Visible-Optical to near InfraRed (VOIR) emission of electron excited H_2

Evelyne Roueff (1)

Hervé Abgrall (1)

J.M. Ajello (2)

A. Aguilar (2)

R.S. Mangina (2)

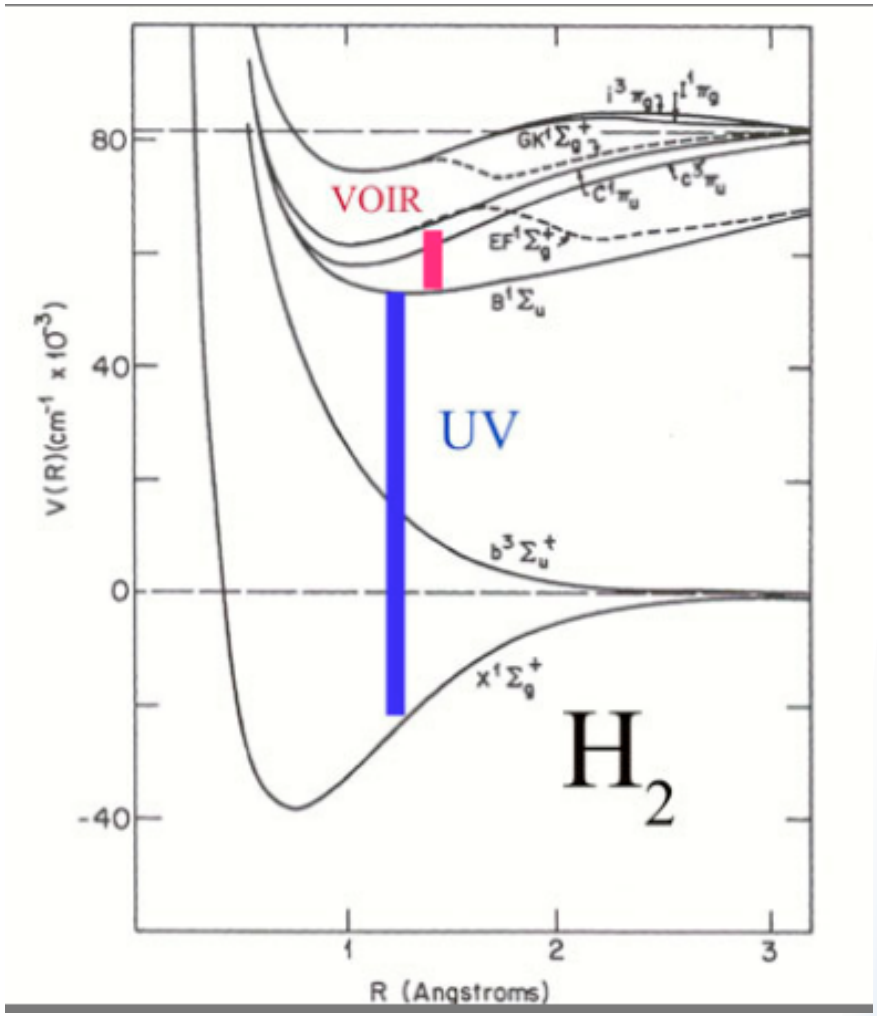
G.K. James

(1) LUTh & UMR 8102, Observatoire de Paris, France

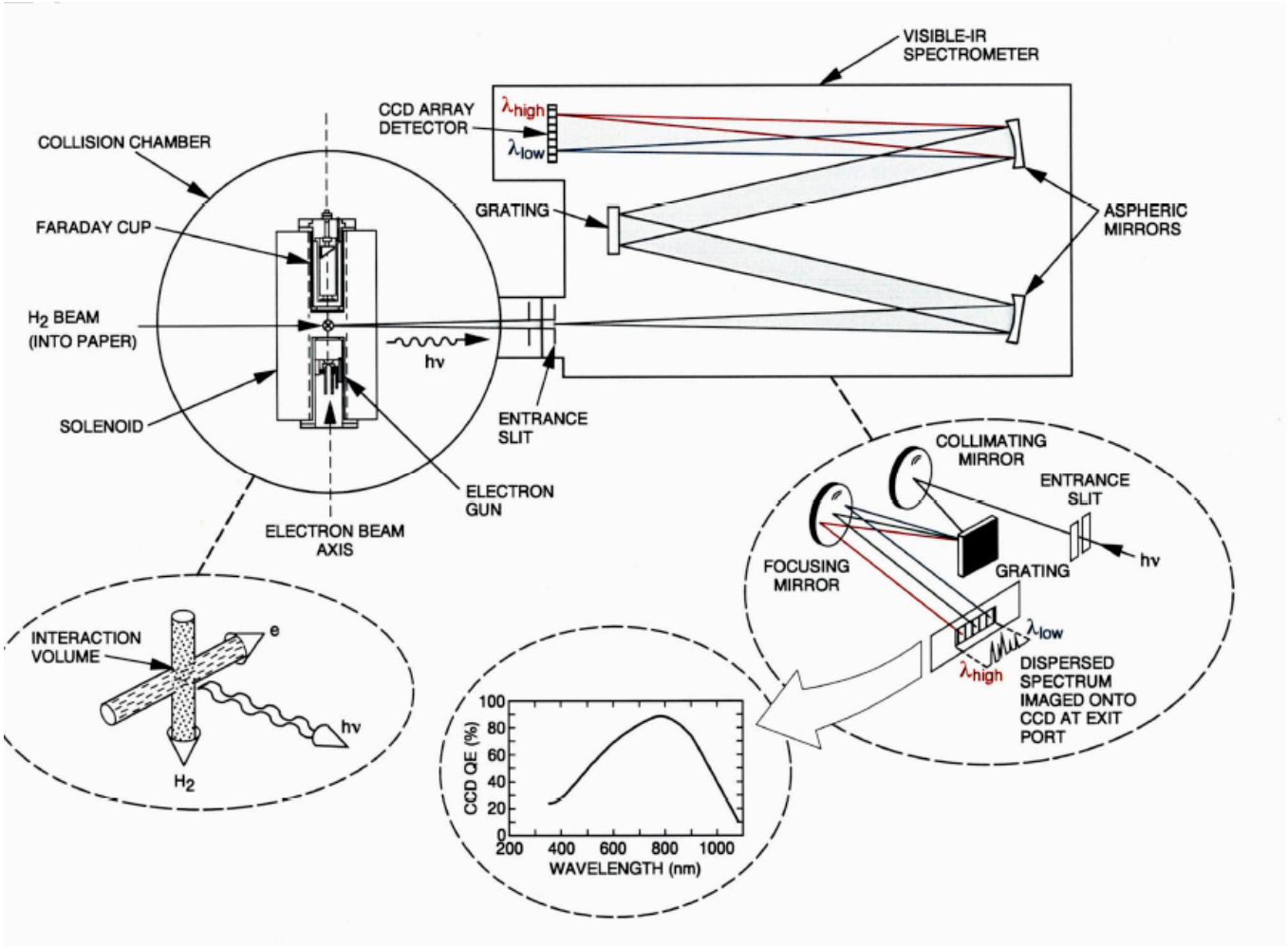
(2) JPL, California Institute of Technology, USA

Electronic excitation and fluorescence

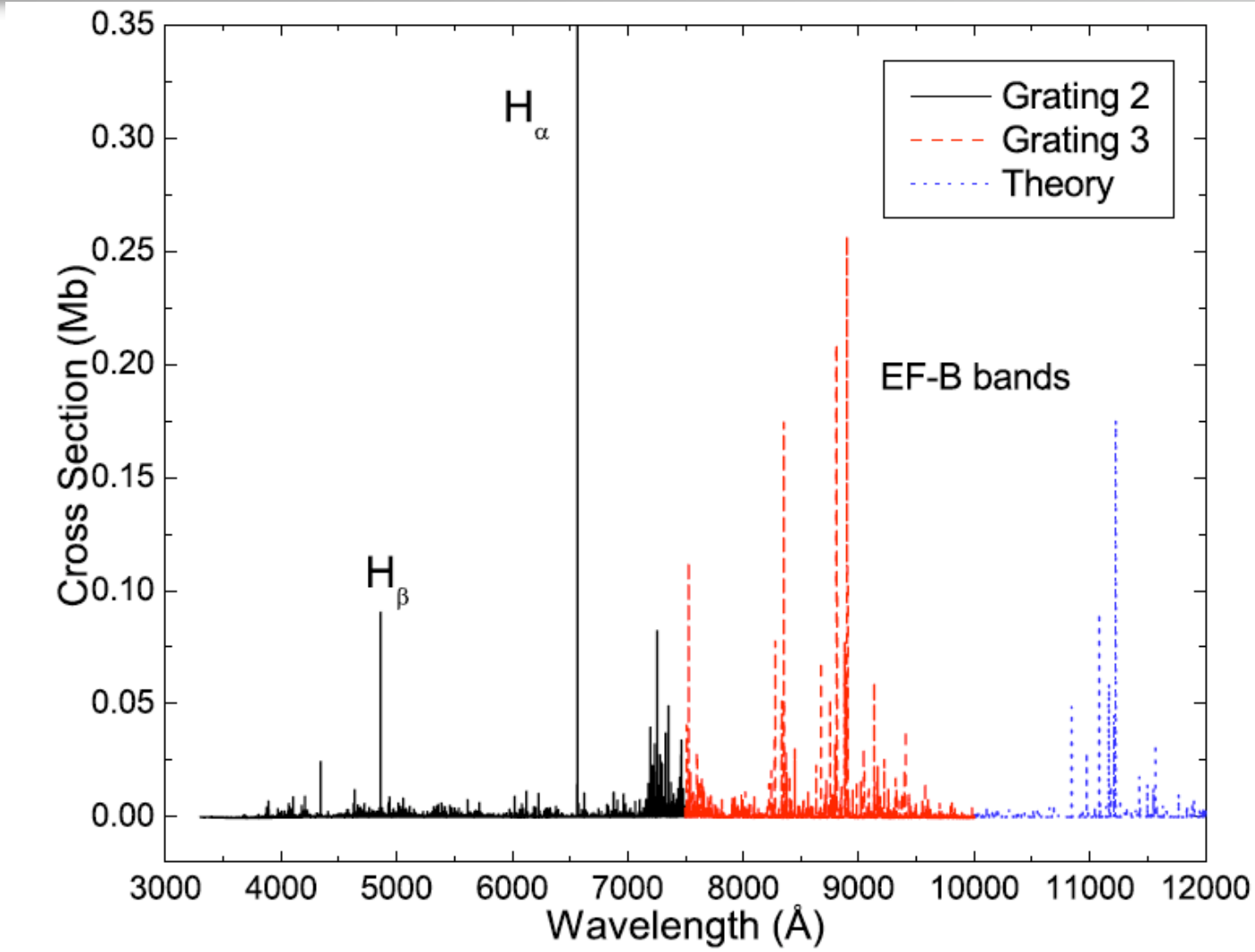
- Fluorescence from u states : essentially UV emission
- Electronic excitation : from g and u states : UV and VOIR emission
- Laboratory studies
- Calculations



Laboratory studies at JPL

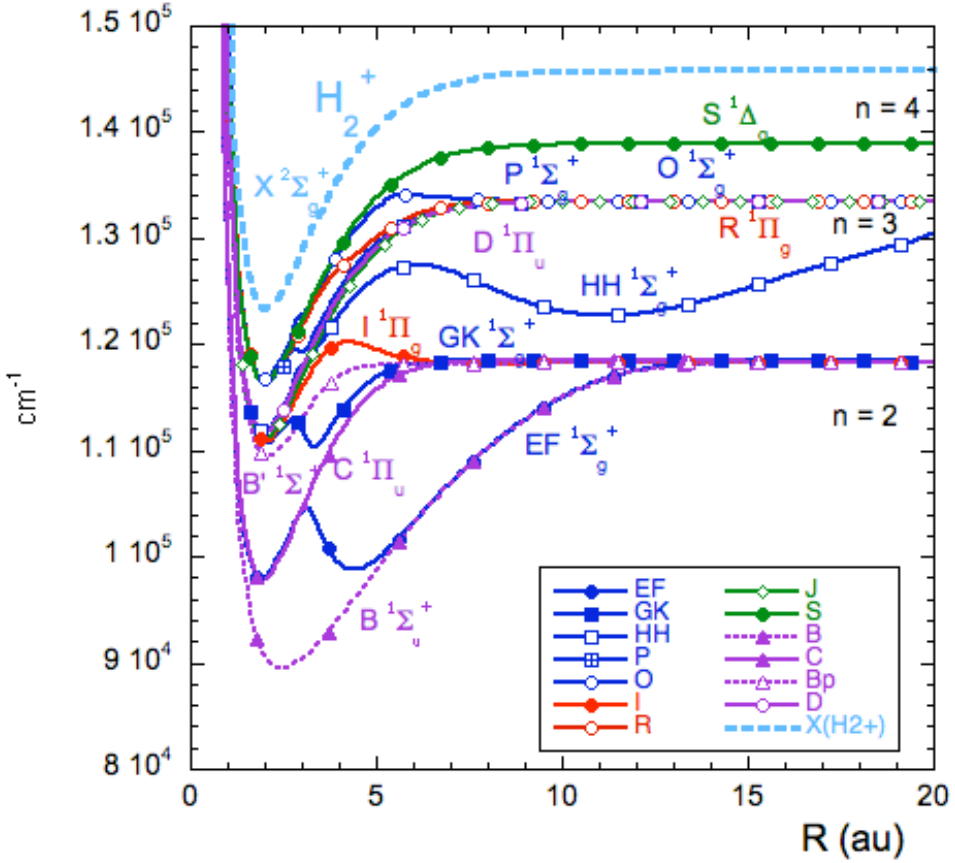


H_2 electronic emission spectrum



Theoretical challenge

- Electronic excitation of excited g Rydberg electronic states of H_2
- Possible infrared and visible cascades between g-u states, followed by VUV emission to the X ground electronic state
- knowledge of potential electronic curves and electronic couplings requested
- Extensive ab-initio studies by Wolniewicz et al. and also by Spielfiedel et al.



Electronic couplings

- Radial coupling between sates of same symmetry

$$EF\ {}^1\Sigma_g^+, GK\ {}^1\Sigma_g^+, HH\ {}^1\Sigma_g^+, P\ {}^1\Sigma_g^+, O\ {}^1\Sigma_g^+$$

$$I\ {}^1\Pi_g, R\ {}^1\Pi_g$$

$$J\ {}^1\Delta_g, S\ {}^1\Delta_g$$

- Rotational coupling between ${}^1\Sigma_g^+$ and ${}^1\Pi_g$ on one hand and ${}^1\Pi_g$ and ${}^1\Delta_g$ on the other hand.
- Similar considerations for u states
- Spin-orbit couplings between singlet and triplet?

Calculation of VOIR spectrum (I)

$$\Phi_{SuJ} = \sum_{T} \Psi_{TJ} f_{STuJ}.$$

- g states : 9 coupled states
- u states : 4 coupled states

$$
\begin{aligned}
M^{R}_{(v_k,v_j J_k)} = &-\sqrt{J_k}\Big[\langle f_{EF v_k J_k}|M_{EF-B}|f_{B v_j J_j}\rangle + \langle f_{EF v_k J_k}|M_{EF-B'}|f_{B' v_j J_j}\rangle + \langle f_{GK v_k J_k}|M_{GK-B}|f_{B v_j J_j}\rangle \\
&+ \langle f_{GK v_k J_k}|M_{GK-B'}|f_{B' v_j J_j}\rangle + \langle f_{H\bar{H} v_k J_k}|M_{H\bar{H}-B}|f_{B v_j J_j}\rangle + \langle f_{H\bar{H} v_k J_k}|M_{H\bar{H}-B'}|f_{B' v_j J_j}\rangle + \langle f_{O v_k J_k}|M_{O-B}|f_{B v_j J_j}\rangle \\
&+ \langle f_{O v_k J_k}|M_{O-B'}|f_{B' v_j J_j}\rangle + \langle f_{P v_k J_k}|M_{P-B}|f_{B v_j J_j}\rangle + \langle f_{P v_k J_k}|M_{P-B'}|f_{B' v_j J_j}\rangle\Big] \\
&+ \sqrt{J_k+1}\big[\langle f_{I^+ v_k J_k}|M_{I-B}|f_{B v_j J_j}\rangle + \langle f_{I^+ v_k J_k}|M_{I-B'}|f_{B' v_j J_j}\rangle + \langle f_{R^+ v_k J_k}|M_{R-B}|f_{B v_j J_j}\rangle + \langle f_{R^+ v_k J_k}|M_{R-B'}|f_{B' v_j J_j}\rangle\big] \\
&-\sqrt{J_k-1}\Big[\langle f_{EF v_k J_k}|M_{EF-C}|f_{C^+ v_j J_j}\rangle + \langle f_{EF v_k J_k}|M_{EF-D}|f_{D^+ v_j J_j}\rangle + \langle f_{GK v_k J_k}|M_{GK-C}|f_{C^+ v_j J_j}\rangle + \langle f_{GK v_k J_k}|M_{GK-D}|f_{D^+ v_j J_j}\rangle \\
&+ \langle f_{H\bar{H} v_k J_k}|M_{H\bar{H}-C}|f_{C^+ v_j J_j}\rangle + \langle f_{H\bar{H} v_k J_k}|M_{H\bar{H}-D}|f_{D^+ v_j J_j}\rangle + \langle f_{O v_k J_k}|M_{O-C}|f_{C^+ v_j J_j}\rangle + \langle f_{O v_k J_k}|M_{O-D}|f_{D^+ v_j J_j}\rangle \\
&+ \langle f_{P v_k J_k}|M_{P-C}|f_{C^+ v_j J_j}\rangle + \langle f_{P v_k J_k}|M_{P-D}|f_{D^+ v_j J_j}\rangle\Big] - \sqrt{\frac{(J_k-1)(J_k+1)}{J_k}}\Big[\langle f_{I^- v_k J_k}|M_{I-C}|f_{C^- v_j J_j}\rangle + \langle f_{I^- v_k J_k}|M_{I-D}|f_{D^- v_j J_j}\rangle \\
&+ \langle f_{R^- v_k J_k}|M_{R-C}|f_{C^- + v_j J_j}\rangle + \langle f_{R^- v_k J_k}|M_{R-D}|f_{D^- + v_j J_j}\rangle\Big] + \sqrt{\frac{(J_k+1)(J_k+2)}{2J_k}}\Big[\langle f_{J^- v_k J_k}|M_{J-C}|f_{C^- v_j J_j}\rangle \\
&+ \langle f_{J^- v_k J_k}|M_{J-D}|f_{D^- v_j J_j}\rangle + \langle f_{S^- v_k J_k}|M_{S-C}|f_{C^- + v_j J_j}\rangle + \langle f_{S^- v_k J_k}|M_{S-D}|f_{D^- + v_j J_j}\rangle\Big],
\end{aligned}
$$

Calculation of VOIR spectrum (II)

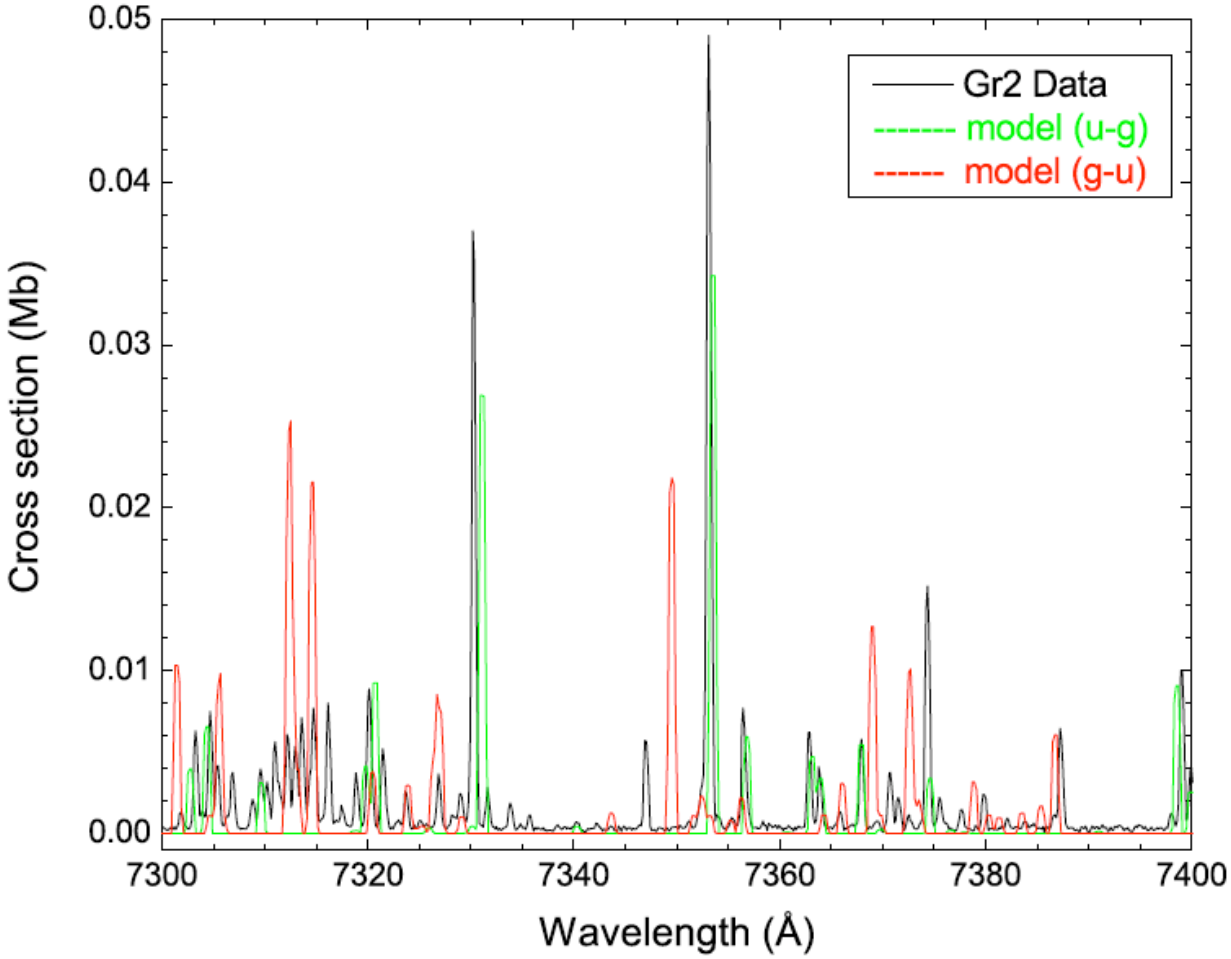
$$
\begin{aligned}
M^{Q}_{(v_k,v_j;J_k)} = &-\sqrt{2J_k+1}\left[\langle f_{I^-v_kJ_k}|M_{I-B}|f_{Bv_jJ_j}\rangle + \langle f_{I^-v_kJ_k}|M_{I-B'}|f_{B'v_jJ_j}\rangle + \langle f_{R^-v_kJ_k}|M_{R-B}|f_{Bv_jJ_j}\rangle + \langle f_{R^-v_kJ_k}|M_{R-B'}|f_{B'v_jJ_j}\rangle\right] \\
&-\sqrt{2J_k+1}\left[\langle f_{EFv_kJ_k}|M_{EF-C}|f_{C^-v_jJ_j}\rangle + \langle f_{EFv_kJ_k}|M_{EF-D}|f_{D^-v_jJ_j}\rangle + \langle f_{GKv_kJ_k}|M_{GK-C}|f_{C^-v_jJ_j}\rangle + \langle f_{GKv_kJ_k}|M_{GK-D}|f_{D^-v_jJ_j}\rangle\right. \\
&+\left\langle f_{H\bar{H}v_kJ_k}\middle|M_{H\bar{H}-C}\middle|f_{C^-v_jJ_j}\right\rangle + \left\langle f_{H\bar{H}v_kJ_k}\middle|M_{H\bar{H}-D}\middle|f_{D^-v_jJ_j}\right\rangle + \langle f_{Ov_kJ_k}|M_{O-C}|f_{C^-v_jJ_j}\rangle + \langle f_{Ov_kJ_k}|M_{O-D}|f_{D^-v_jJ_j}\rangle \\
&\left.+\langle f_{Pv_kJ_k}|M_{P-C}|f_{C^-v_jJ_j}\rangle + \langle f_{Pv_kJ_k}|M_{P-D}|f_{D^-v_jJ_j}\rangle\right] + \sqrt{\frac{(2J_k+1)}{J_k(J_k+1)}}\left[\langle f_{I^+v_kJ_k}|M_{I-C}|f_{C^+v_jJ_j}\rangle + \langle f_{I^+v_kJ_k}|M_{I-D}|f_{D^+v_jJ_j}\rangle\right. \\
&+\left.\langle f_{R^+v_kJ_k}|M_{R-C}|f_{C^+v_jJ_j}\rangle + \langle f_{R^+v_kJ_k}|M_{R-D}|f_{D^+v_jJ_j}\rangle\right] - \sqrt{\frac{(2J_k+1)(J_k+2)(J_k-1)}{2J_k(J_k+1)}}\left[\langle f_{J^+v_kJ_k}|M_{J-C}|f_{C^+v_jJ_j}\rangle\right. \\
&\left.+\langle f_{J^+v_kJ_k}|M_{J-D}|f_{D^+v_jJ_j}\rangle + \langle f_{S^+v_kJ_k}|M_{S-C}|f_{C^+v_jJ_j}\rangle + \langle f_{S^+v_kJ_k}|M_{S-D}|f_{D^+v_jJ_j}\rangle\right],
\end{aligned}
$$

$$
A(v_k,v_j;J_k,J_j) = \frac{4}{3\hbar^4c^3(2J_k+1)}\left(E_{v_kJ_k}-E_{v_jJ_j}\right)^3\left|M^{\alpha}_{(v_k,v_j;J_k)}\right|^2,
$$

same phase conventions wanted !!

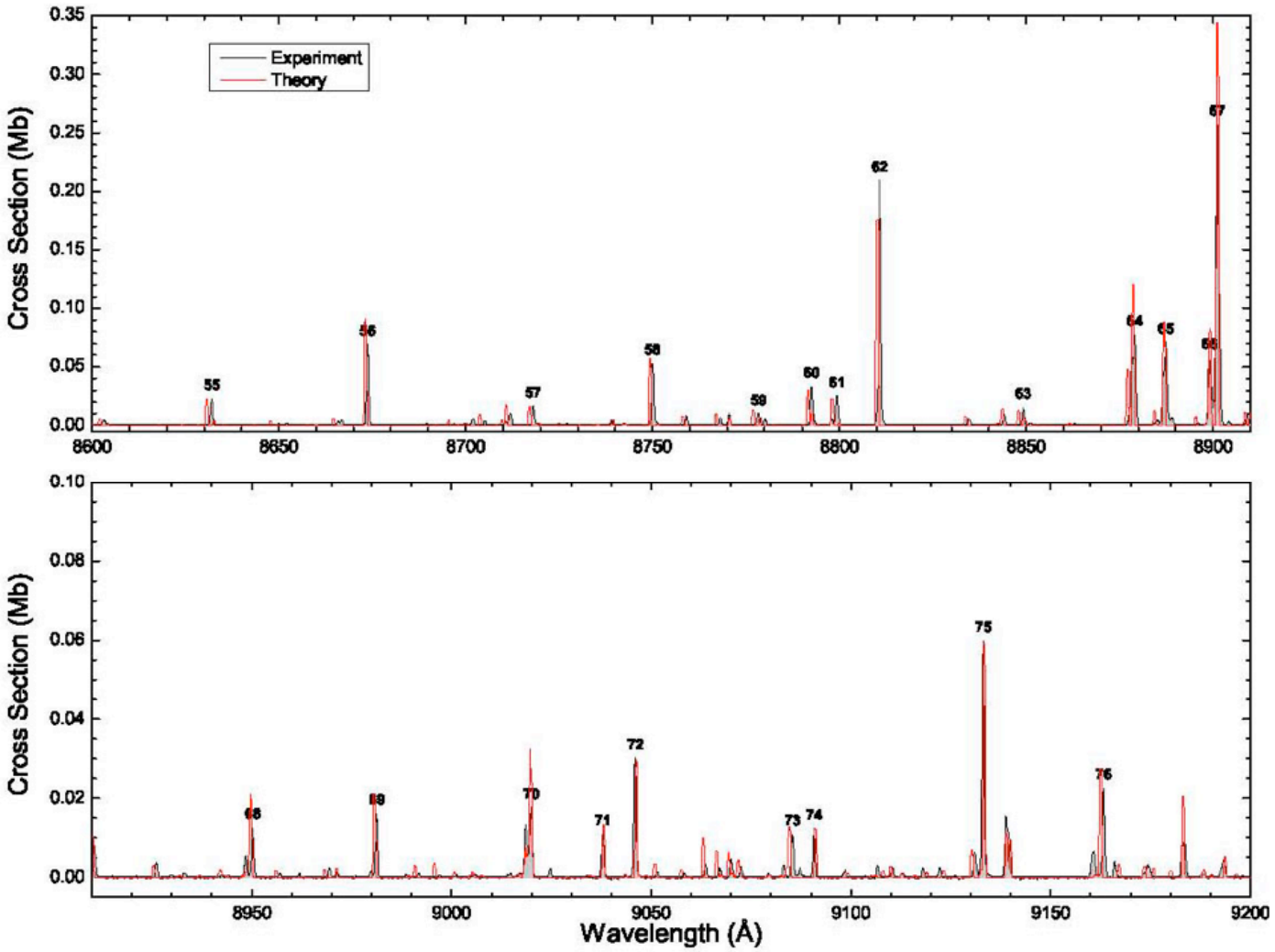
Comparison theory-experiment (1)

- Results reported in Aguilar et al. 2008, ApJS 177, 388
- essential features recovered by theoretical model
- both g->u and u->g emission
- Some failures present



Comparison theory-experiment (2)

- E-F->B transitions
- features identified unambiguously
- in agreement with Diecke's positions and assignments
- Positions and intensities well reproduced



Conclusions

- ✓ VOIR spectrum of H_2 is a potential probe of (exo)planetary atmospheres
- ✓ Experimental spectrum available from 1000 to 70 nm
- ✓ Qualitative agreement with theoretical predictions
- ✓ Origin of the discrepancies
  - Assumption on the form of the emission cross section
  - Temperature of the sample
  - Possible difference of phase conventions in the potentials and couplings
- ✓ Work in progress, NASA support; extension to HD and D_2