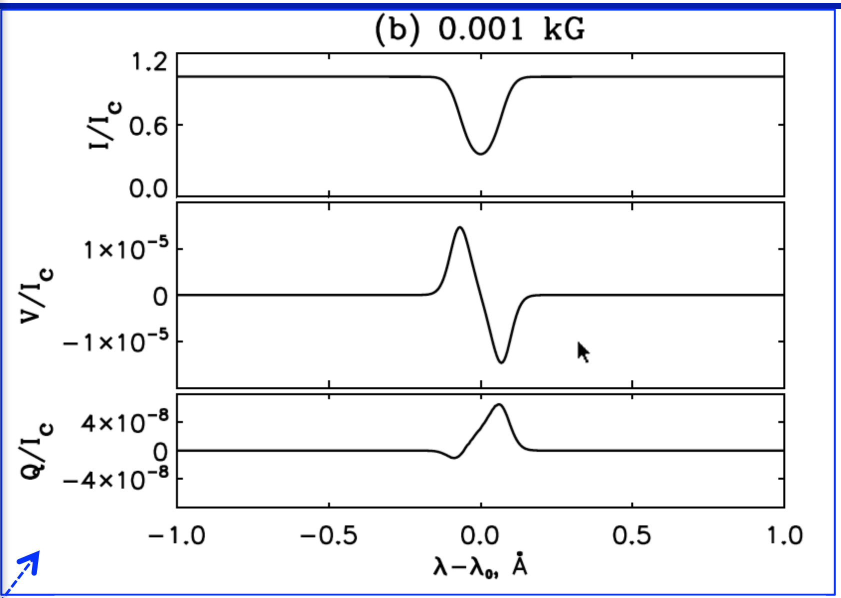
Magnetic response : NOT MUCH ...

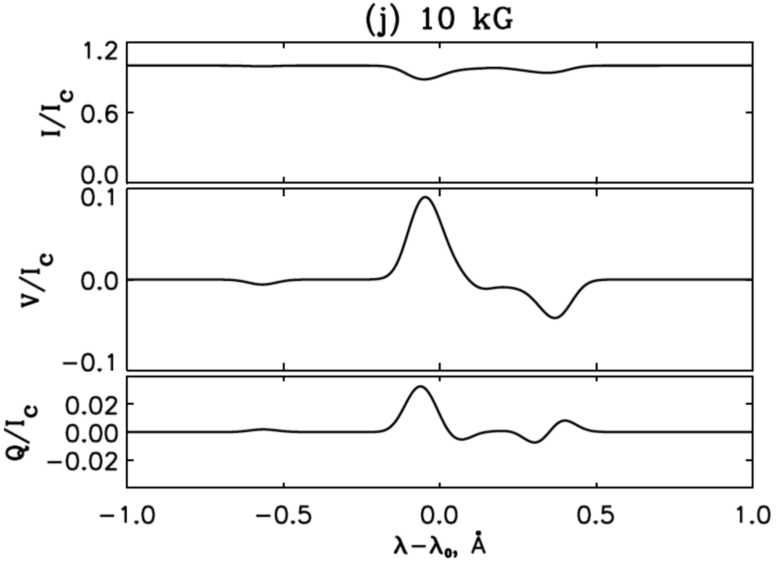
- LMR /discharge : *X* $^2\Delta$, v''=0, N"<6 :
  S.Corkery et al, J. Mol. Spectrosc. 149,257 (1991)
- LIF/beam A-*X* , J"<5 v'=0,1 :
  J. Chen et al, PCCP, 9, 949 (2007)
- *Heff* model for A-X (0-0) :
  O. Kuzmychov, A&A, 558, A120 (2013).
  Spectropolarimetry simulation : strong asymmetric splitting for Stokes Q @ B > 1 G Paschen-Back regime
  "a considerable signal in both circular and linear polarization, up to 30% @ B ≥3 kG in early L dwarfs"

=> Needs from the lab :

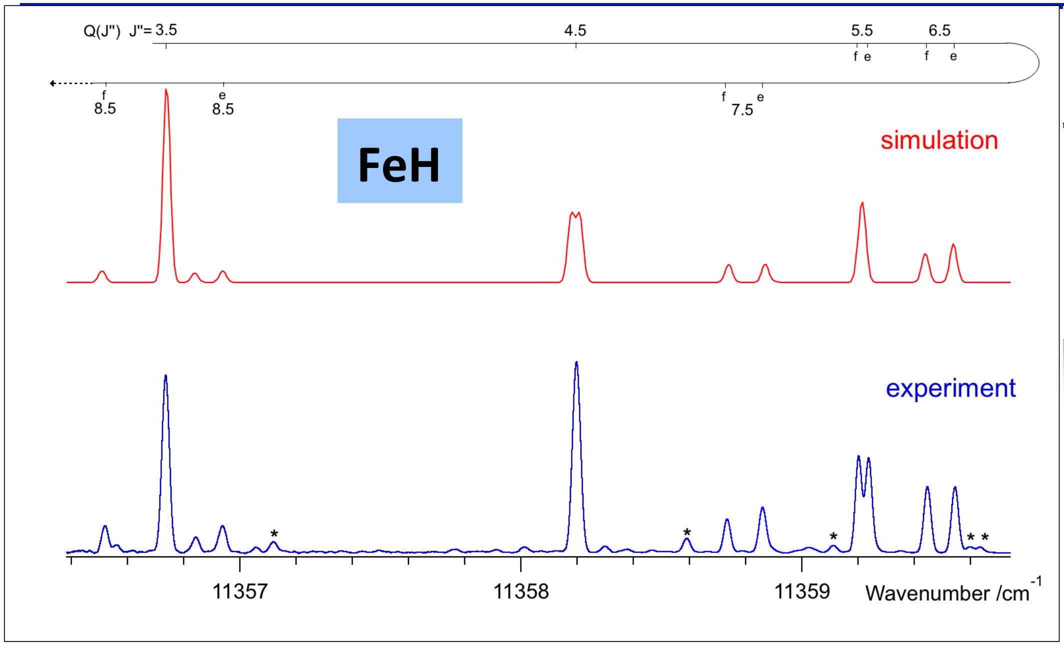
*** absorption cross-sections(B=0)**

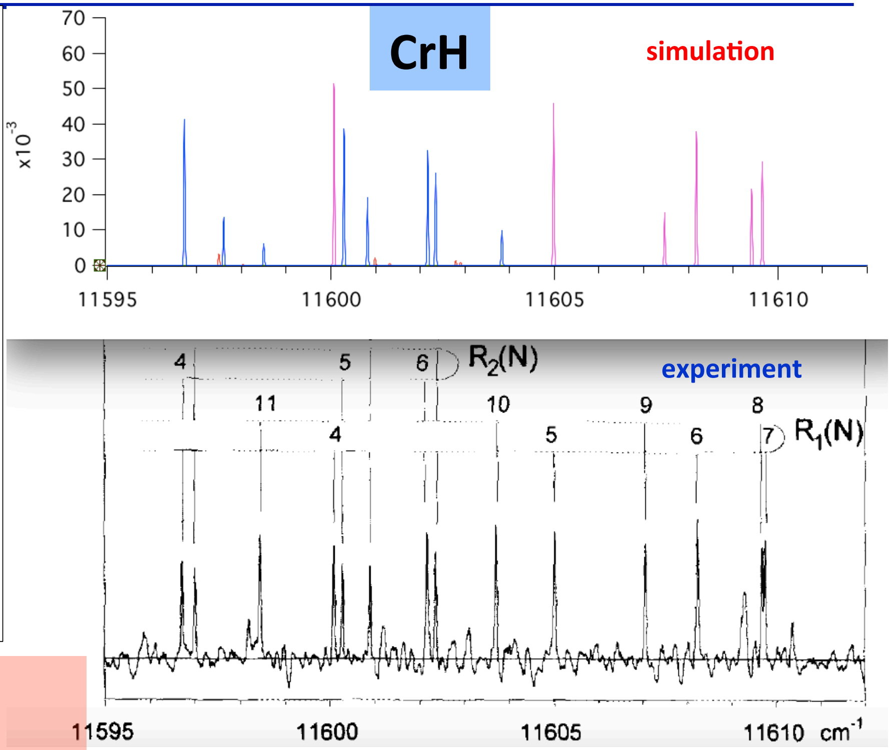
***** g_{eff}





3. Etat de l'Art au labo / **Atlases : caveat ...**





Ram et al, J. Mol. Spectrosc.,161, 445(1993)

Atlas de P.W. Bernath en champ nul

FeH : Dulick et al, ApJ, 594:651–663 (2003).
CrH : Burrows et al, ApJ, 577:986–992 (2002).

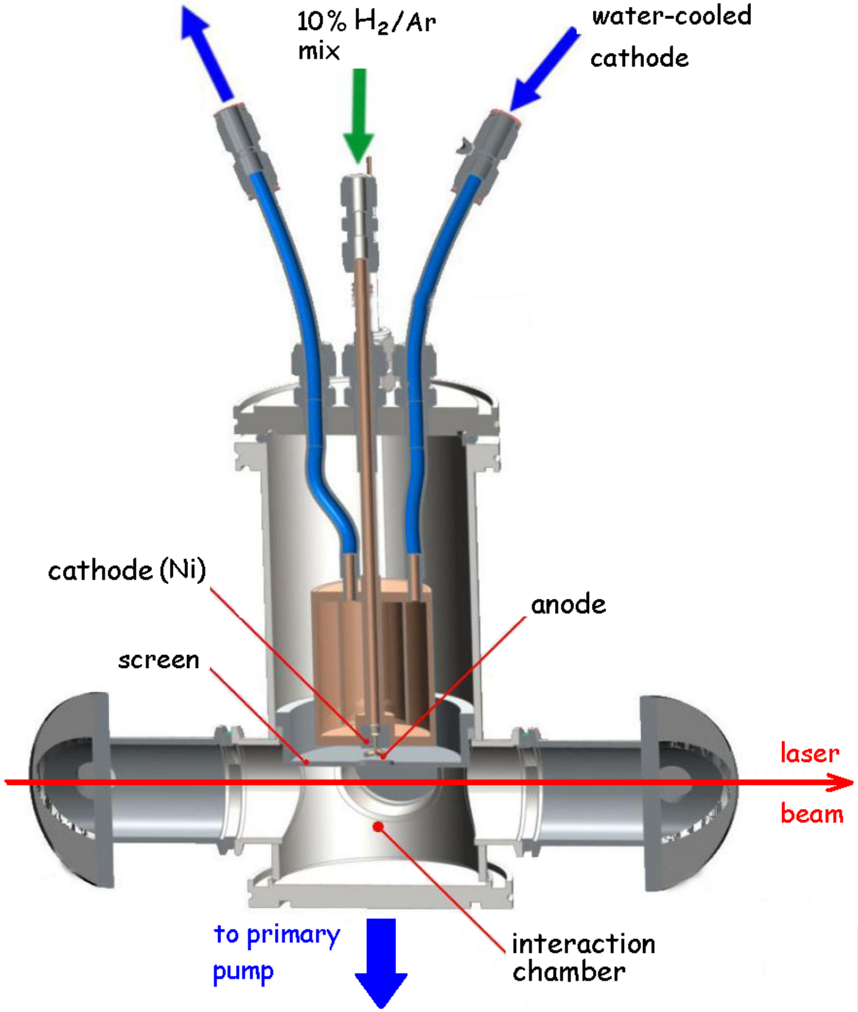
Les simulations stellaires nécessitent les fréquences, opacités et réponses magnétiques précises des raies moléculaires.
Atlas : les fréquences et coeff. A d'Einstein des transitions (v',J') <— (v'',J'') sont obtenus par extrapolation de données de laboratoire, à partir de calculs ab-initio, peu fiables en raison de l'imbrication des états électroniques et vibrationnels (approximation B-O non valide)
=> **mesures directes nécessaires, même en champ nul, et même à bas J.**

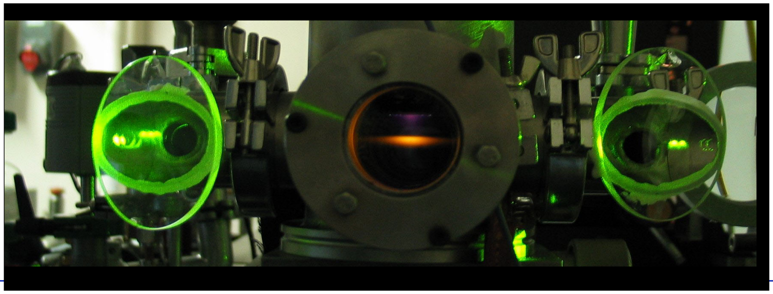
Simulation du profil d'absorption :

$$I = I_0\, e^{-Sg(\nu-\nu_0)Nl}$$

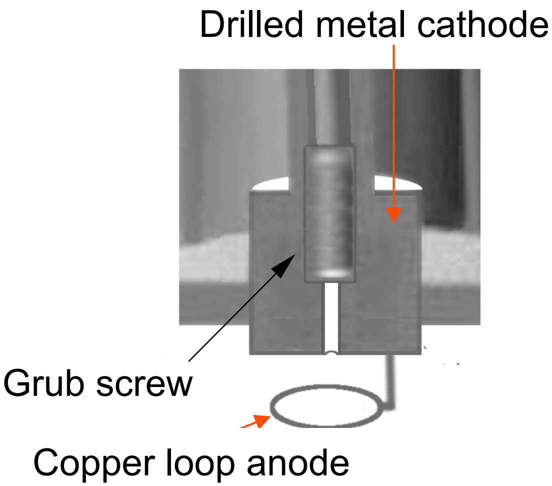
$$S = \frac{A_{J'J''}}{8\pi\nu_0^{2}}(2J'+1)\,\frac{e^{-\frac{E''}{kT}}\left(1-e^{-\frac{h\nu_0}{kT}}\right)}{Q(T)}$$

3. Etat de l'Art au labo / **MH production : hollow cathode discharge**





décharge : 250 V_{DC}, i=100 mA.
pression : 0.5 - 2 torr
débit : 5 10^{-5} mol/s



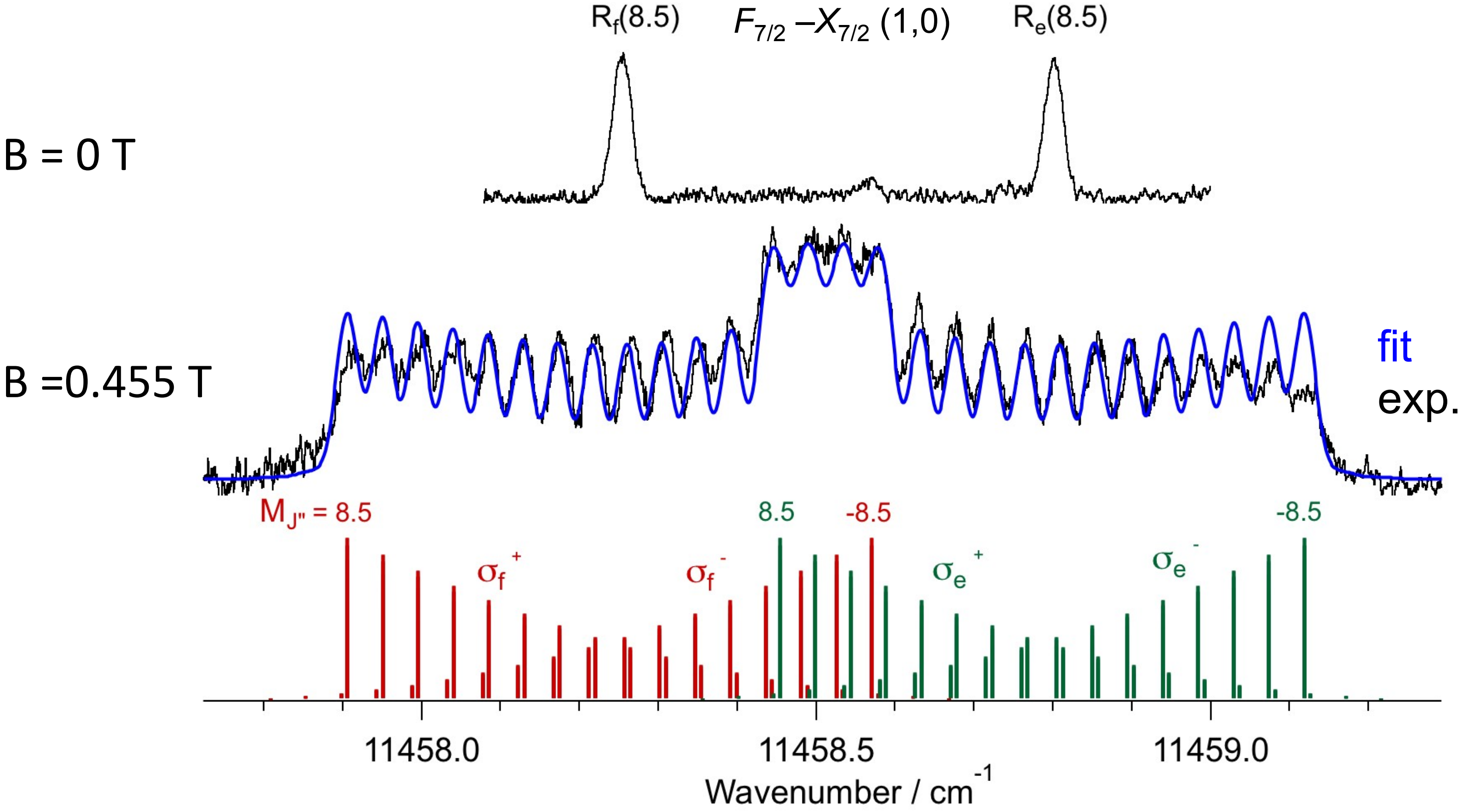
Source 'froide' (T_{rot} = 400 K) :

- fréquences des raies d'absorption précises
- splittings Zeeman résolus

Mais : J<10

=> gagner en sensibilité !

3. Etat de l'Art au labo / **Measurement of FeH g_J factors**



Line profile model (*Igor pro*) : $I(\nu) = \eta \,.\delta\, .\, I_{Laser}\, .\sigma_{12}(\nu - \nu_{12})\, N_1$

η : quantum yield of level 2, δ : detection efficiency

$\sigma_{12}(\nu - \nu_{12}) = B_{12}(\nu_0).\, g_D(\nu - \nu_{12}).\, h\nu_0/c$

$B_{12}(\nu_{12}) = (1/6\varepsilon_0\hbar^2)\, \langle 1|\mu_{12}|2\rangle^2$

$1 = |\alpha'', J'', M''_J\rangle$

$2 = |\alpha', J', M'_J\rangle$

$$\nu_{12} = \nu_0 + \frac{g'_{J'} M'_{J'} \mu_B \,\mathrm{B}}{J'(J'+1)} - \frac{g''_{J''} M''_{J''} \mu_B \,\mathrm{B}}{J''(J''+1)}$$

parameters : σ_{12} , N_1 , g'_J , g''_J , B .

B calibrated (0.5%) with Ar* lines

$g''_{J''}$: constrained to FIR exp. values (J.M. Brown, J. Chem. Phys.,124 (2006)

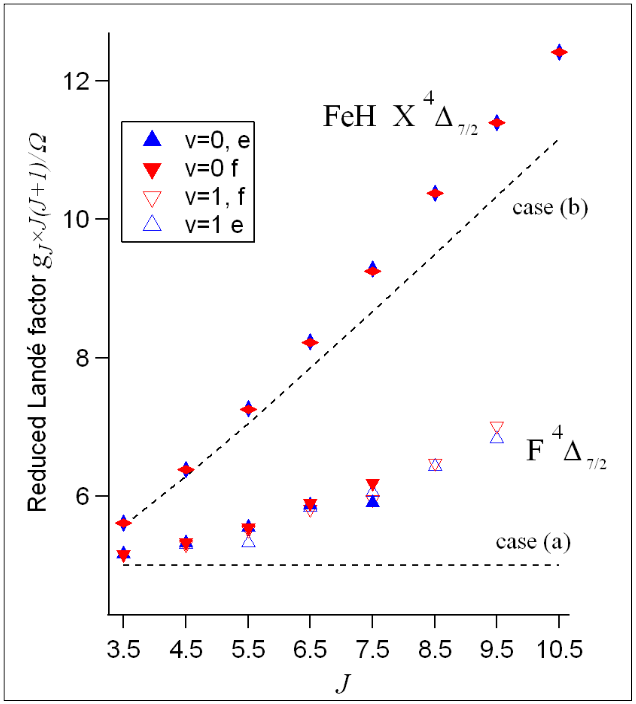
3. Etat de l'Art au labo / **New FeH laboratory Landé factors :**

P. Crozet , G. Dobrev , C. Richard, A. J. Ross, J. Mol. Spectrosc., 303, 46 (2014)

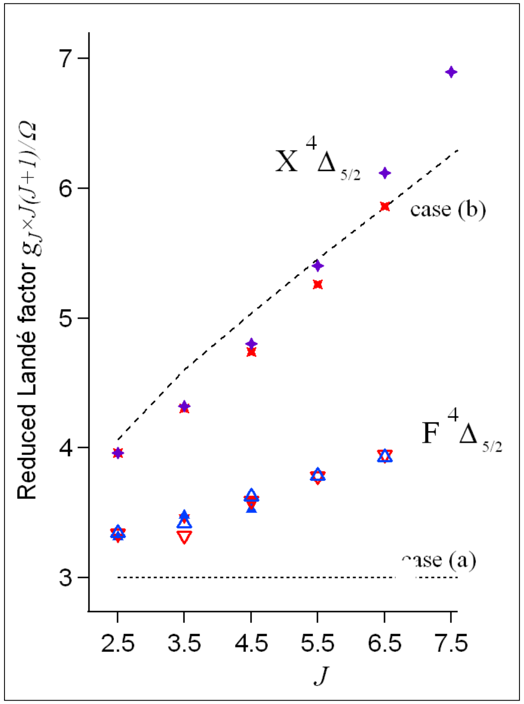
Electronic Landé factors $g_J * J(J+1)/\Omega$

Fit data from B = 0.2-0.6 T, and examine results for two nominally $^4\Delta$ states

X, *F* $^4\Delta$ Ω =7/2



X, *F* $^4\Delta$, Ω = 5/2



X : v=0 from LMR results of Brown, Evenson et al JCP, 124, 234309 (2006)

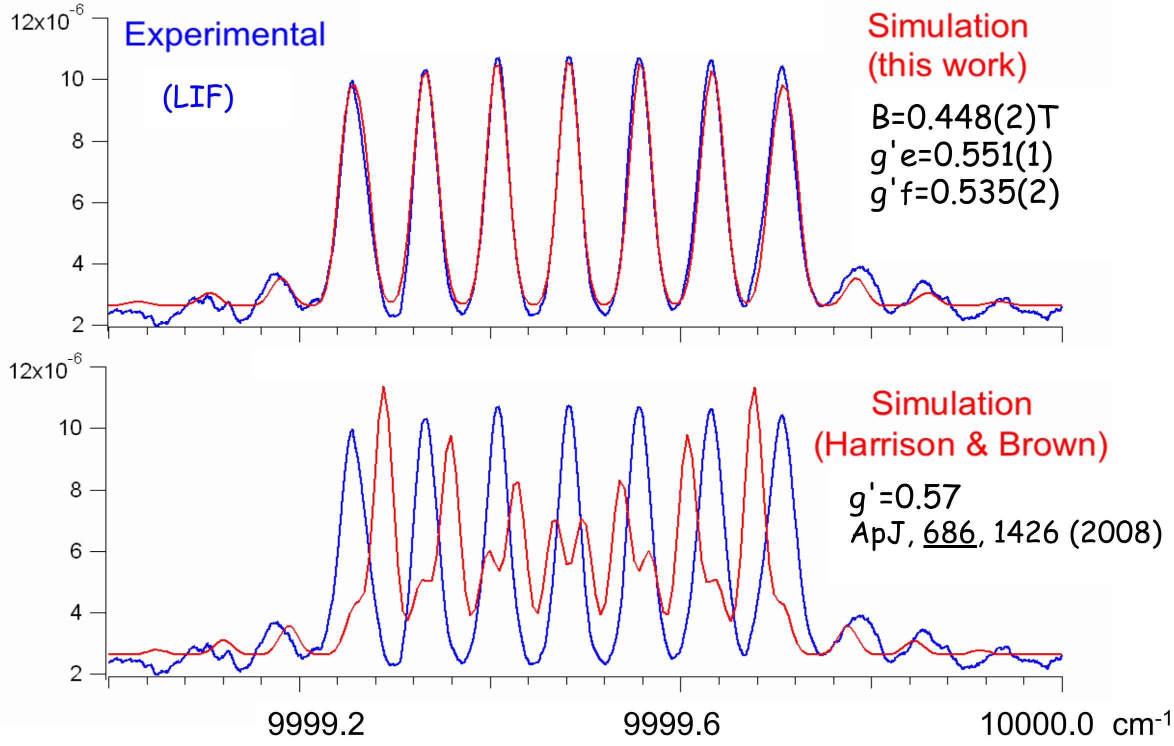
***F* : Match** for v=1, J=3.5 from molecular beam study (Harrison *et al.* ApJ 679 854 (2008)

Mismatch ~4% wrt sunspot-derived g-factors Harrison & Brown, ApJ, 686 1426 (2008)

3. Etat de l'Art au labo / **Does a 4% difference in g'_J really matter?**

Previous Landé factors were deduced from molecular simulation of sunspot data, using Zeeman splittings of Ti lines to calibrate the local magnetic flux *B* .

F-*X* (0,0) R(4.5), σ polar



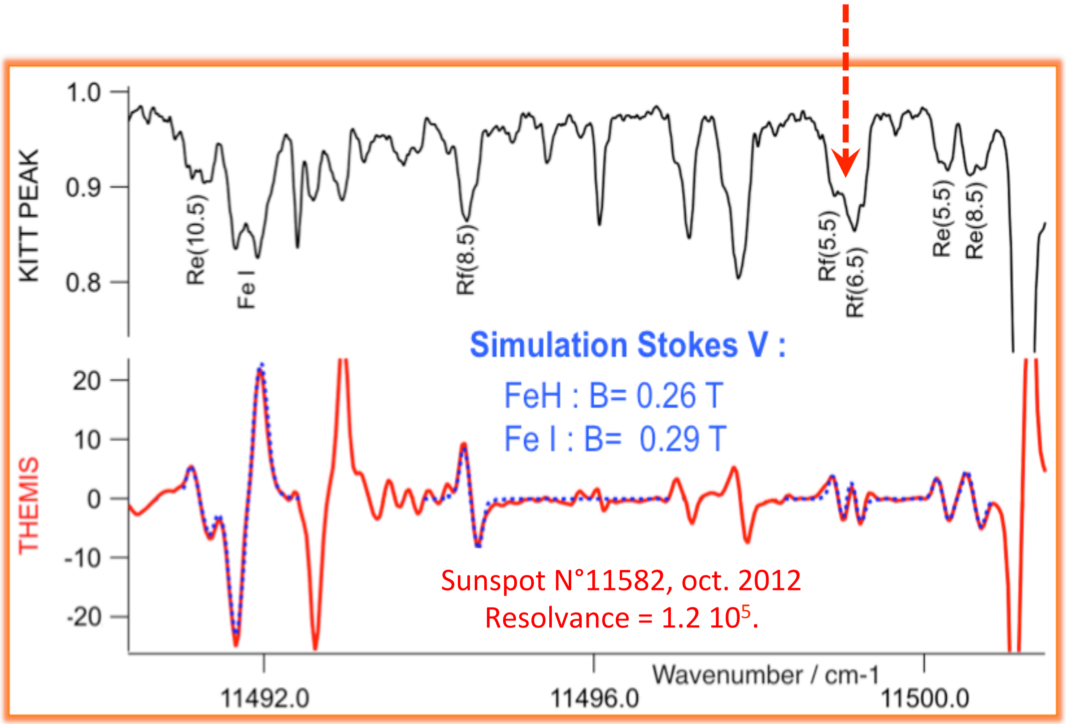
B=0.448(2)T
g'e=0.551(1)
g'f=0.535(2)

g'=0.57
ApJ, 686, 1426 (2008)

uncertainty in sunspot magnetic flux *B* may explain previous overestimation of *F* state Landé factors.

3. Etat de l'Art au labo / **Application to sunspots**

Our new Landé factors involve also the spin-orbit component F_2 (1-0) Ω=5/2...



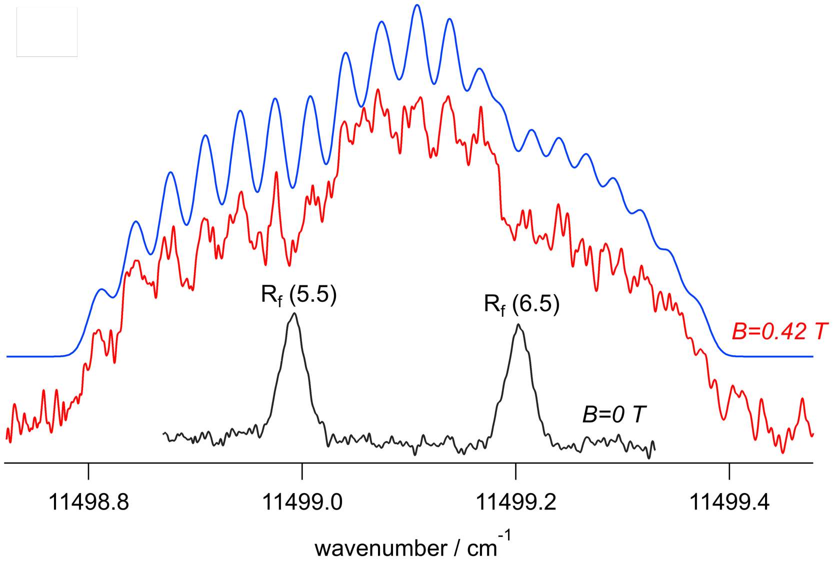
Simulation Stokes V :

FeH : B= 0.26 T

Fe I : B= 0.29 T

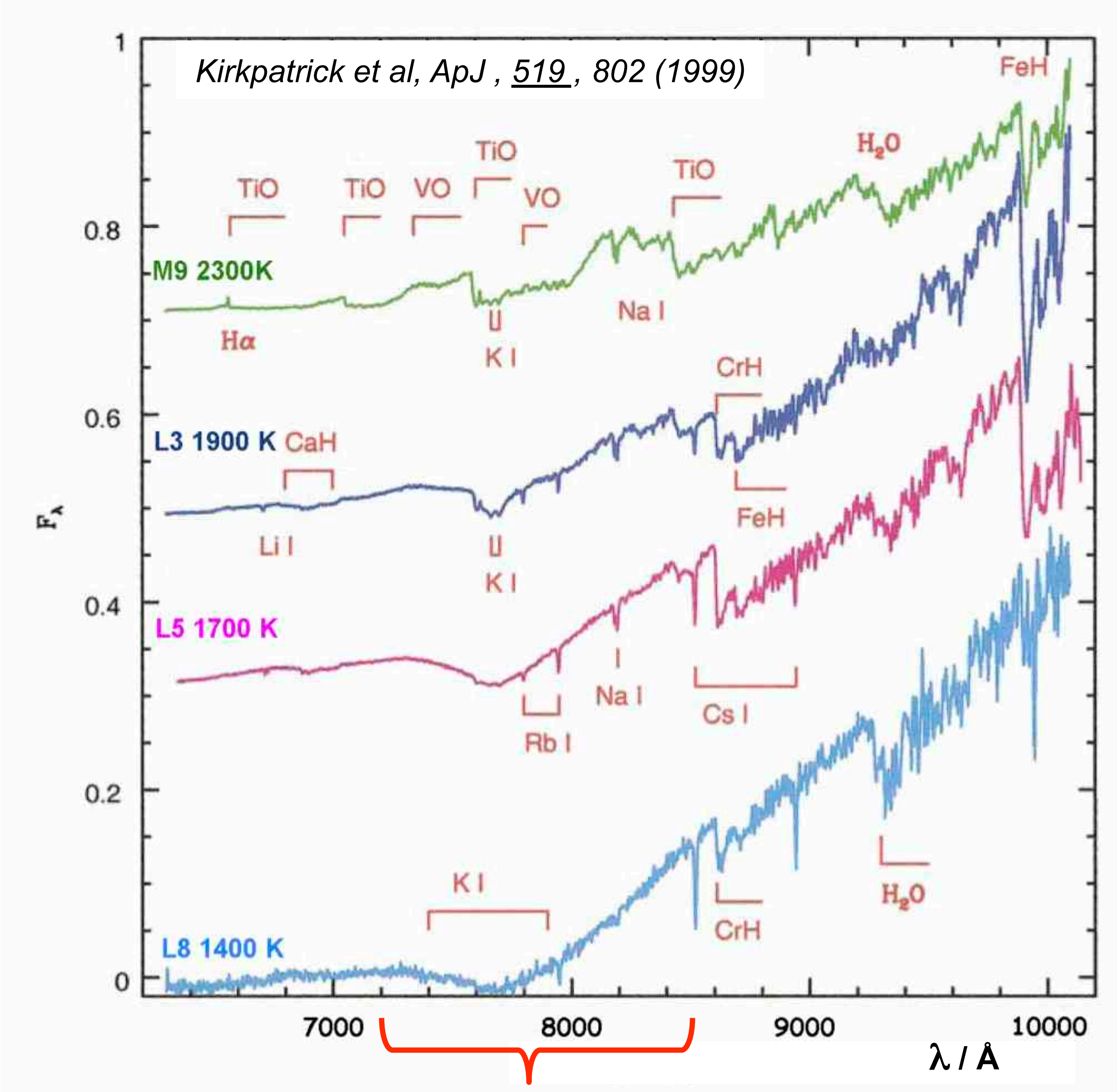
Sunspot N°11582, oct. 2012

Resolvance = 1.2 10^5.



P. Crozet, A. J. Ross, N. Alleq, A. López Ariste, C. Le Men and B. Gelly,
Magnetic Fields throughout *Stellar Evolution*,
Proc. IAU Symposium 302 (2013)164-165, I.A.U. 2014, P. Petit, M. Jardine & H. Spruit, eds.

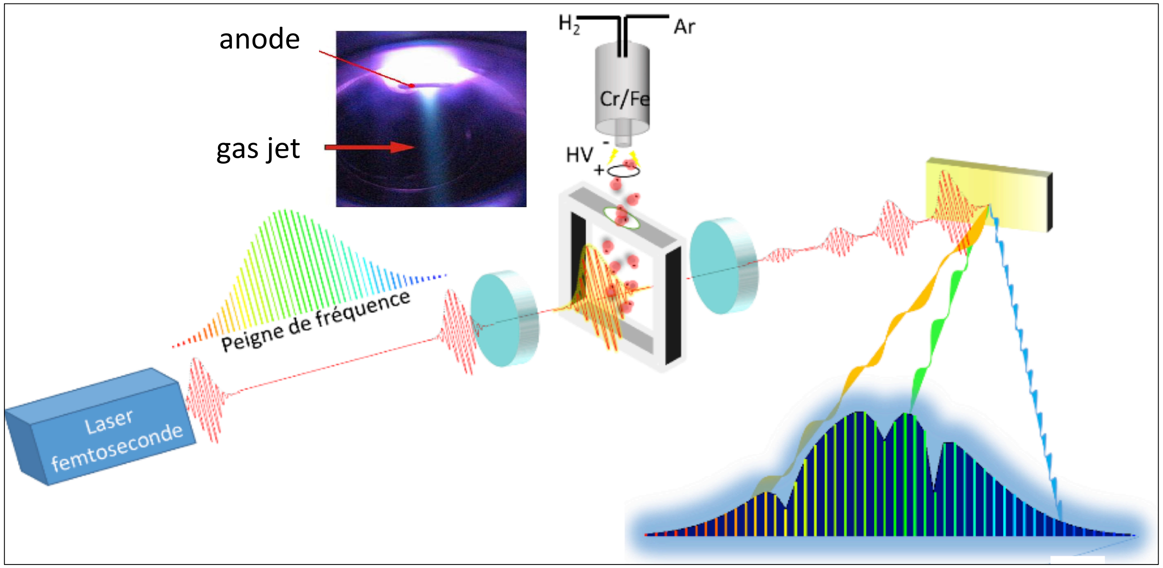
4.Projet en cours/ **Nouvelle approche instrumentale**

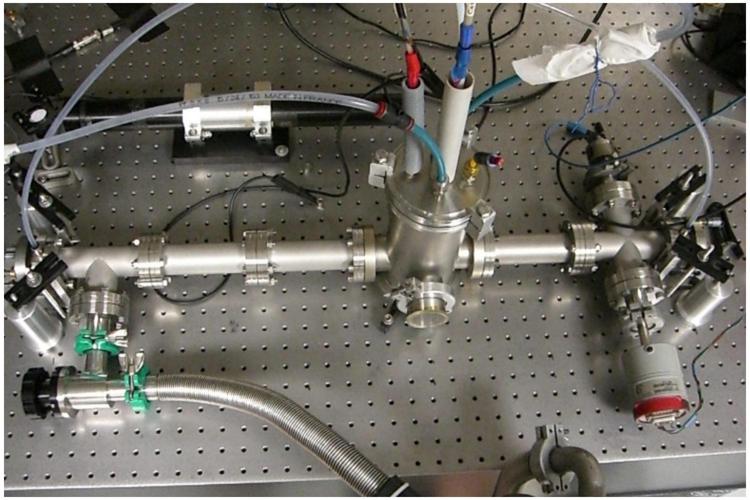


Expérience peigne de fréquence / cavité optique

4.Projet en cours/ **Spectromètre Vernier**

L. Rutkowski & J. Morville, Opt. Lett. 39 (23), 6664 (2014)

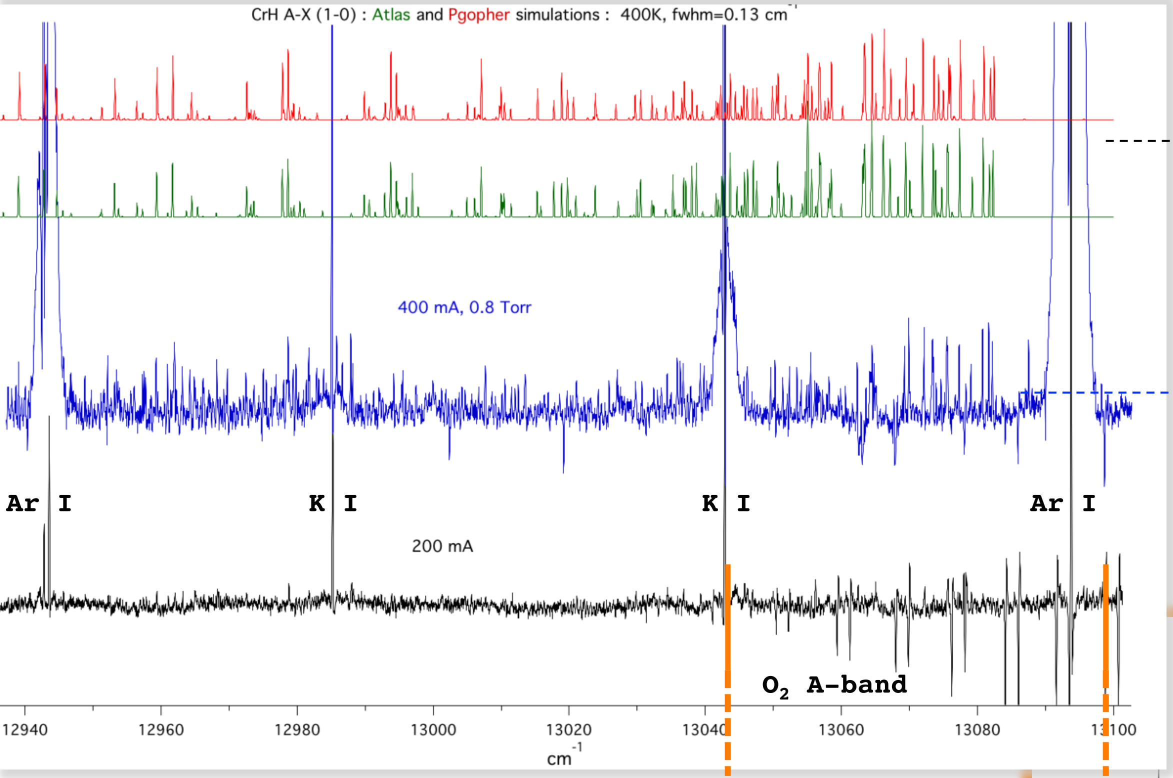




Avantages :

- fenêtre d'enregistrement : 20 THz (40 nm @780 nm)
- sensibilité : détection intracavité L_{eq} ~ 400 m.
- résolution : $\mathcal{F}_V = \mathcal{F}_C = FSR_C/\Gamma_C$
- échantillonnage rapide : 100 spectres moyennés en 1s.

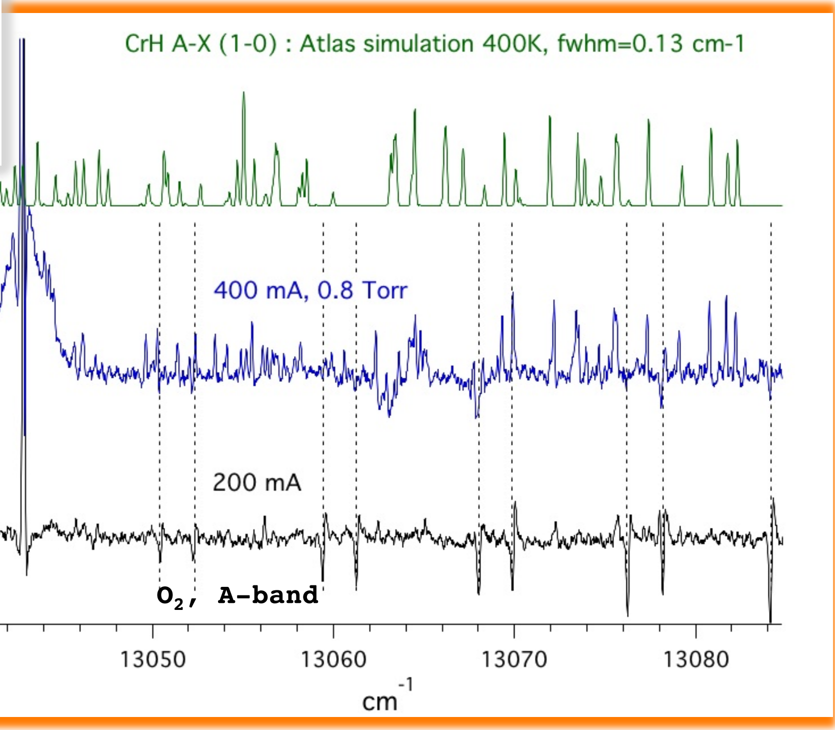
4/ Résultats préliminaires : CrH $A\ {}^6\Sigma^+$-$X\ {}^6\Sigma^+$ (1-0)



Simulations CrH : Atlas et Pgopher :
400 K, fwhm=0.13 cm^{-1}

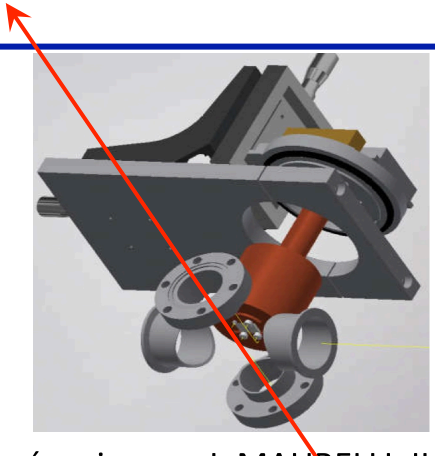
Paramètres d'enregistrement :

- flux gazeux Ar + H_2 5% : 50 sccm @ 0.8 Torr
- décharge plasma : 400 mA , 250 V_{DC}.



^{52}CrH détecté dans la bande *A*-*X* (1-0) à 764 nm, **10 fois plus faible que la bande (0-0)** vers 861 nm observée dans les spectres de naines brunes.

4.Conclusion / **perspectives**



mécanique : J. MAURELLI, ILM

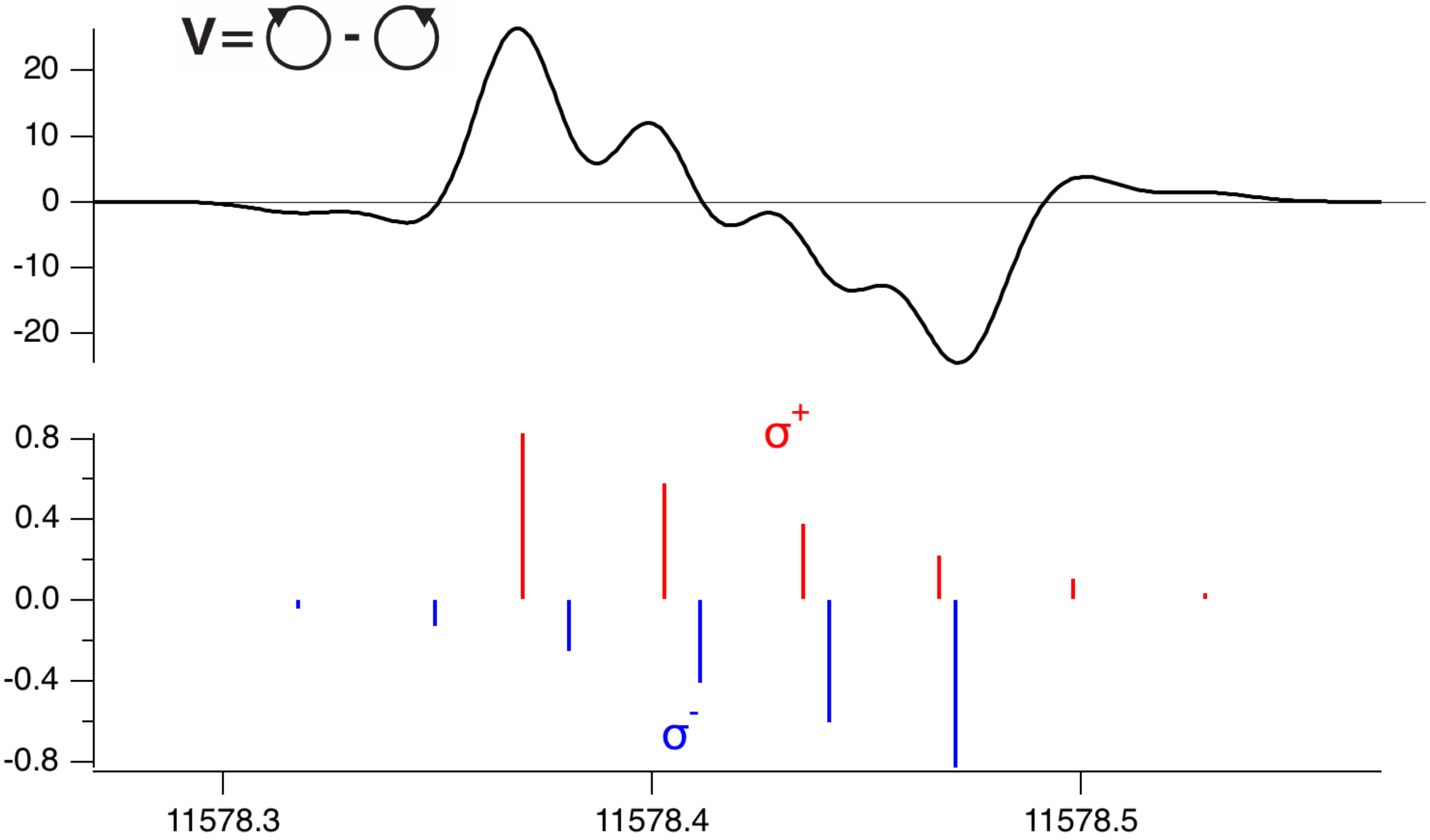
- **Source MH en construction (financement PNPS 2016) :**
  - décharge / fente-source : longueur d'absorption ↗
  - réglages micrométriques de la tête-cathode : signal optimal.

- **Enregistrement des spectres d'absorption /Spectromètre Vernier**

Objectifs : - Spectres d'absorption large bande de CrH 0-0 et 1-0 @B=0 et B<0.6 T à résolution Doppler (0.002 nm) → nouvelle cavité.
- accès aux grands J (≈20.5), grâce à une sensibilité accrue (*).
- mesure des réponses magnétiques σ^+, σ^-, π.

(*) **Défis pour augmenter la sensibilité :** - élimination des franges (*etalonning* de cavité)
- bande passante de l'asservissement (AOM shifter)
- caractériser la fonction d'appareil du spectromètre.

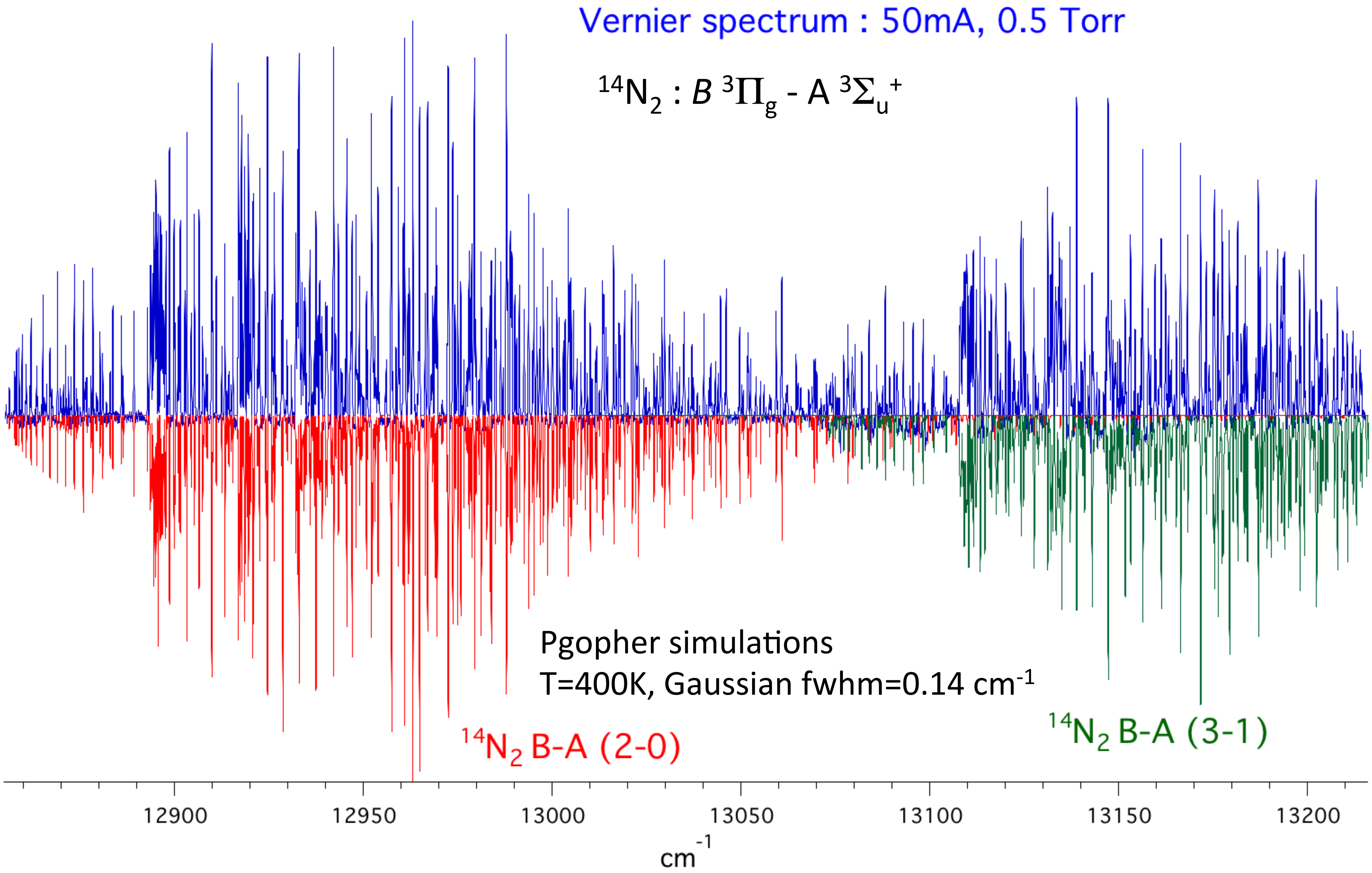
5.Conclusion / Autre défis : **simulations de CrH**



Simulation moléculaire *Pgopher*

CrH $^{r}R_4(2.5)$: B=0.2 T, $\text{fwhm}_{\text{Gauss}}$=0.024 cm^{-1}

Spectre du premier système positif de l'azote moléculaire:



Vernier spectrum : 50mA, 0.5 Torr

$^{14}N_2 : B\,^3\Pi_g - A\,^3\Sigma_u^+$

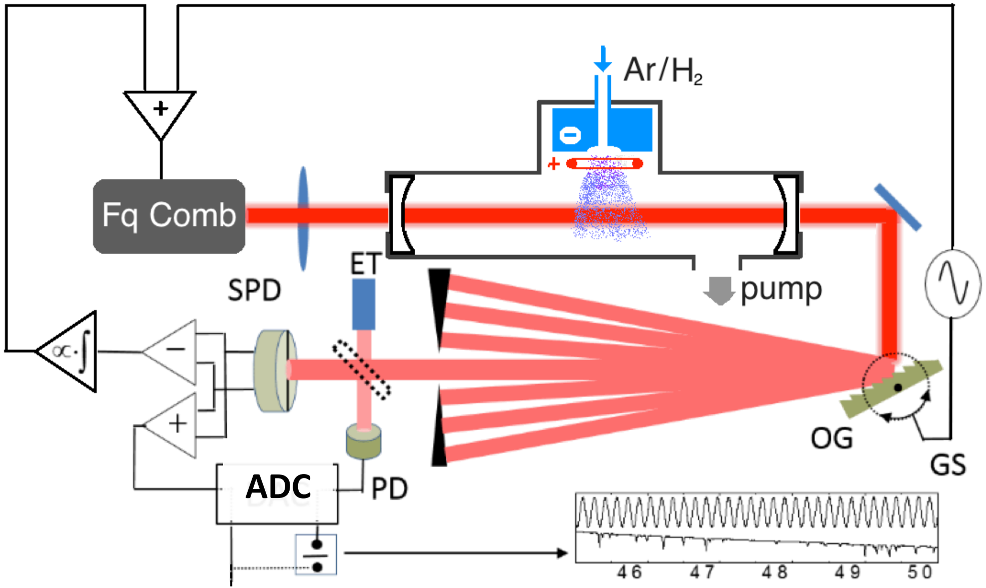
Pgopher simulations
T=400K, Gaussian fwhm=0.14 cm^{-1}

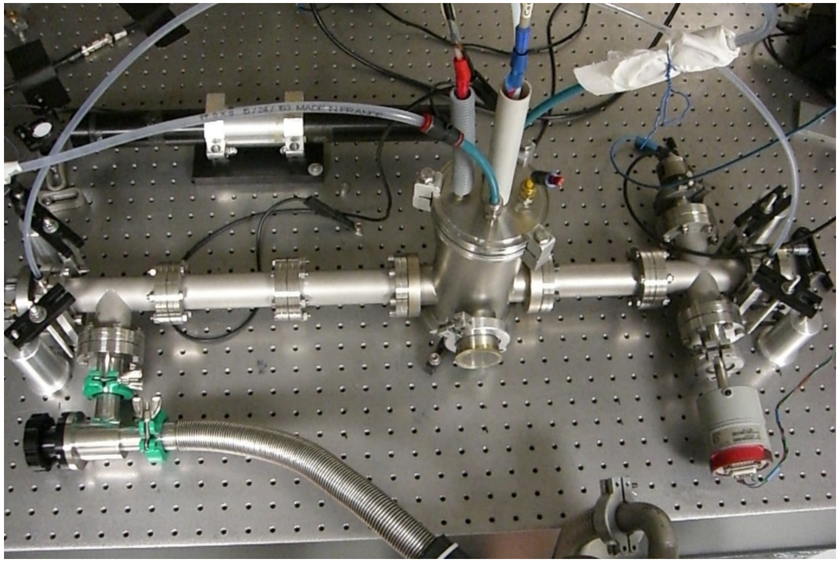
$^{14}N_2$ B-A (2-0)

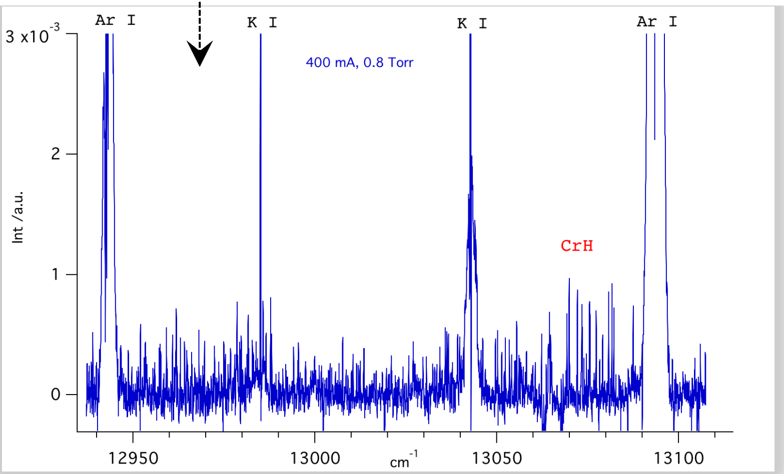
$^{14}N_2$ B-A (3-1)

Spectromètre Vernier : une nouvelle approche instrumentale

L. Rutkowski & J. Morville, Opt. Lett. 39 (23), 6664 (2014)

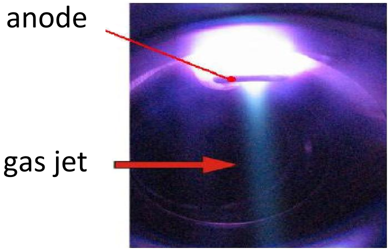




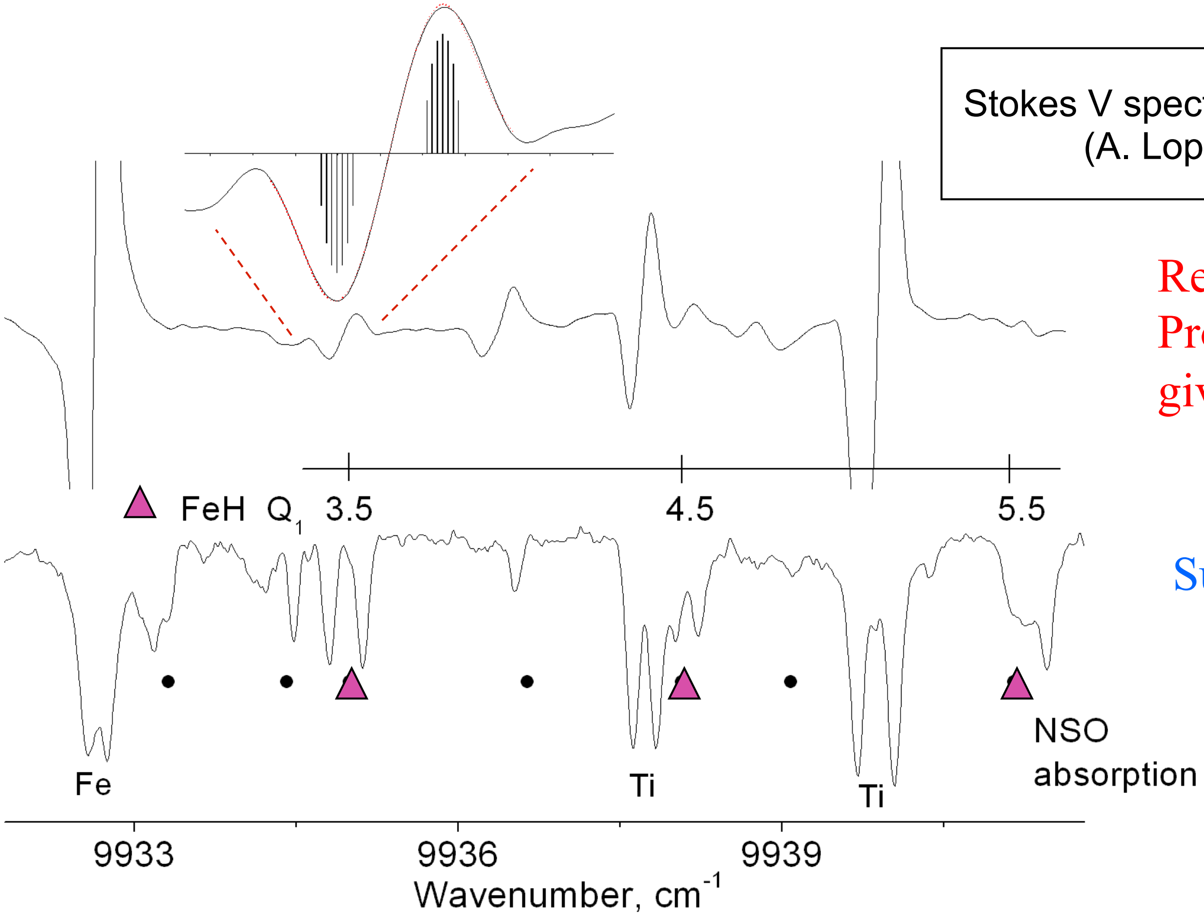


Legend

OG : Optical Grating
GS : Galvo-Scanner
SPD : Split-Photodiode
PD : Photodiode
ET : Etalon (1mm)
ADC : Analog to Digital Converter.



Using our parameters, we can determine the magnetic field for FeH in sunspots



Stokes V spectrum from Themis telescope
(A. Lopez-Ariste, F Paletou)

Res 0.046 cm^{-1}
Profile simulations
give B = 0.22 Tesla

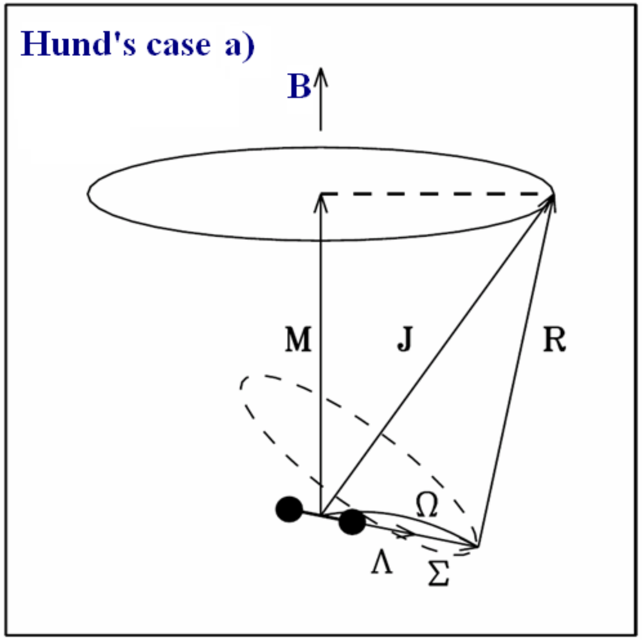
Sunspot Atlas ~ 0.3 T

Dots indicate FeH lines from higher spin components

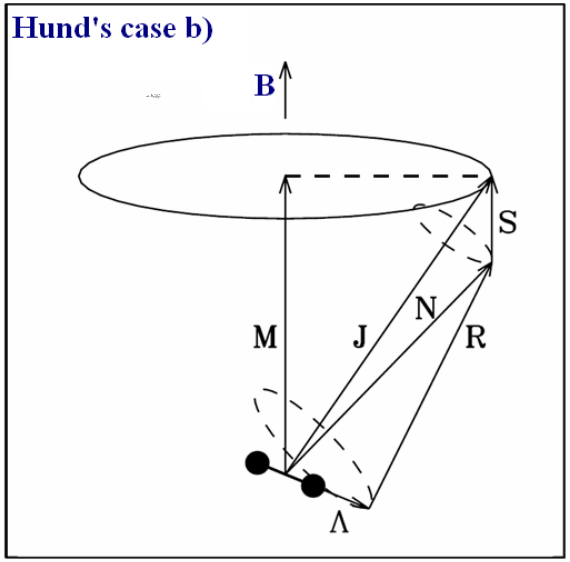
FeH Landé factors give B = 0.22 Tesla for the Themis spectrum.
Atomic lines give B = 0.25 T. Molecules are likely formed at higher altitudes.

Aim of this work = find g_J for many J in the F $^4\Delta$ state.

LMR studies (Brown, Evenson & co-workers) established molecular Landé factors are close to Hund's case b) limit for the X $^4\Delta$ ground state. What about F $^4\Delta$?



$$\boxed{\Delta E = \frac{g_J M_J \mu_B \mathrm{B}}{J(J+1)}}$$



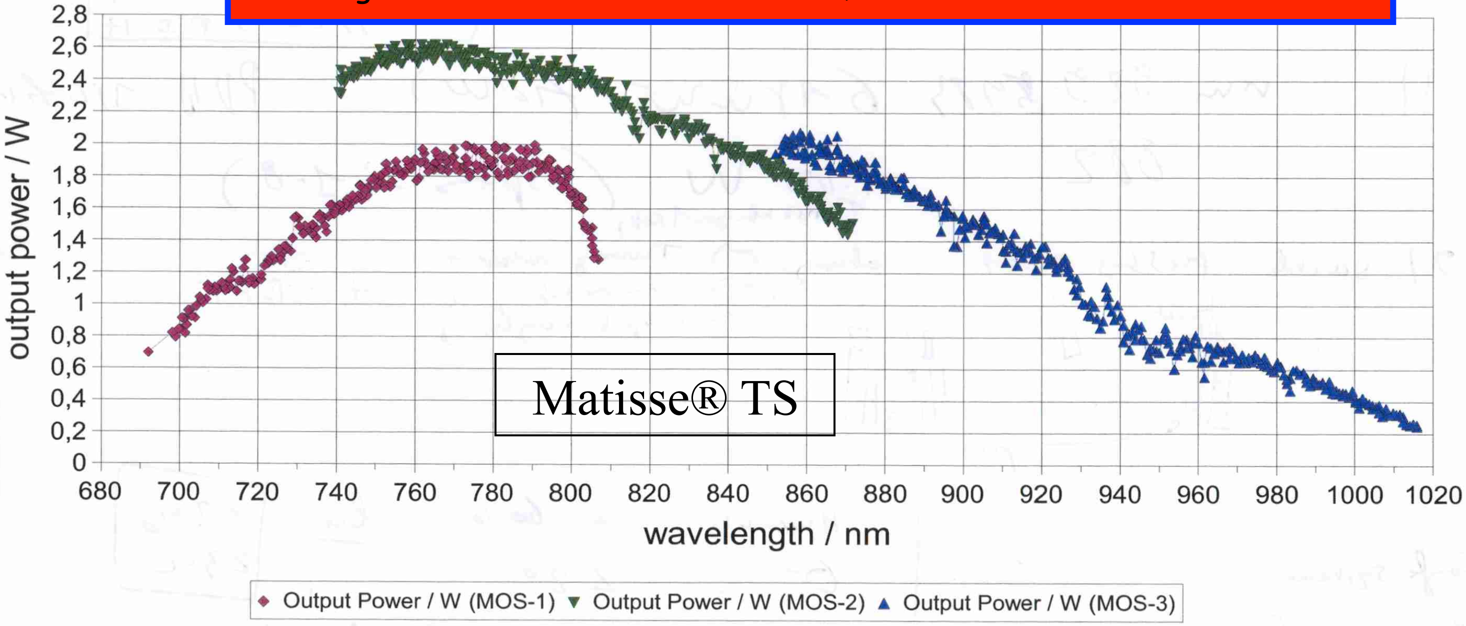
$$\Delta E = \frac{(\Lambda + 2.003\Sigma)\Omega \, M_J \, \mu_B \, \mathrm{B}}{J(J+1)}$$

$$\Delta E = \frac{M_J \mu_B \mathrm{B}}{2J(J+1)} \left[\frac{\mathrm{g_L} \Lambda^2 \left(J(J+1) + N(N+1) - S(S+1)\right)}{N(N+1)} + \mathrm{g_s}\left[J(J+1) - N(N+1) + S(S+1)\right] \right]$$

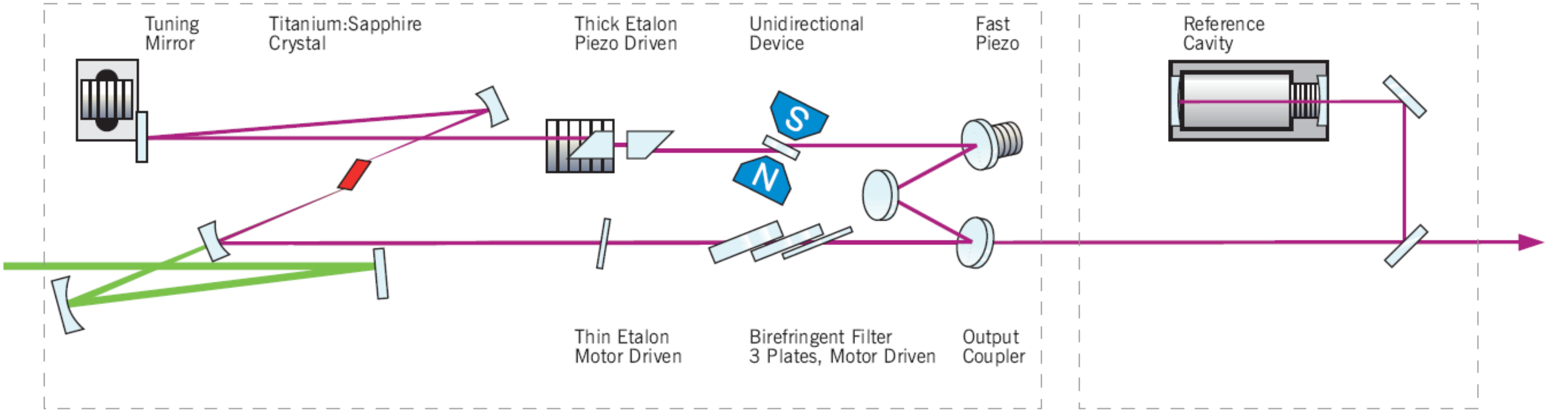
From : S. V. Berdyugina and S. K. Solanki, A&A 385(2002)701

We have now (thanks to ANR) a benchmark cw tunable laser

<u>Specs at FeH *F-X* bands</u> (10W pump @ 532 nm)
(1,0) λ=880 nm : P= 1.8 W ,
(0,0) λ=989 nm : P= 0.6 W
single mode scans : 2 cm^{-1} = 60 GHz, fwhm <150kHz.

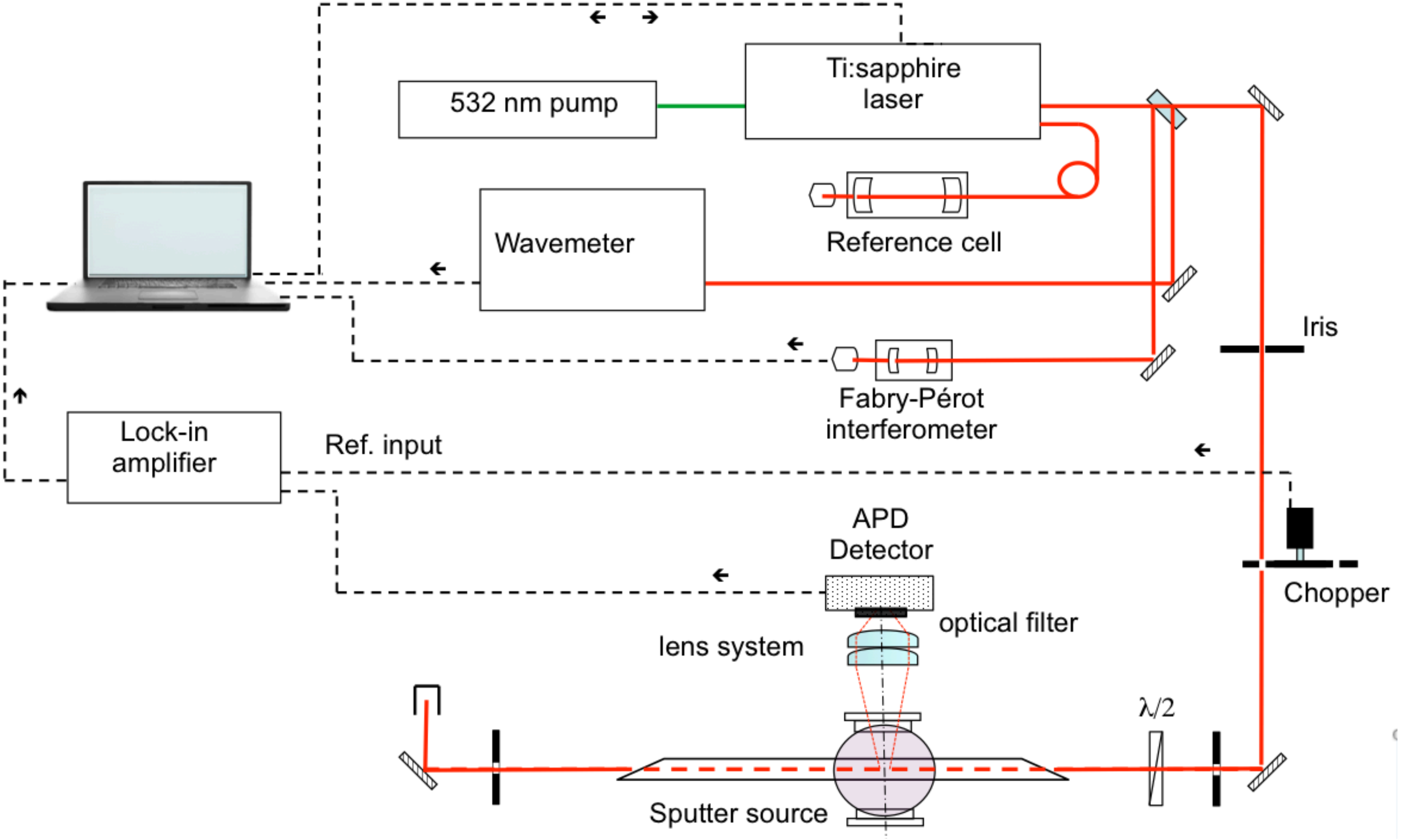


Optical Layout



ANR *LASSA (ILM/IRAP,2009-2011)*

the experimental setup ...

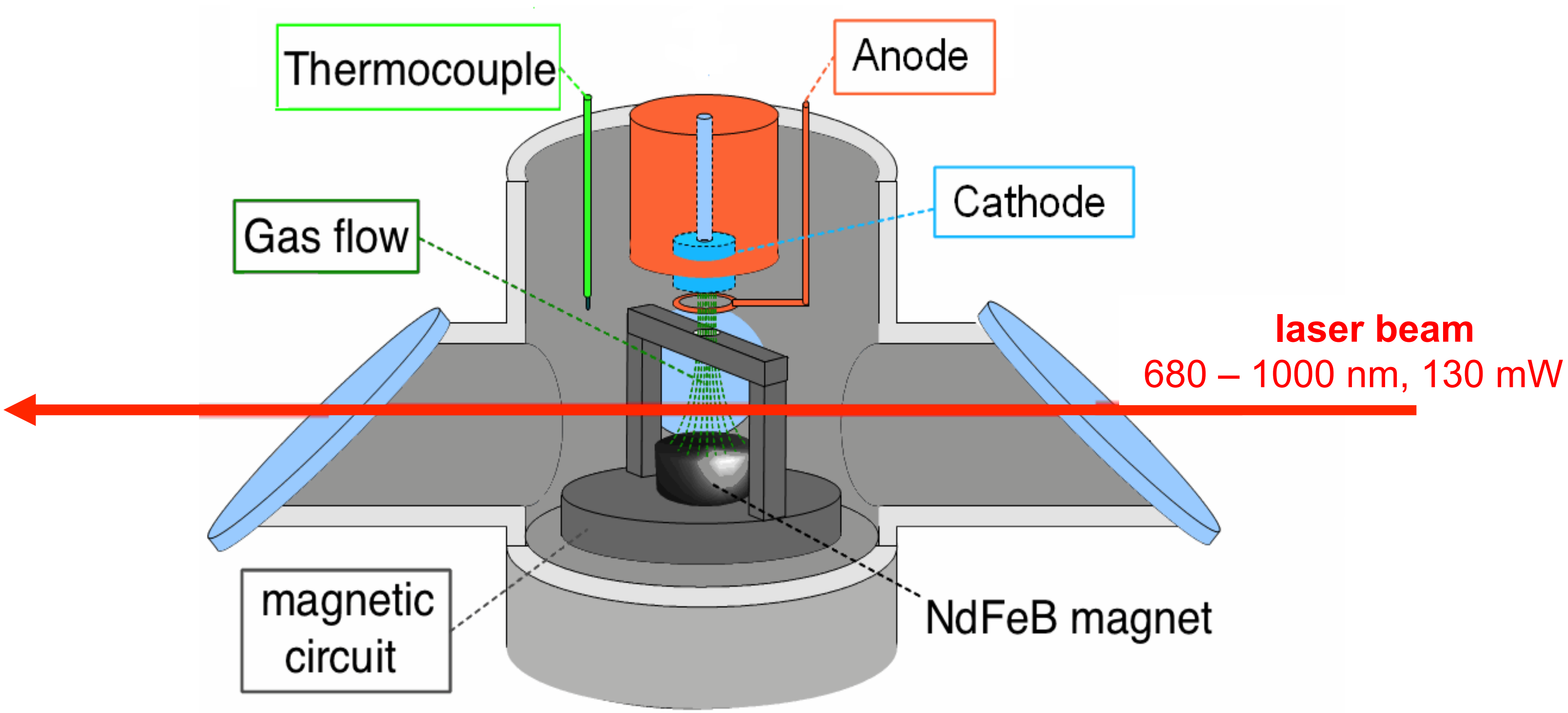


Source à MH

FeH is formed at ~ 400 K, populating J<10.5 in $X\,^4\Delta_{7/2}$ and 8.5 in $^4\Delta_{5/2}$

Sputter source : Fe cathode, located above a permanent magnet.

i=350 mA , gas flow ~ 40 sccm (10% H_2 in argon), p = 1 torr



Magnetic field calibration from Ar* lines

$3s^2\,3p^5\,(^2P^\circ_{3/2})\,4p\;J'=1$

$g' = 1.985$

↑

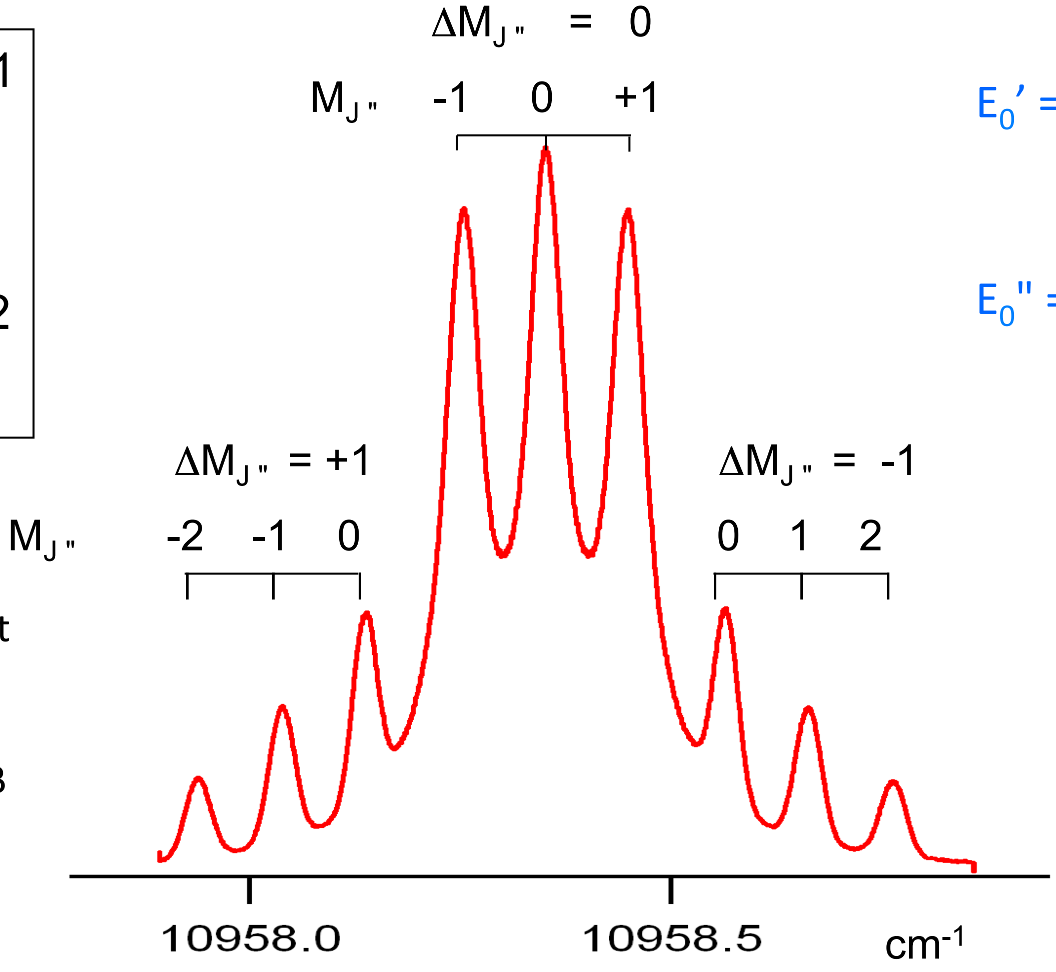
$3s^2\,3p^5\,(^2P^\circ_{3/2})\,4s\;J'=2$

$g' = 1.506$

$E_0' = 104102.099\ \text{cm}^{-1}$

↑

$E_0'' = 93143.770\ \text{cm}^{-1}$

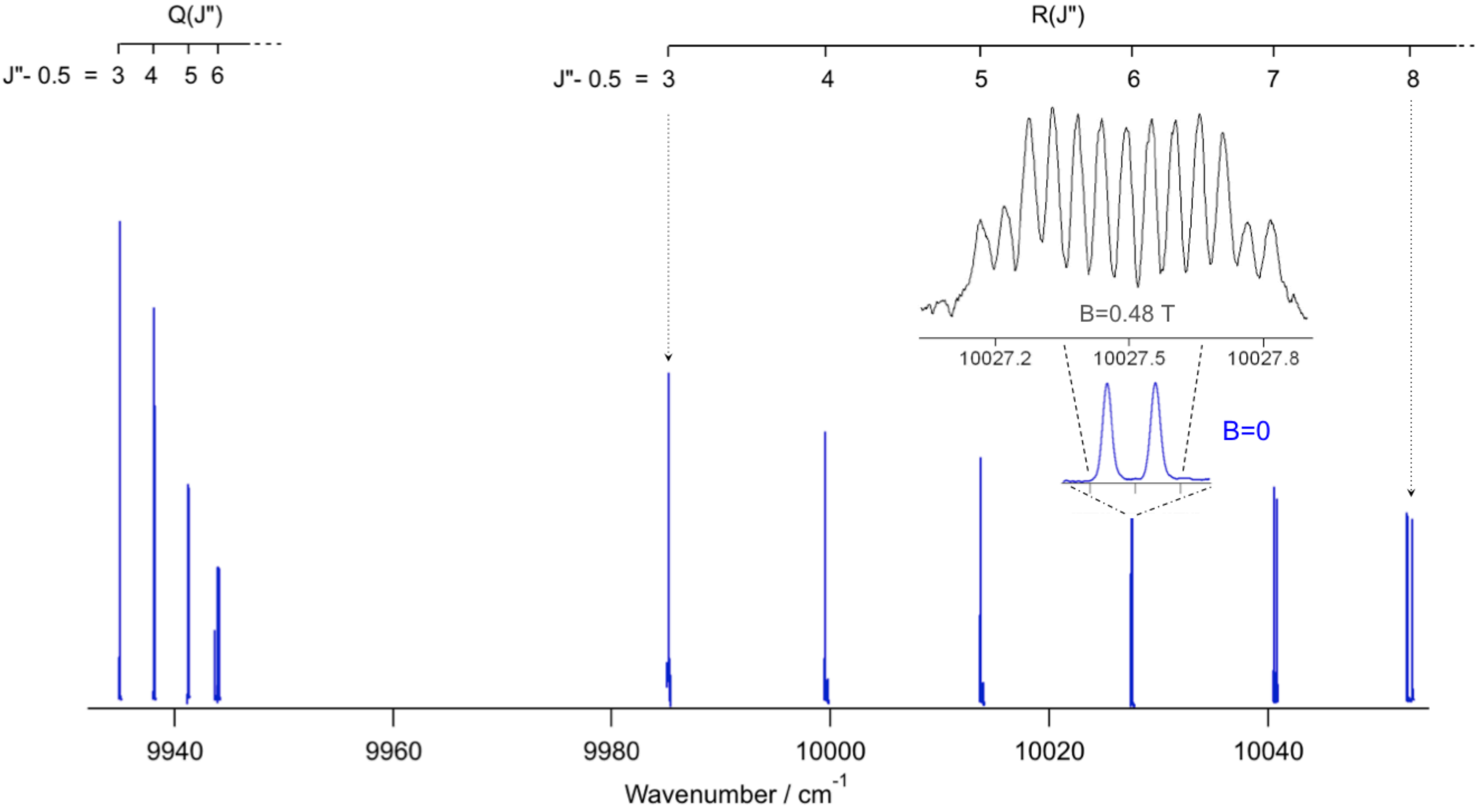


Separations depend on <u>product</u> Field x Landé factor.

Knowing g' and g" we deduce B = 0.443(2) Tesla

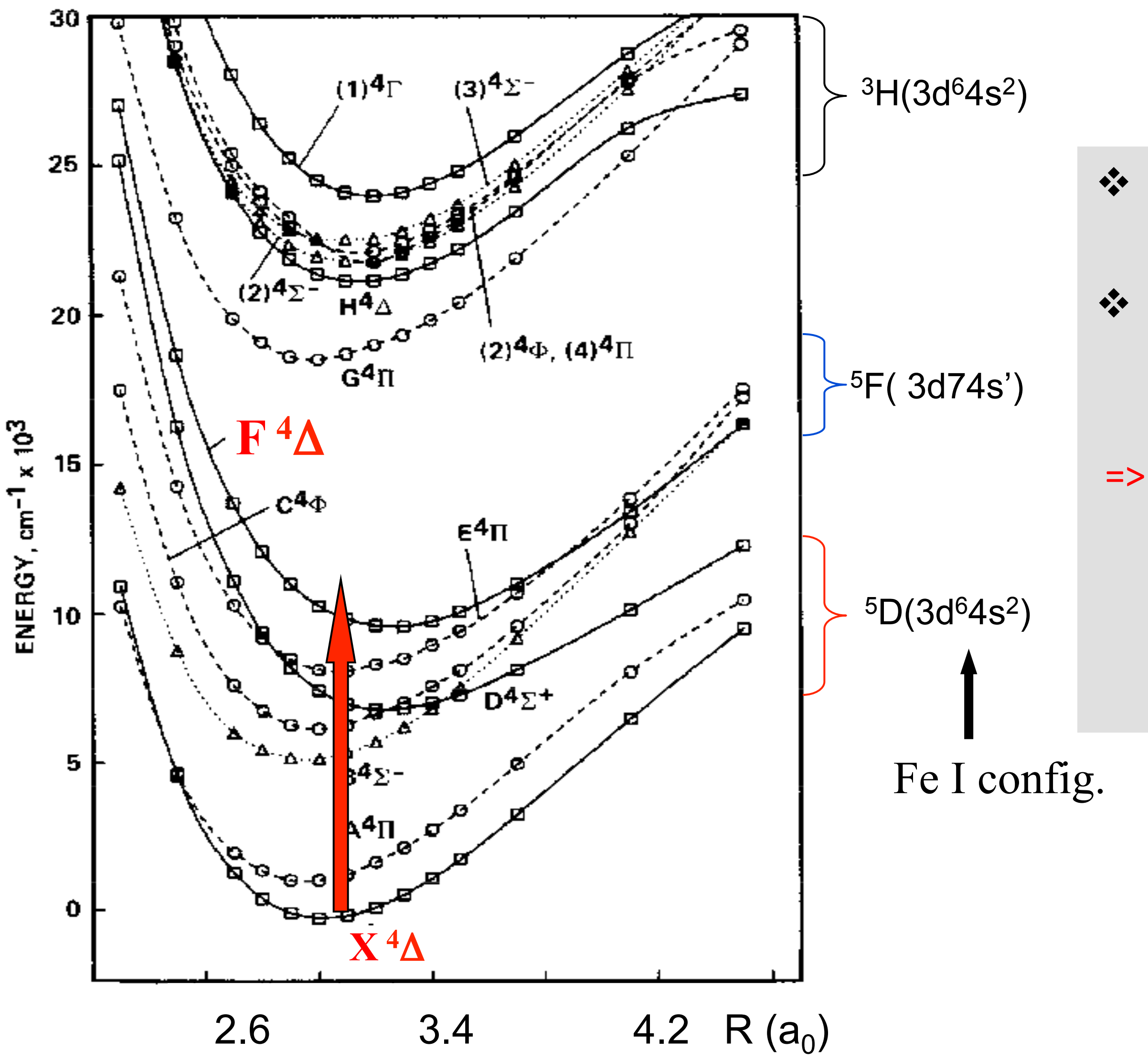
Peak positions can give B in Tesla. PROFILES are important for variation in B.

Wing-Ford band of FeH*: some results*



FeH electronic structure from ab initio calculations

Langhoff & Bauschlicher, *J Mol Spectrosc*. 141, 243-257 (1990)



❖ 6 electronic states have been identified within 5000 cm^{-1} of the ground state;

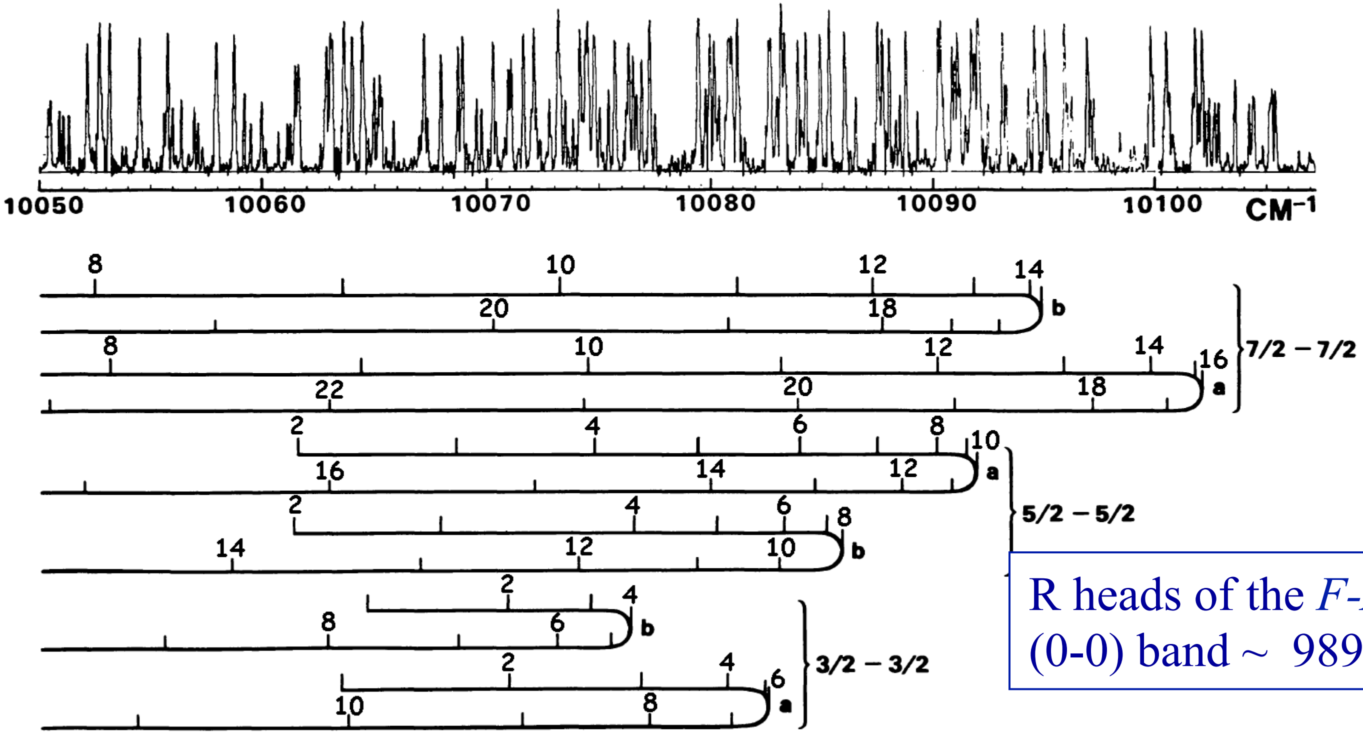
❖ the A state lies only 970 cm^{-1} above the X state, while the first vibrational level at 1759 cm^{-1}.

=> Born-Oppenheimer approximation fails.

Calculations are not reliable.

FeH absorption near 1μm (laboratory spectrum, Kitt Peak)

J.G. Phillips *et al*, ApJS, 65 (1975)721, then
M. Dulick et al, ApJ, 594:651–663 (2003), with full linelist available http://bernath.uwaterloo.ca/FeH



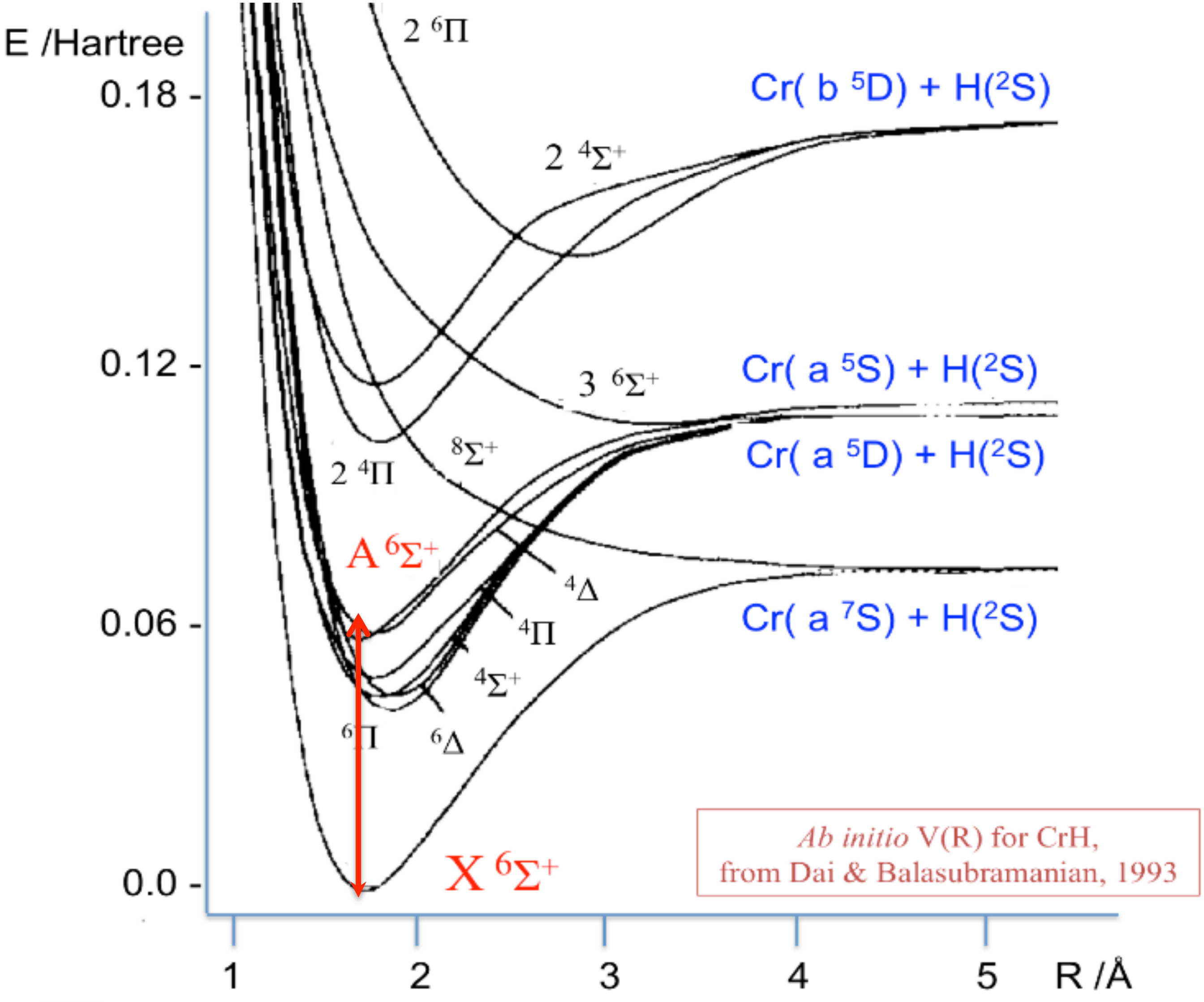
R heads of the F-X $^4\Delta_i$- $^4\Delta_i$ (0-0) band ~ 989.6 nm

Source : King furnace (2200-2450 °C) , $\delta\sigma_D$ = 0.05 cm^{-1}
FTS : McMath telescope , NSO at Kitt Peak

We rely completely on this analysis, but we need improved wavenumber accuracy and resolution, to distinguish Zeeman splittings from Λ doubling

CrH electronic structure from ab initio calculations

Langhoff & Bauschlicher, *J Mol Spectrosc*. 141, 243-257 (1990)



Ab initio V(R) for CrH,
from Dai & Balasubramanian, 1993

A $^6\Sigma^+$

$1\sigma^2\ 2\sigma^1\pi^2\delta^2$ (49%)

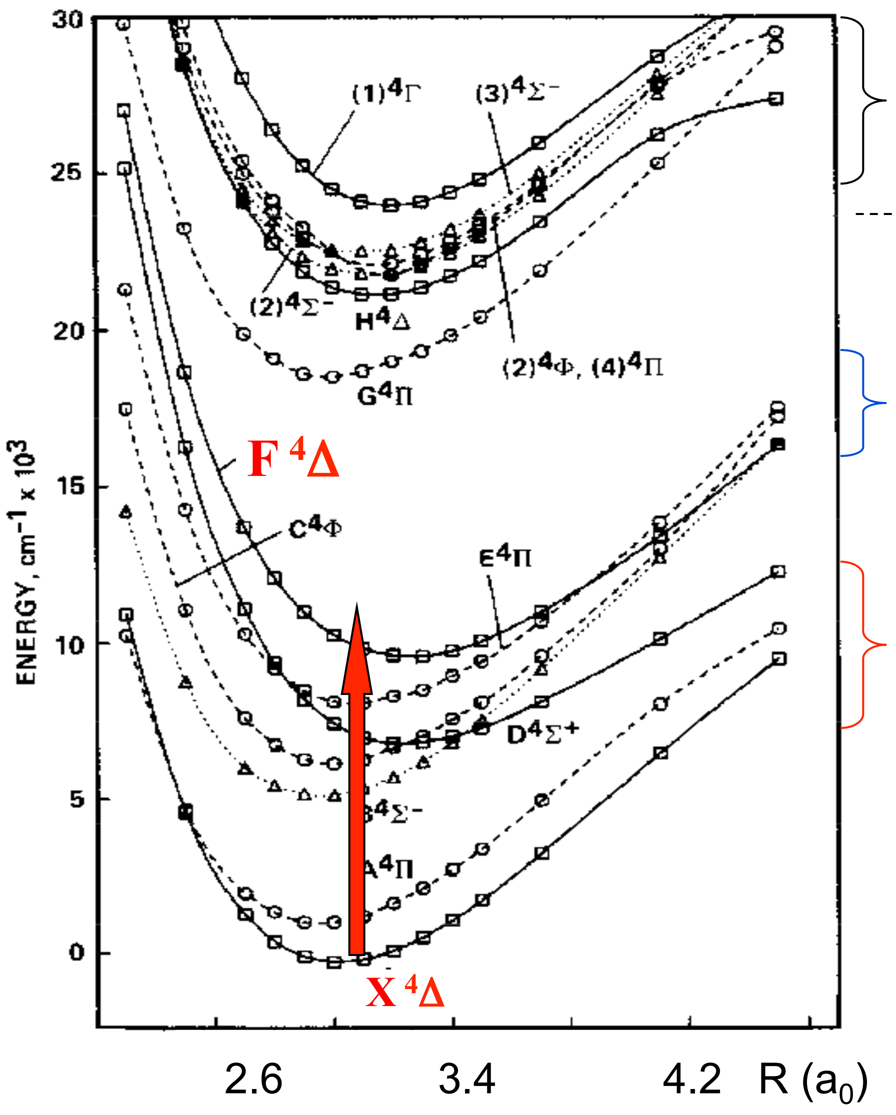
+ …

X $^6\Sigma^+$

$1\sigma^2\ 2\sigma^1\pi^2\delta^2$ (92%)

FeH electronic structure from MRCI calculations

Langhoff & Bauschlicher, *J Mol Spectrosc*. 141, 243-257 (1990)



^{3}H(3d^{6}4s^2) $^4\Gamma$, $^4\Phi$, $^4\Delta$, (2x) $^4\Pi$ and (2x) $^4\Sigma^-$

(3d^{6}4s^1) ^{6}D 4p^1

$^6\Phi$, $^6\Delta$, b $^6\Pi$, and $^6\Sigma^-$ states (not shown)

^{5}F(3d74s') B $^4\Sigma^-$,C $^4\Phi$, E $^4\Pi$, and F $^4\Delta$ states

^{5}D(3d^{6}4s^2) X $^4\Delta$, A $^4\Pi$, and D $^4\Sigma^+$ states

and

a $^6\Delta$, b $^6\Pi$, and c $^6\Sigma^+$ states (not shown)

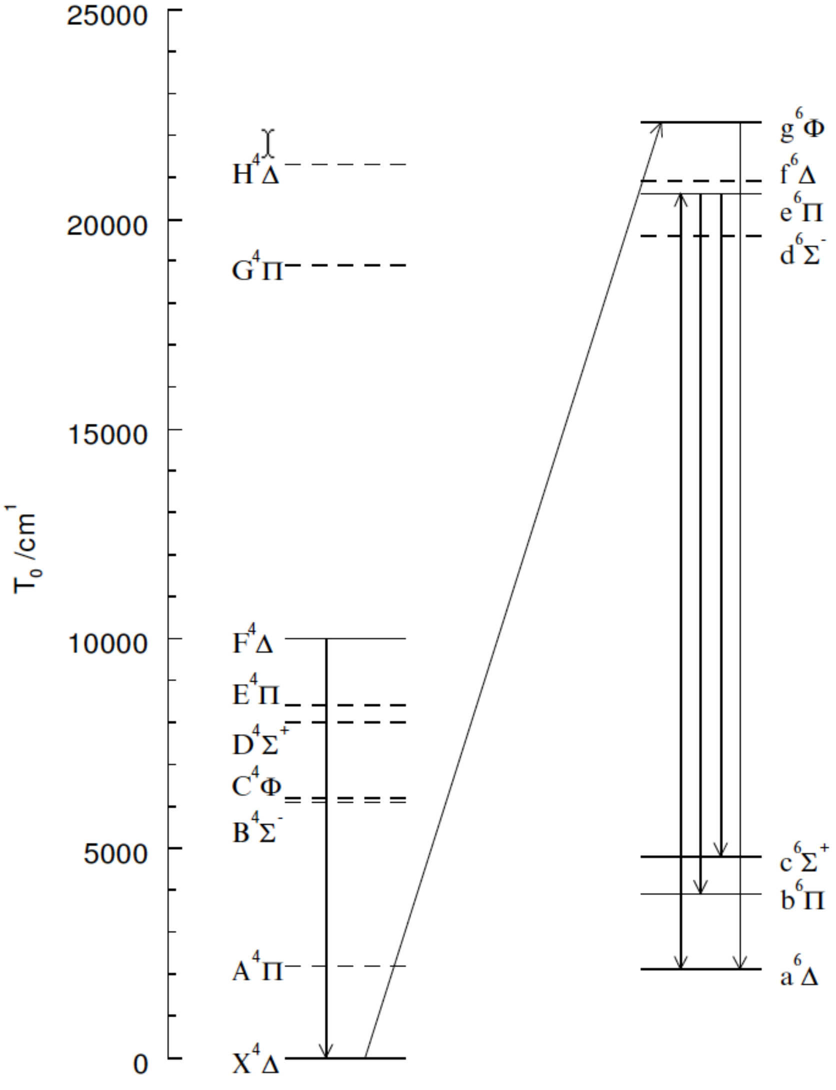
Fe I config.

Difficult spectrum !

But F $^4\Delta$ ← X $^4\Delta$ has been "sorted out"

FeH electronic energy diagram

D.F.Hullah et al, Mol. Phys., 97(1),93 (1999)



Diatomics with transitions in the optical & near IR
Zeeman → PBE

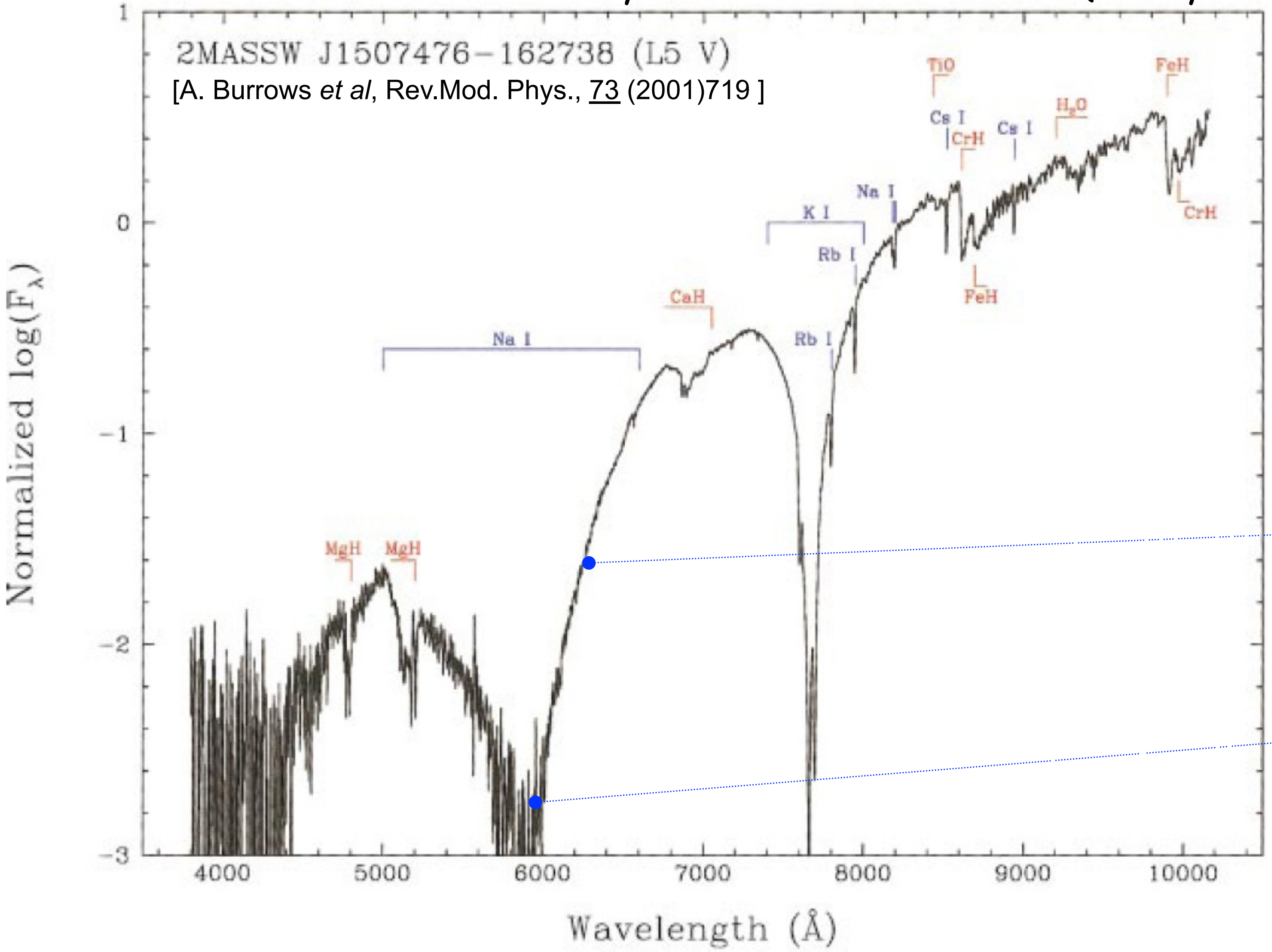
	State	Mult. split.$^{(1)}$ (cm^{-1})	Rot. split.$^{(1)}$ (cm^{-1})	Mag. field$^{(2)}$ (G)	Hund's case
TiO	$X^3\Delta$	96	2.2	4.7×10^4	a
	$A^3\Phi$	170	3.1	6.6×10^4	a
	$B^3\Pi$	16	1.0	2.1×10^4	a–b$^{(3)}$
	$C^3\Delta$	90	2.0	4.3×10^4	a
	$a^1\Delta$	-	3.2	6.9×10^4	a
	$b^1\Pi$	-	2.0	4.3×10^4	a
	$c^1\Phi$	-	4.2	9.0×10^4	a
C_2	$a^3\Pi$	15.3	3.3	7.1×10^4	a–b
	$d^3\Pi$	16.9	3.5	7.5×10^4	a–b
CH	$X^2\Pi$	27.9	57.6	6.0×10^5	b
	$A^2\Delta$	2.0	89.4	4.3×10^4	b
OH	$X^2\Pi$	139	56.7	1.2×10^6	a–b
	$A^2\Sigma$	0.1	34.8	2100	b
CN	$X^2\Sigma$	0.0036	3.8	77	b
	$A^2\Pi$	52.6	26.1	5.6×10^5	a–b
	$B^2\Sigma$	0.0078	3.9	167	b
MgH	$X^2\Sigma$	0.013	11.6	280	b
	$A^2\Pi$	35.3	7.8	1.7×10^5	a–b
	$B'^2\Sigma$	…$^{(4)}$	12.4	…$^{(4)}$	b
CaH	$X^2\Sigma$	0.022	8.6	470	b
	$A^2\Pi$	79	12.9	2.8×10^5	a–b
	$B^2\Sigma$	0.0069	8.6	148	b
FeH	$^4\Delta$	191	19.5	4.1×10^5	a–b
	$^4\Delta$	214	17.5	3.7×10^5	a–b

S. V. Berdyugina and S. K. Solanki, A&A 385, 701-715 (2002)

band	system	ν_{00} / cm^{-1}
α	C-X	19334.03, 19343.66, 19341.68
β	c-a	17840.6
γ	A-X	14163.00, 14095.88, 14019.43
γ'	B-X	16066.7, 16151.6, 16226.4
δ	b-a	11272.82
ε	E-X	11871, 11886, 11899
Swan	d-a	19400
Phillips	A-X	8268.16
G	A-X	23200
Meinel	X(Δv)	2243-18950
	A-X	32402.3
	B-X	25797.84 (near UV)
	A-X	(16570-22760)
	B-X	22081
	A-X	19278
	B-X	15754.9
	A-X	14430.39
Wing-Ford	$F^4\Delta$-$X^4\Delta$	9929, 10026, 10039, 9984
	$E^4\Pi$-$A^4\Pi$, E-X :	5500-7500

Atomic lines are a bad choice …

L-dwarfs : 1400-2000 K ;
atomic lines collisionally broadened and shifted (mainly alkali atoms)



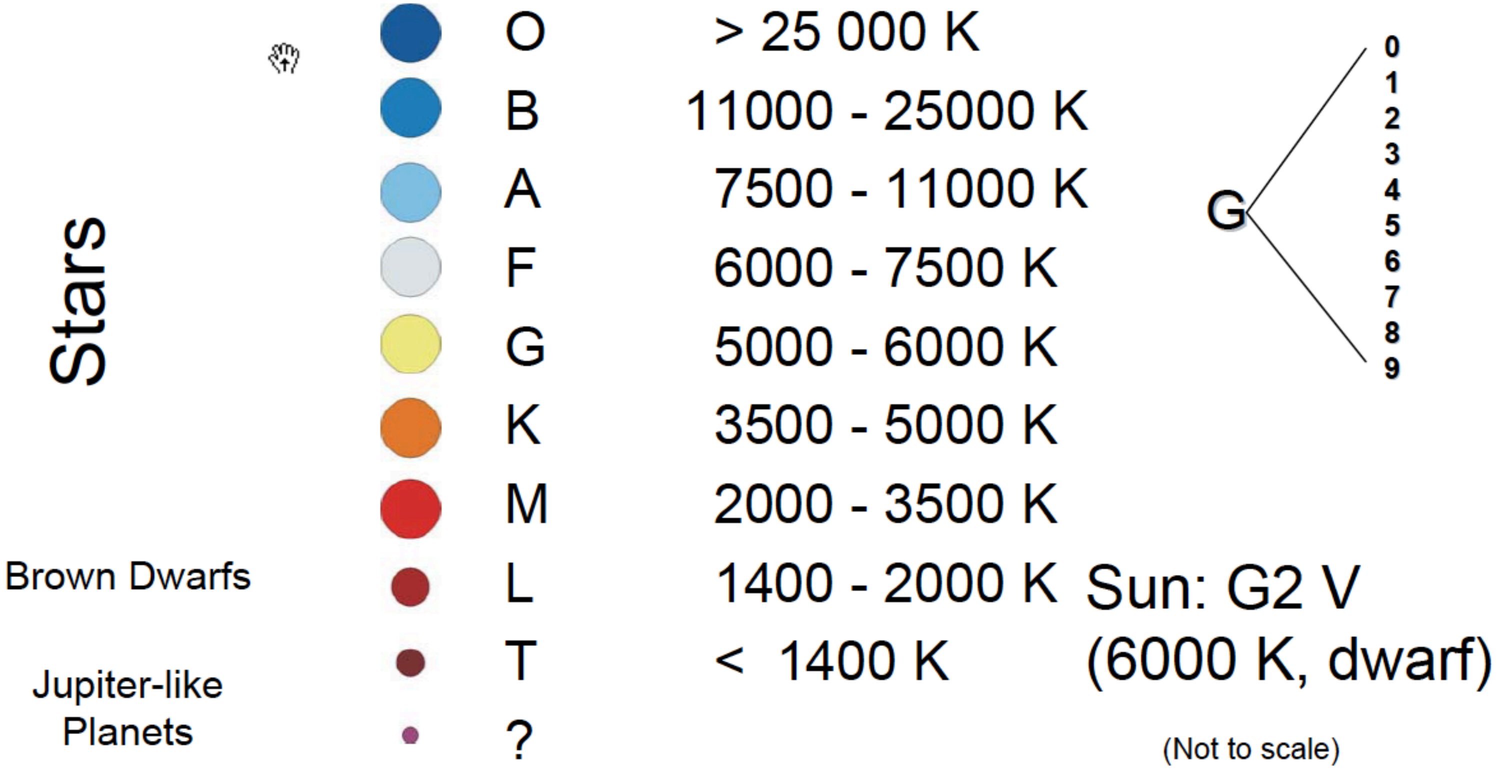
[A. Burrows *et al*, Rev.Mod. Phys., 73 (2001)719]

wings : high p (lower atmosphere)
~ 10-50 bars

cores : low p
(upper atmosphere)
~1 bar

Stellar Spectral Classification System ("normal" oxygen-rich stars)

from P.W. Bernath



Stars	●	O	> 25 000 K
	●	B	11000 - 25000 K
	●	A	7500 - 11000 K
	●	F	6000 - 7500 K
	●	G	5000 - 6000 K
	●	K	3500 - 5000 K
	●	M	2000 - 3500 K
Brown Dwarfs	●	L	1400 - 2000 K
	●	T	< 1400 K
Jupiter-like Planets	●	?	

Sun: G2 V
(6000 K, dwarf)

(Not to scale)

Luminosity (Size): I (Supergiant), II, III (Giant), IV, V (dwarf)