



UCL

The **ExoMol** project : Progress and Updates

Jonathan Tennyson

Physics and Astronomy, University College London, UK

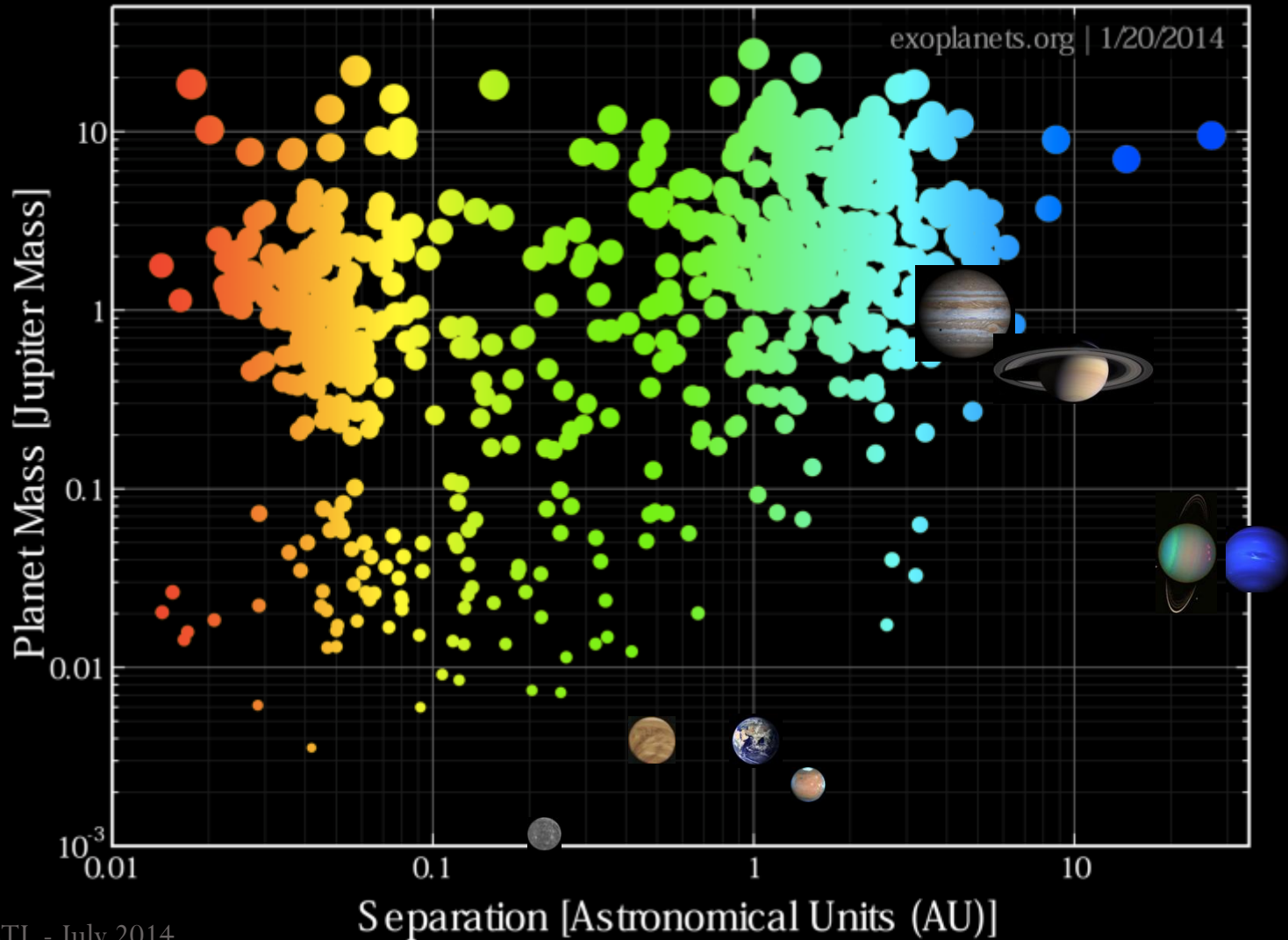


ExoMol conference
June, 2025
Broxbourne

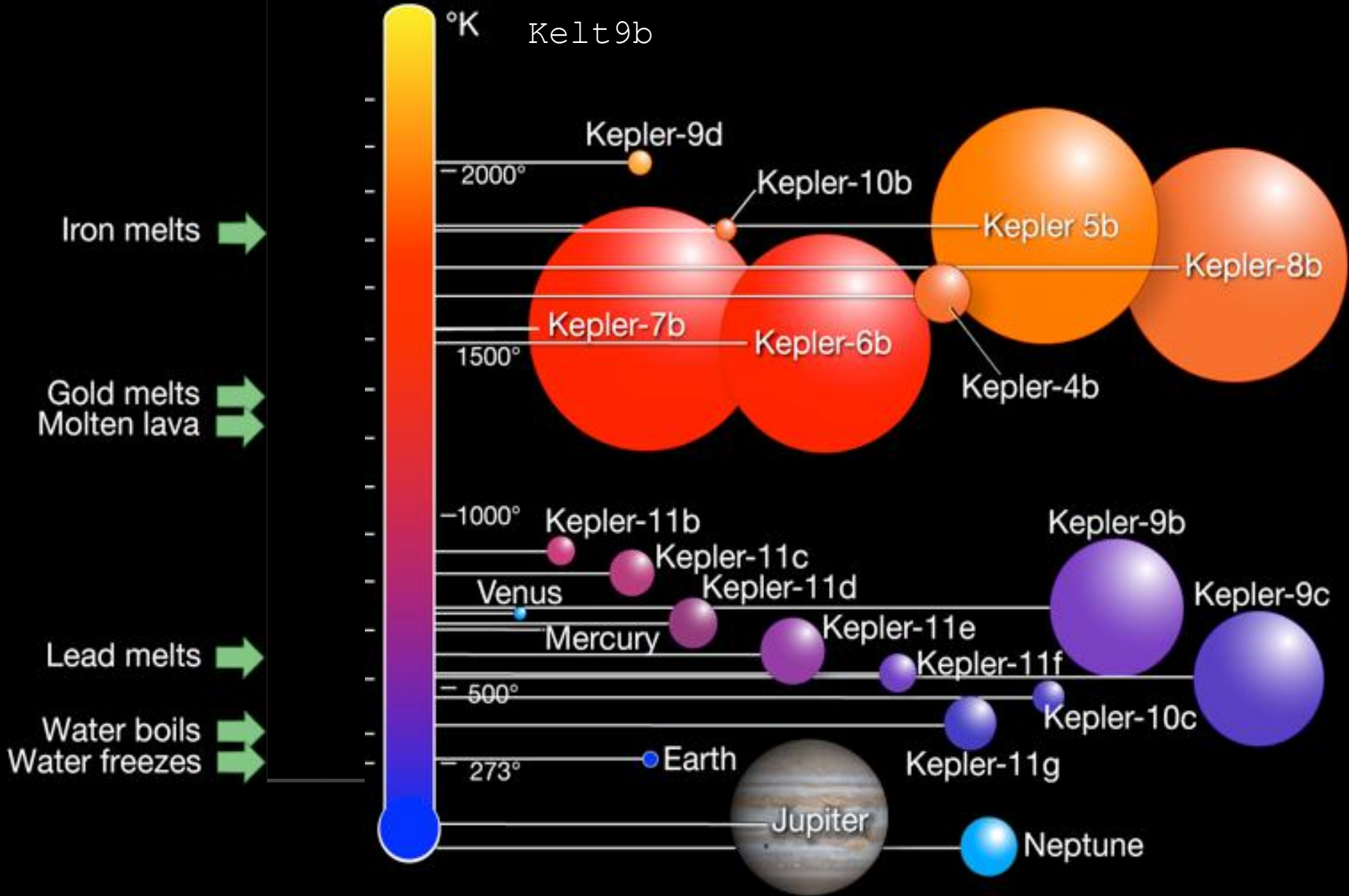
Image credit Shutterstock

The Exoplanet Revolution

October 2023: 5523 planets / 4250 planetary systems



Planet Temperature & Size



ExoMol

5 year project: 2011-16

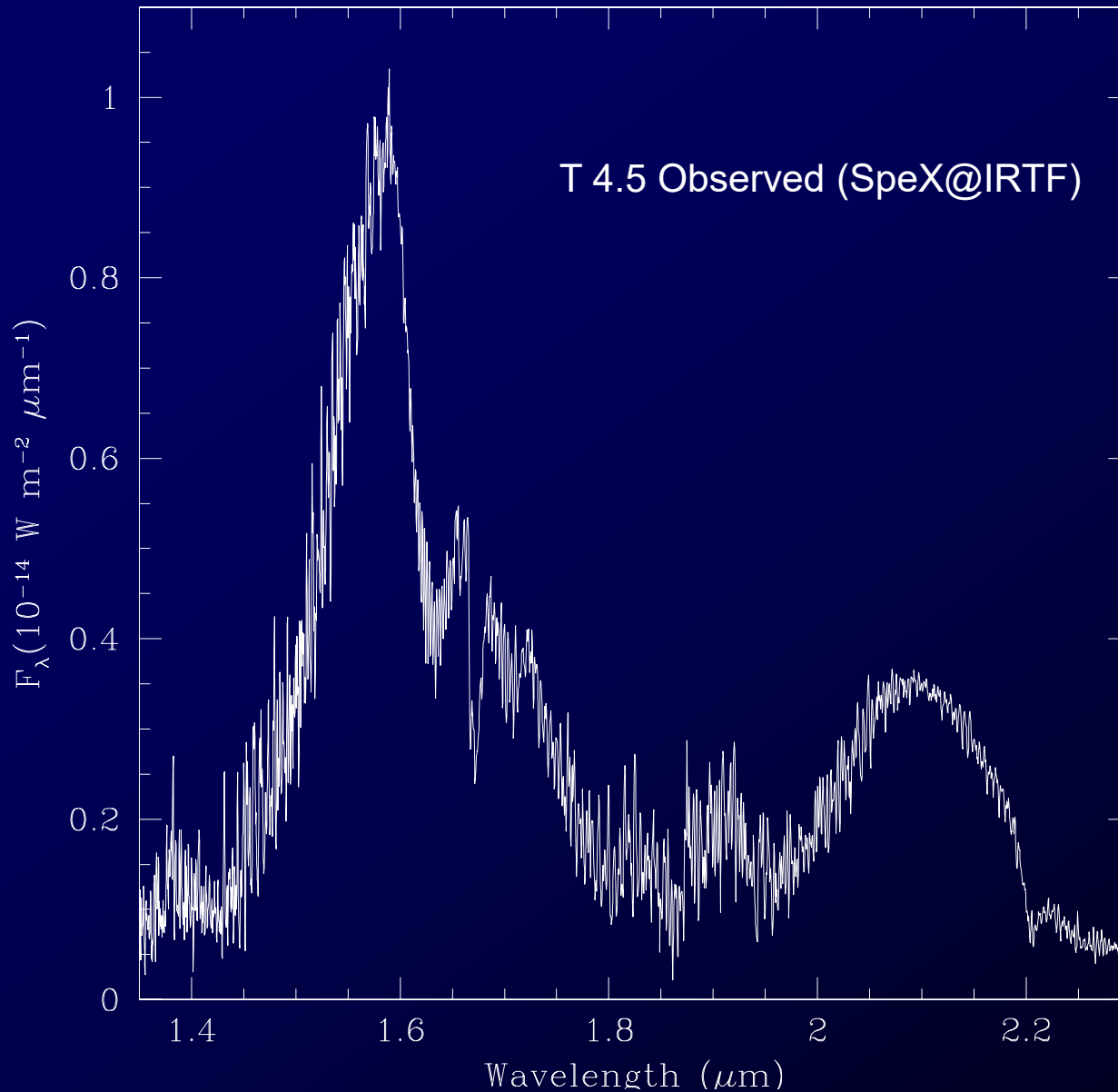
Provide data for all molecular transitions important for exoplanet atmospheres

Methodology: first principles quantum mechanical calculations, informed by experiment

J Tennyson and S.N. Yurchenko,
Monthly Not. Roy. Astro. Soc. (MNRAS) 425, 21 (2012).



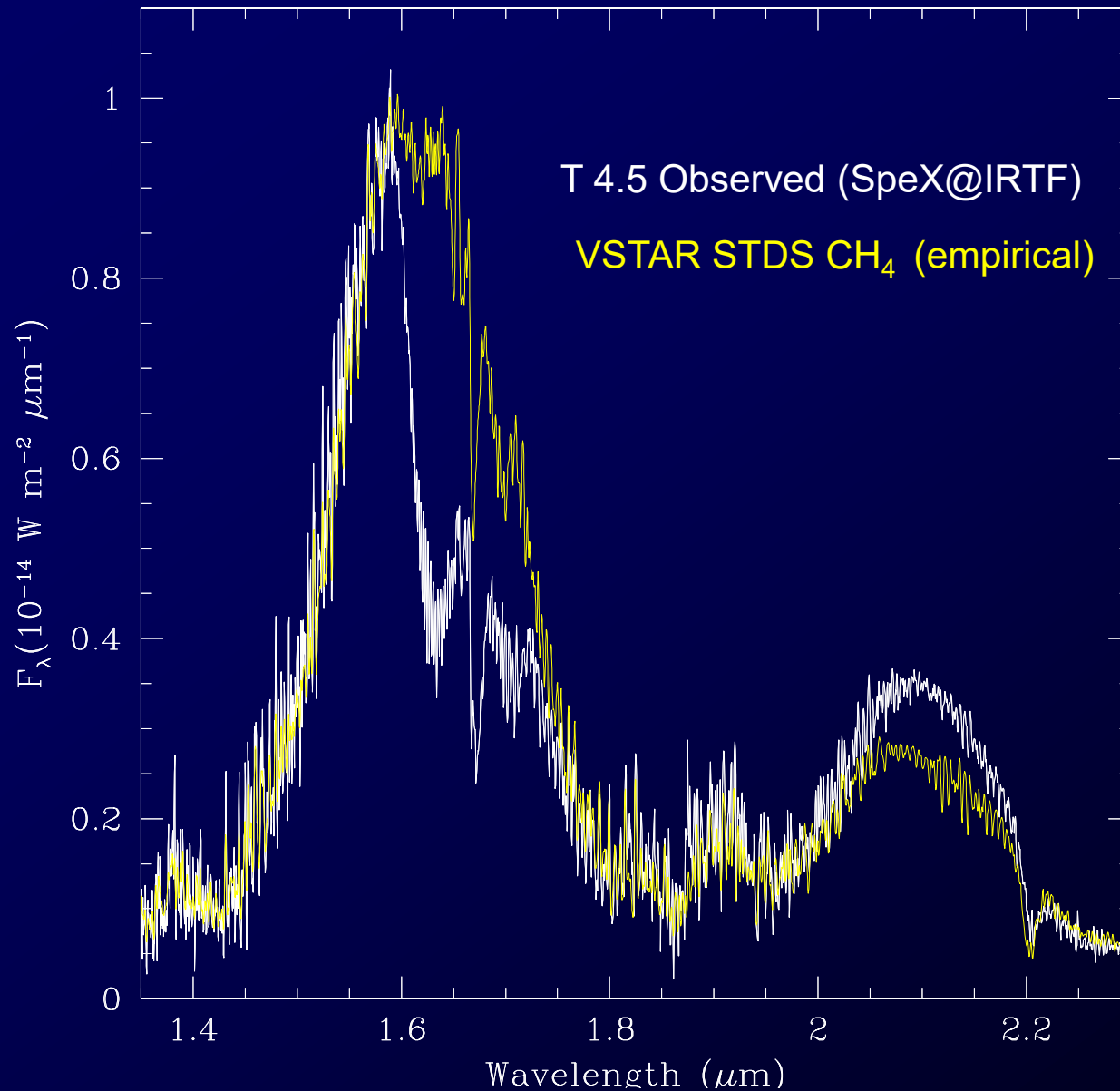
Spectrum T4.5 brown dwarf: a “methane dwarf”



2MASS 0559-14

Cushing, Rayner, Vacca (2005)

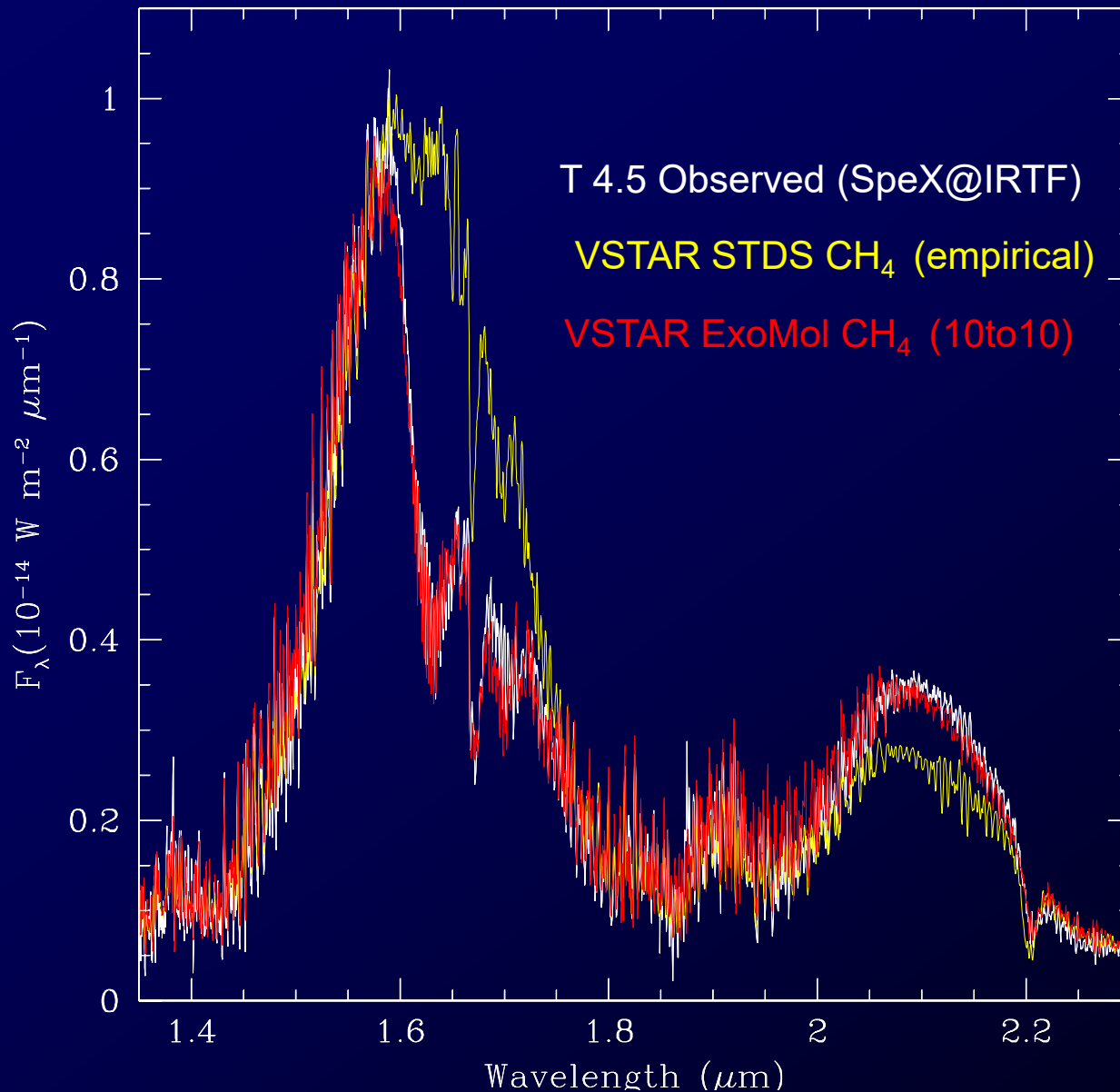
Spectrum T4.5 brown dwarf: a “methane dwarf”



2MASS 0559-14

Cushing, Rayner, Vacca (2005)

Spectrum T4.5 brown dwarf: a “methane dwarf”



2MASS 0559-14

T 4.5 Observed (SpeX@IRTF)

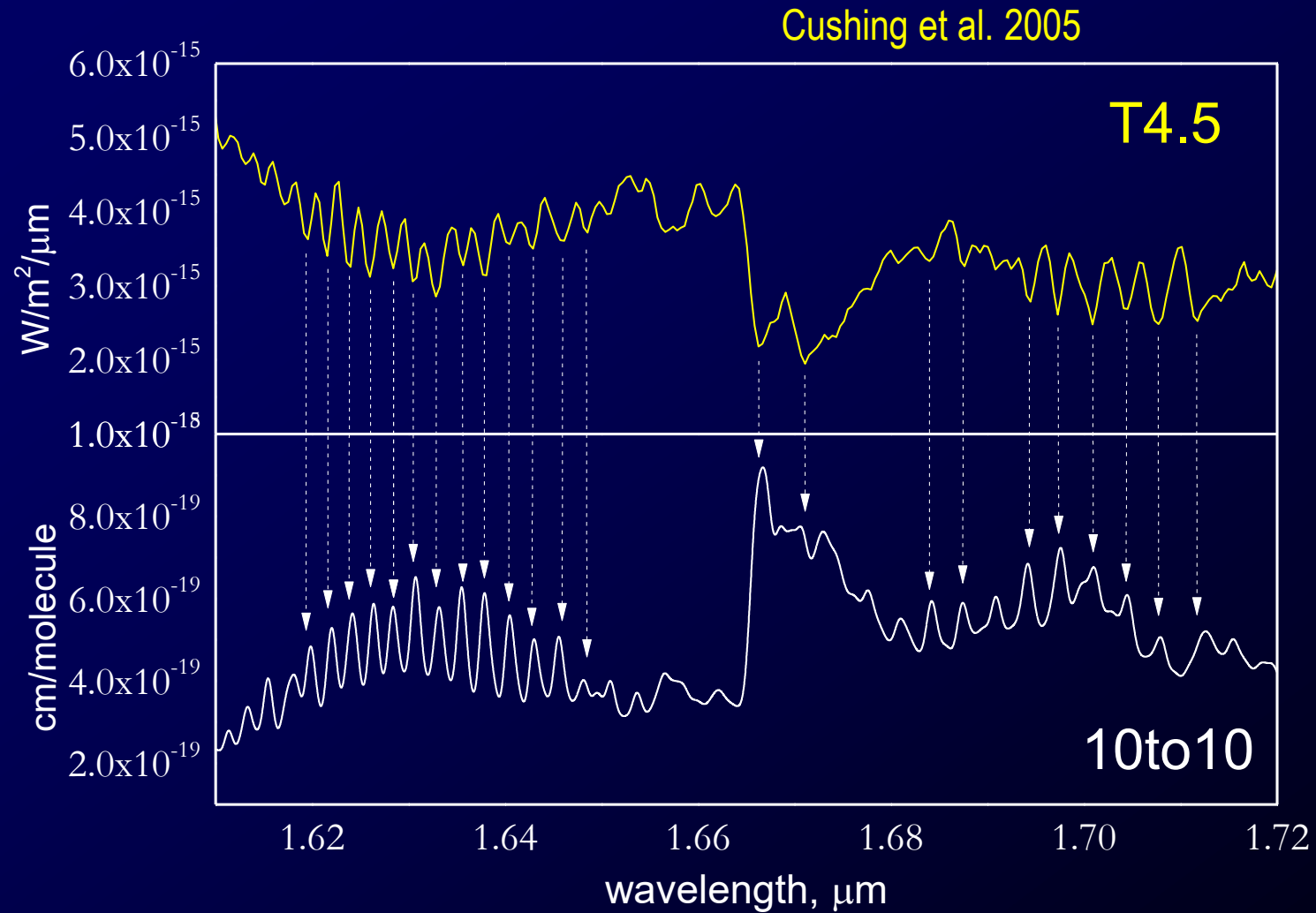
VSTAR STDS CH_4 (empirical)

VSTAR ExoMol CH_4 (10to10)

SN Yurchenko, J
Tennyson, J Bailey,
MDJ Hollis, G Tinetti,
PNAS, 111, 9379 (2014)

Cushing, Rayner, Vacca (2005)

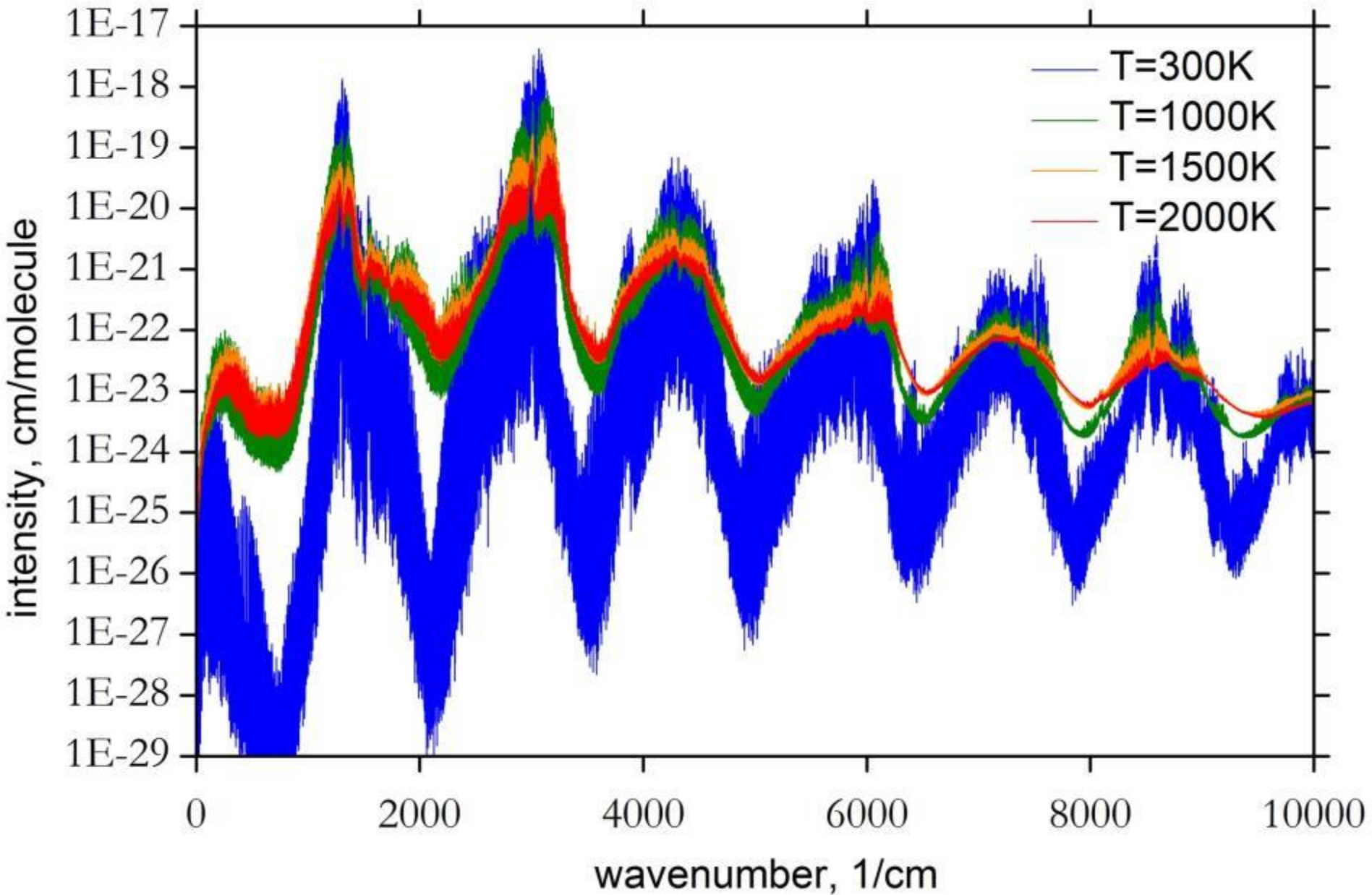
The spectrum of the T4.5 Brown Dwarf 2MASS J0559-1404



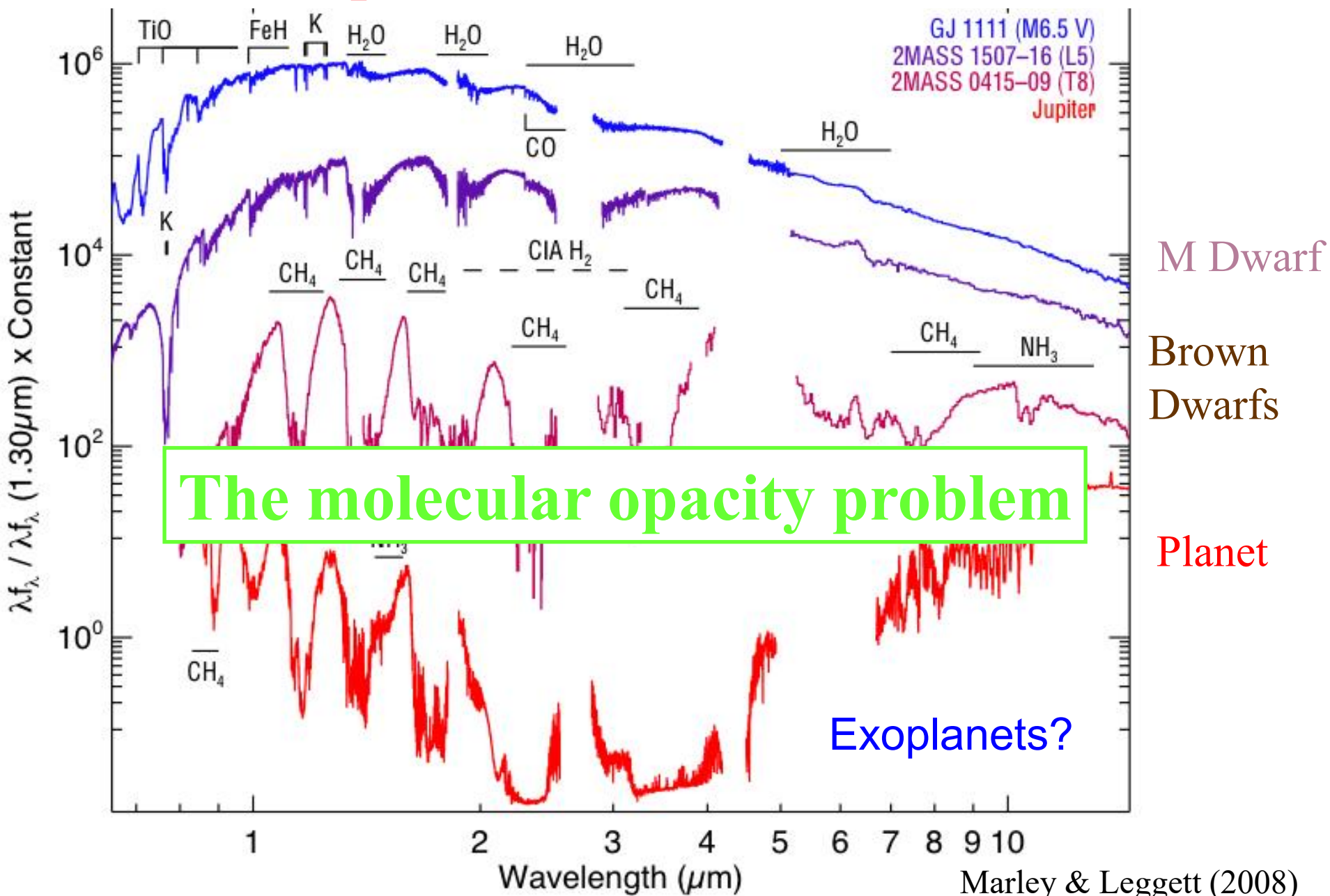
R=2000

SN Yurchenko & J Tennyson, MNRAS 440, 1649 (2014)

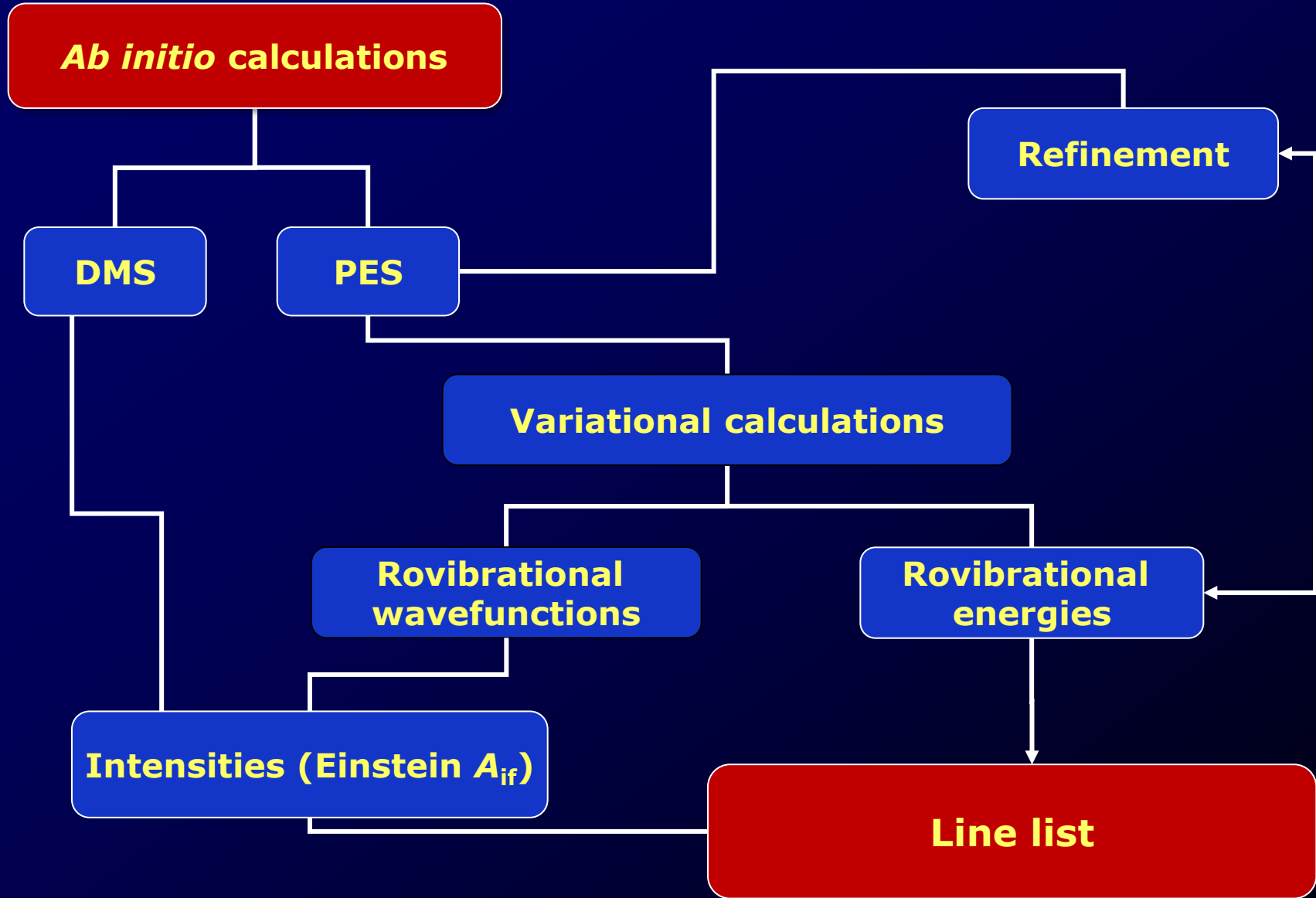
Absorption spectrum of methane



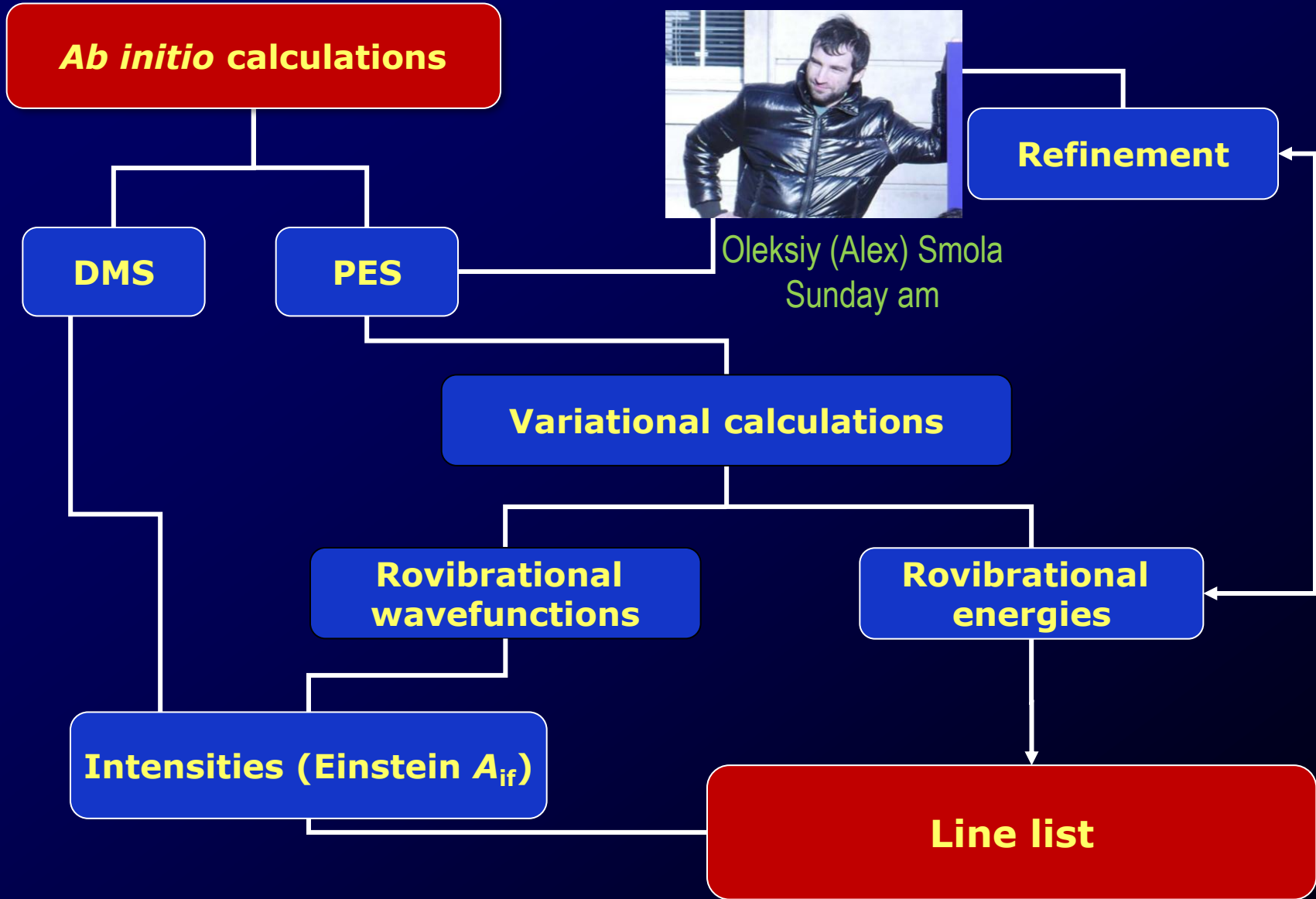
Cool atmospheres: dominated by molecular absorption



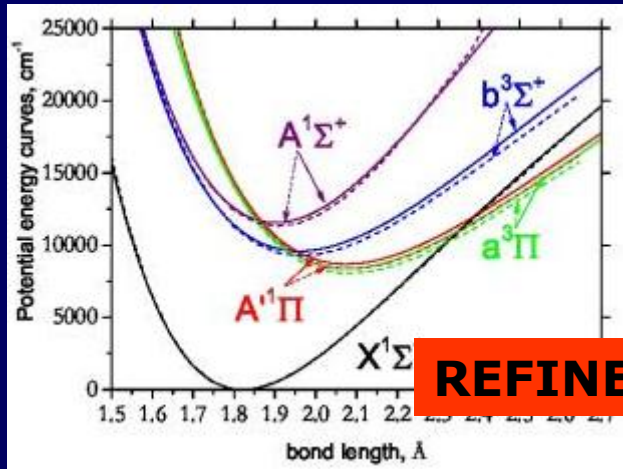
Method: Spectrum from the “first-principles”



Method: Spectrum from the “first-principles”

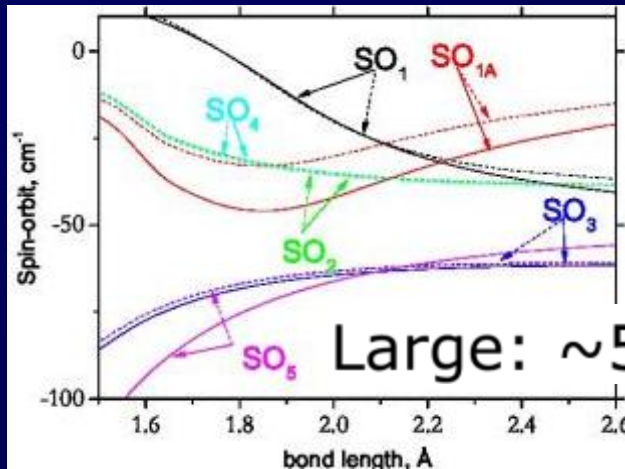


Potential energy



Khalil et al
(2011)

CaO observed in
meteorite spectra
Berezjnoj et al. (2018)



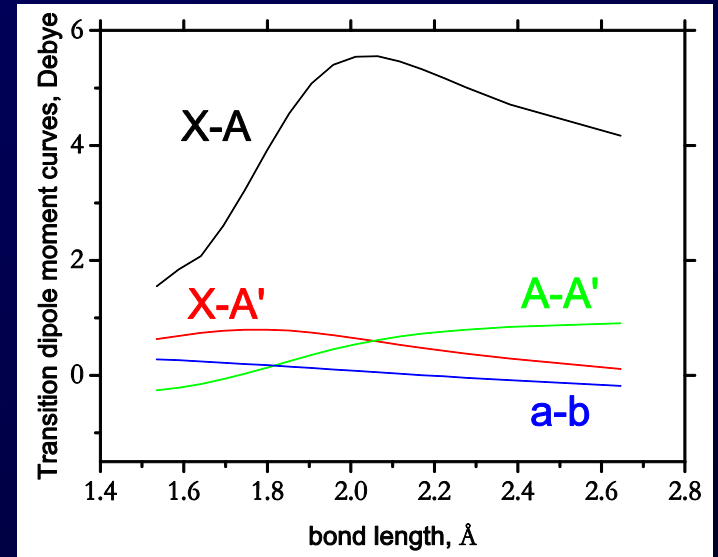
Solve for the motion
of the nuclei

Duo

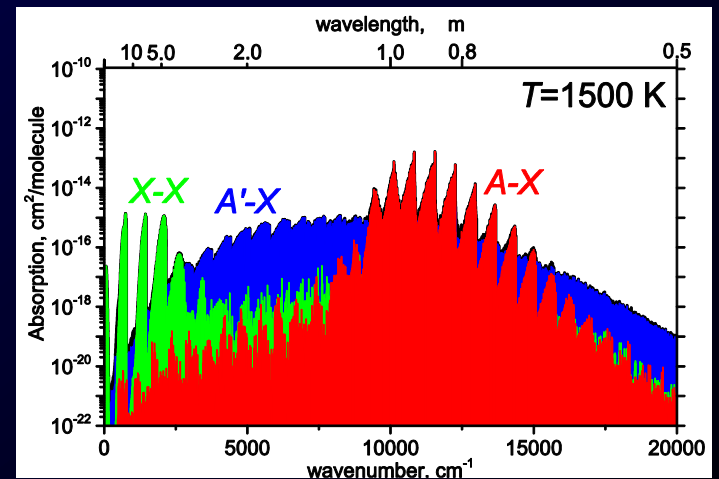
SN Yurchenko et al, MNRAS 456, 4524 (2016)

Line list: CaO

Dipole moment

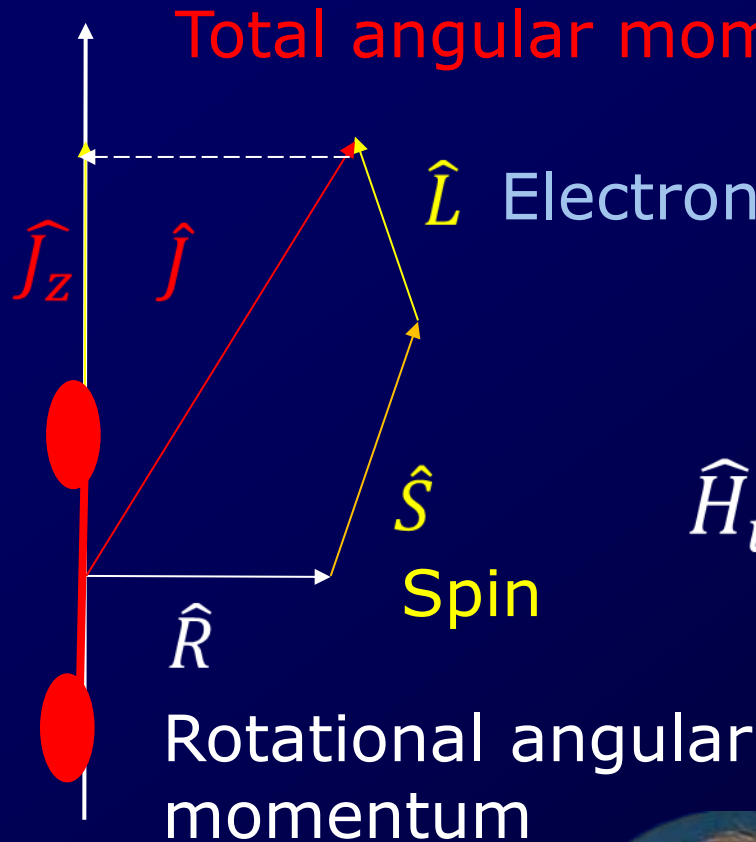


Line list: 22 M lines



Duo: a general diatomic nuclear motion code

S.N. Yurchenko, L. Lodi, J. Tennyson & A.V. Stolyarov, Computer Phys. Comm. **202**, 262 (2016).



$$\hat{R}^2 = (\hat{J} - \hat{L} - \hat{S})^2$$

$$\hat{H}_{ii} = \frac{\hbar^2}{2\mu r^2} \hat{R}^2 - \frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial r^2} + V_i(r)$$

Variational basis set
Hund's case (a)

$$\phi_n = |v\rangle |J\Omega\rangle |S\Sigma\rangle |L\Sigma\rangle$$

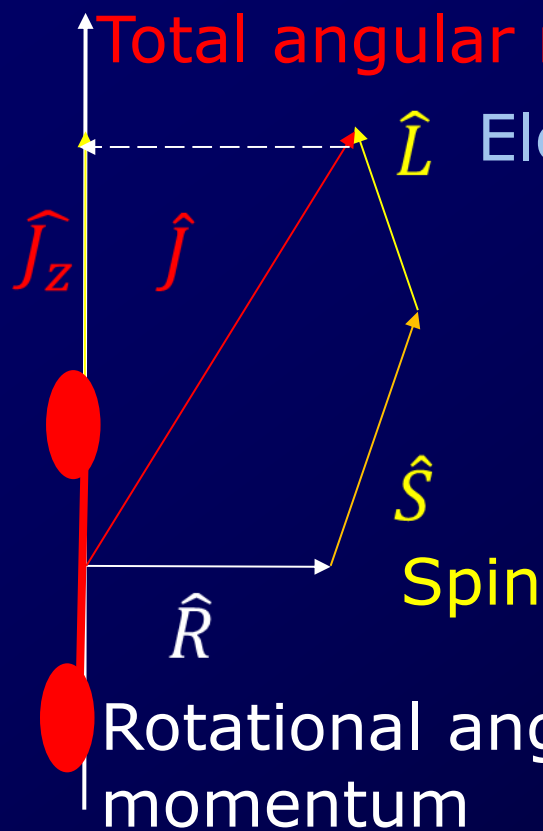
vibrational Spin
Rotational Electronic

Sergey Yurchenko



Duo: a general diatomic nuclear motion code

S.N. Yurchenko, L. Lodi, J. Tennyson & A.V. Stolyarov, *Computer Phys. Comm.* **202**, 262 (2016).



\hat{L} Electronic angular momentum

$$\hat{R}^2 = (\hat{J} - \hat{L} - \hat{S} - I)^2$$

$$\hat{H}_{ii} = \frac{\hbar^2}{2\mu r^2} \hat{R}^2 - \frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial r^2} + V_i(r)$$

Variational basis set, Hund's case (a_β)

Rotational Electronic

$$\phi_n = |v\rangle |J\Omega\rangle |S\Sigma\rangle |L\Sigma\rangle$$

Dipole + quadrupole transitions

Hyperfine effects

vibrational Spin

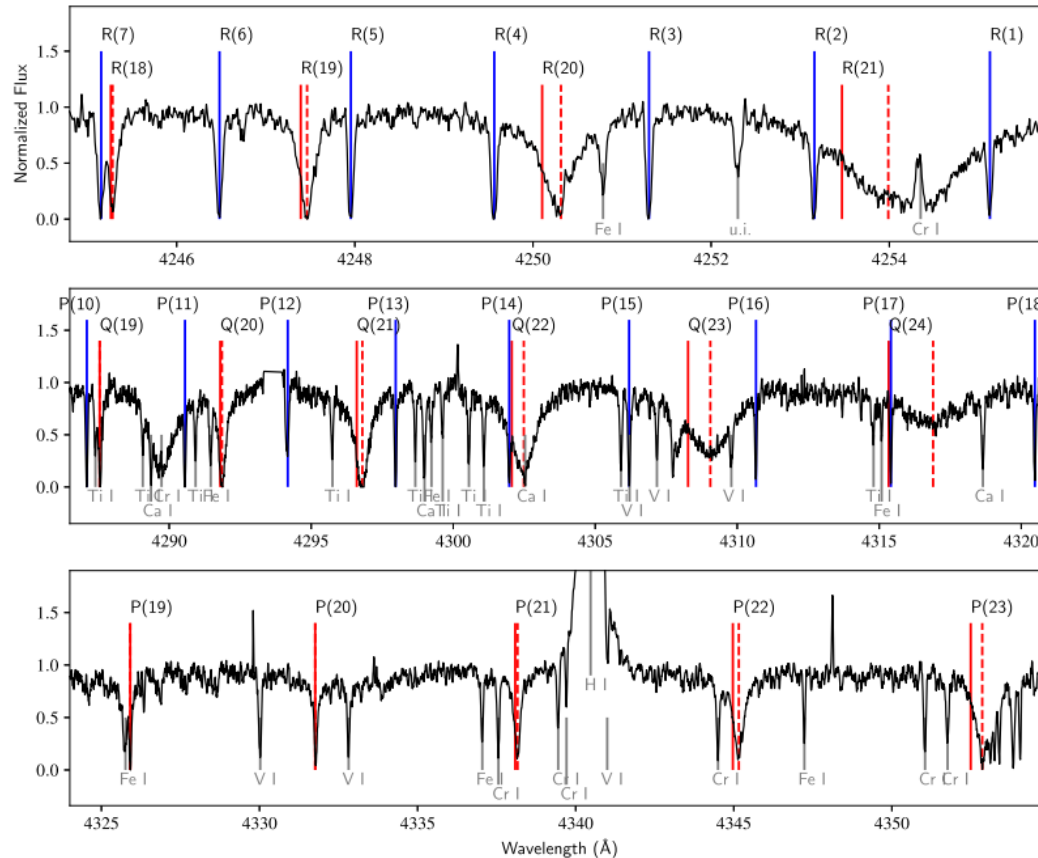
$$\phi_n = |v\rangle |J\Omega\rangle |S\Sigma\rangle |L\Sigma\rangle |IFM_F\rangle$$

Nuclear Spin



Qianwei Qu

AIH in Proxima Cen spectrum



Bound-bound transitions

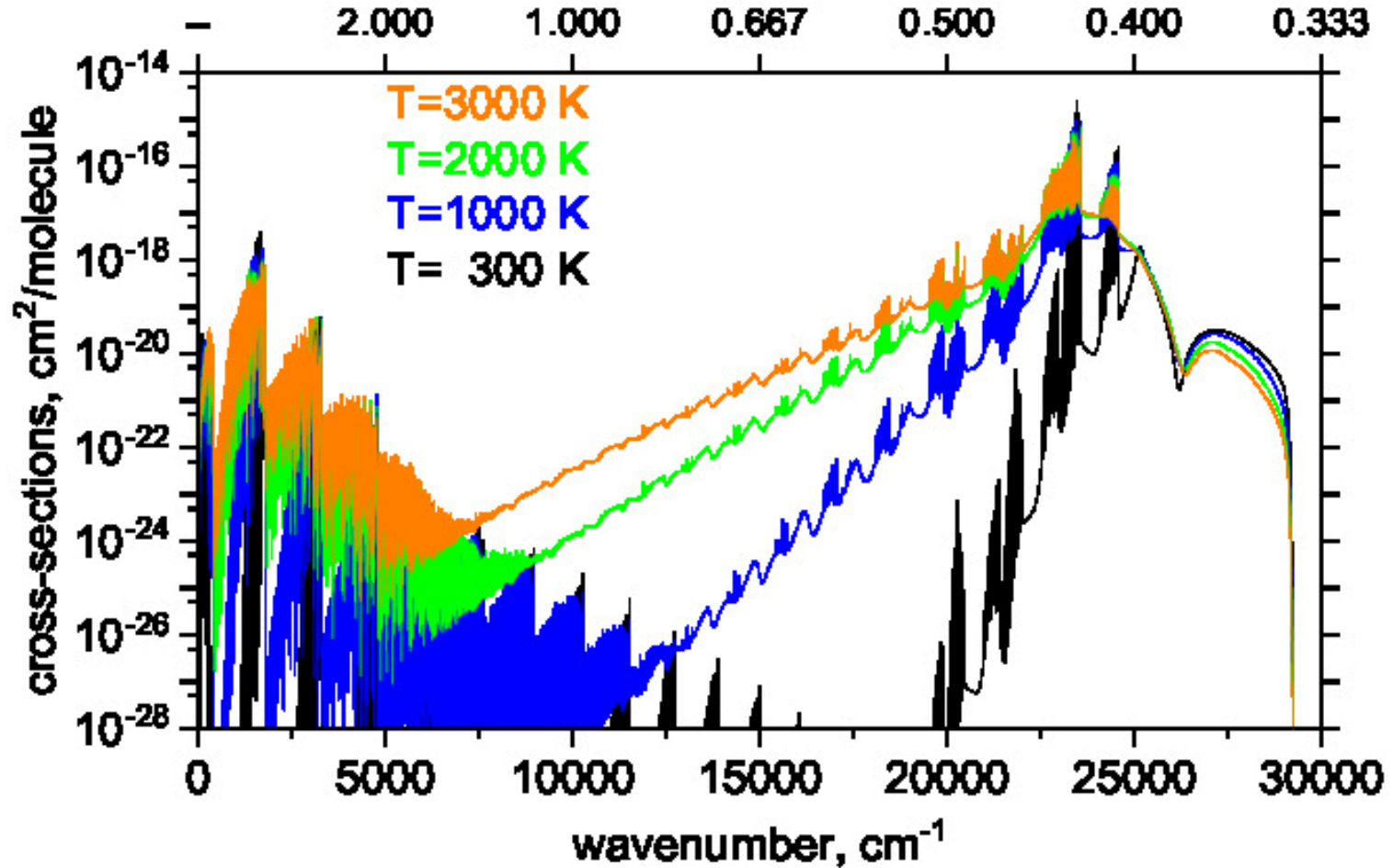
Line broadened due to predissociation

Figure 4. Spectrum of Proxima Cen in the spectral range covering selected intervals of the $^{27}\text{AlH } A^1\Pi - X^1\Sigma^+ 0-0$ band. The lines of diffuse nature are marked in red. The vertical lines mark calculated positions of lines, while the dashed ones mark the observed positions; the R(21) in the top panel is heavily blended by the CrI resonance line and not marked. Atomic lines are marked in grey.

Y.V. Pavlenko, J. Tennyson, S.N. Yurchenko, H.R.A. Jones, Y. Lyubchik & A. Suárez Mascareño,
Mon. Not. R. astr. Soc., **516**, 5655-5673 (2022).

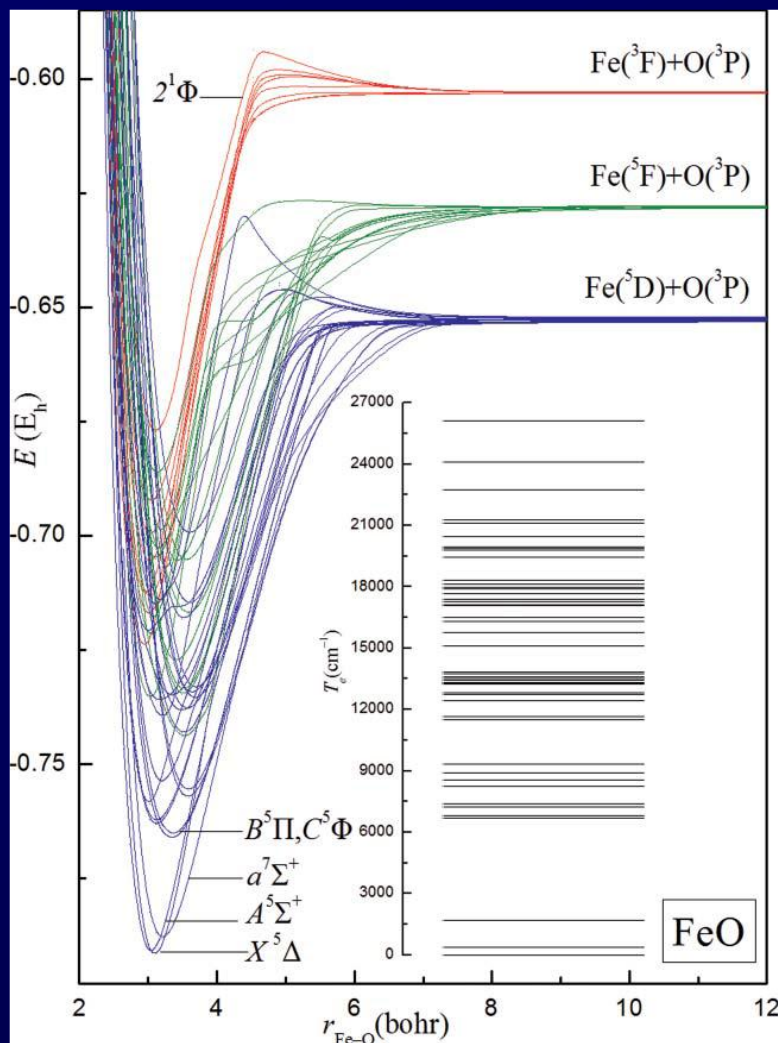
AloHA: "line list"

- Bound-bound
- Continuum absorption
- Predissociation



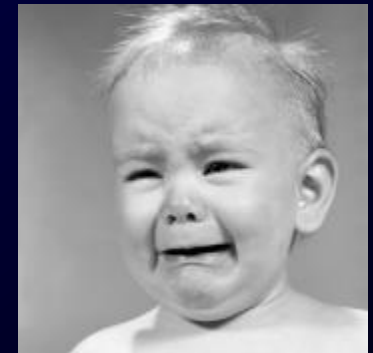
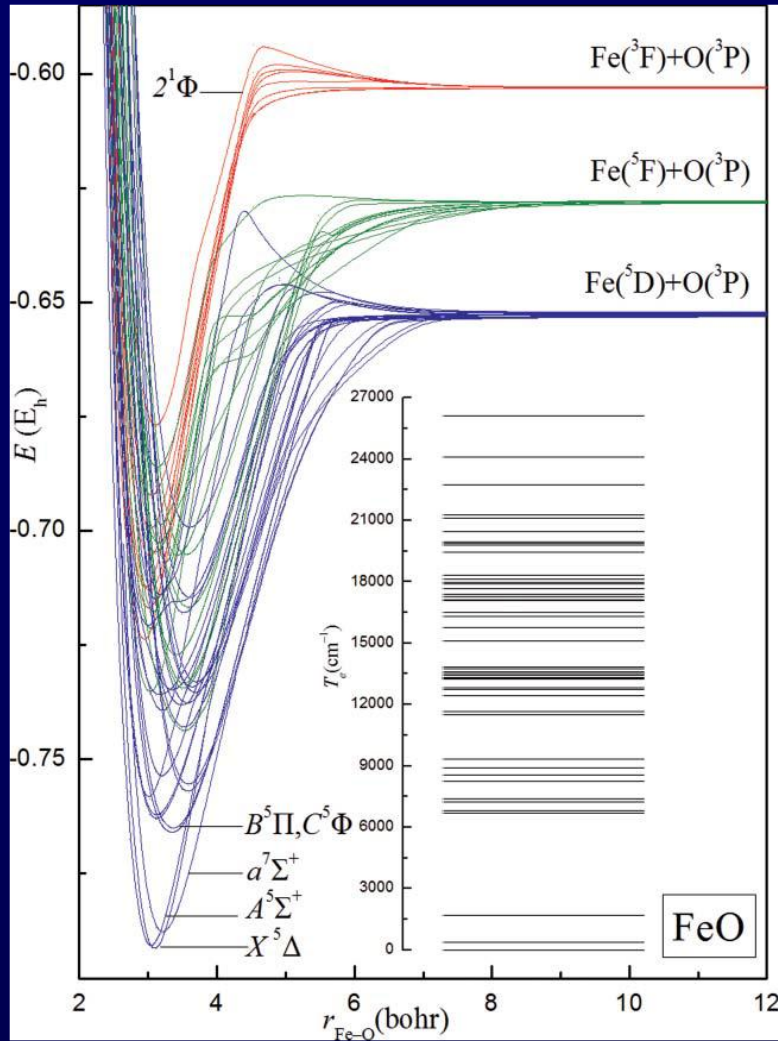
S.N. Yurchenko, W. Szajna, R. Hakalla, M. Semenov, J. Tennyson, Y. Pavlenko & M.R. Schmidt,
Mon. Not. R. astr. Soc., **527**, 9736-9756 (2024)

FeO



30000 cm^{-1}

FeO



I. BeH, MgH, CaH	XIX. H ₂ ¹⁸ O, H ₂ ¹⁷ O	XXXVII HCCH	LVI. SO
II. SiO	XX. H ₃ ⁺	XXXVIII SiO ₂	LVII. CH ₄
III. HCN/HNC	XXI. NO	XXXIX CO ₂	LVIII. OCS
IV. CH ₄	XXII. SiH ₄	XL. H ₃ O ⁺	LIX. N ₂ O
V. NaCl, KCl	XXIII. PO, PS	XLI. NaOH, KOH	LX. ¹⁵ NH ₃
VI. PN	XXIV. SiH	XLII. NO (UV)	LXI. OH
VII. PH ₃	XXV. SiS	XLIII. SiO (UV)	LXII. C ₃
VIII. H ₂ CO	XXVI. SN, SH	XLIV. NaO	LXIII. HDO
IX. AlO	XXVII. AlH	XLV. MgH (UV), CaH (UV)	LXIV. PN
X. NaH	XXVIII. C ₂ H ₄	XLVI. SiN	LXV. NiH
XI. HNO ₃	XXIX. CH ₃ Cl	XLVII. CaOH	In progress
XII. CS	XXX. H ₂ ¹⁶ O	XLVIII AlCl	O ₂ , CS ₂ , HCO ⁺ , NO ⁺ ,
XIII. CaO	XXXI. C ₂	XLVIII H ₂ CS	OH ⁺ , BH, etc
XIV. SO ₂	XXXII. TiO	L. H ₃ ⁺ , H ₂ D ⁺ , D ₂ H ⁺ , D ₃ ⁺	
XV. HOOH	XXXIII. MgO	Li. LiOH	
XVI. H ₂ S	XXXIV. PH	LII. CH ⁺	
XVII. SO ₃	XXXV. NH ₃	LIII. YO	
XVIII. VO	XXXVI SH (UV)	LIV. VO (hyperfine)	
		LV. AlH (predissociation)	

2024 data releases:
 J. Tennyson *et al.*,
 JQSRT, **326**, 109083 (2024)

I. BeH, MgH, CaH
II. SiO
III. HCN/HNC
IV. CH₄
V. NaCl, KCl
VI. PN
VII. PH₃
VIII. H₂CO
IX. AlO
X. NaH
XI. HNO₃
XII. CS
XIII. CaO
XIV. SO₂
XV. HOOH
XVI. H₂S
XVII. SO₃
XVIII. VO

XIX. H₂¹⁸O, H₂¹⁷O
XX. H₃⁺
XXI. NO
XXII. SiH₄
XXIII. PO, PS
XXIV. SiH
XXV. SiS
XXVI. SN, SH
XXVII. AlH
XXVIII. C₂H₄
XXIX. CH₃Cl
XXX. H₂¹⁶O
XXXI. C₂
XXXII. TiO
XXXIII. MgO
XXXIV. PH
XXXV. NH₃
XXXVI SH (UV)

XXXVII HCCH
XXXVIII SiO₂
XXXIX CO₂
XL. H₃O⁺
XLI. NaOH, KOH
XLII. NO (UV)
XLIII. SiO (UV)
XLIV. NaO
XLV. MgH (UV), CaH (UV)
XLVI. SiN
XLVII. CaOH
XLVIII AlCl
XLVIII H₂CS
L. H₃⁺, H₂D⁺, D₂H⁺, D₃⁺
Li. LiOH
LII. CH⁺
LIII. YO
LIV. VO (hyperfine)
LV. AlH (predissociation)

LVI. SO
LVII. CH₄
LVIII. OCS
LIX. N₂O
LX. ¹⁵NH₃
LXI. OH
LXII. C₃
LXIII. HDO
LXIV. PN
LXV. NiH

In progress
O₂, CS₂, HCO⁺, NO⁺,
OH⁺, BH, CrH, etc

Others?

2024 data releases:
J. Tennyson *et al.*,
JQSRT, **326**, 109083 (2024)



Ryan Brady
poster

Databases

[ExoMol](#)

[ExoMolOP](#)

[LIDB](#)

[ExoMolHR](#)

[ExoPhoto](#)

ExoMol Database

[ExoMol](#) is the main database of molecular line lists for exoplanets and other hot atmospheres.

ExoMol Secondary databases

- [ExoMolOP: Opacities](#)
- [LIDB: Database of molecular radiative lifetimes for plasma processes](#)
- [ExoMolHR: High Resolution Database](#)
- [ExoPhoto: Photo-dissociation cross sections](#)

ExoMol is funded by the ERC under the Advanced Investigator Projects 267219 and 883830



New Databases

Databases

[ExoMol](#)

[ExoMolOP](#)

[LIDB](#)

[ExoMolHR](#)

[ExoPhoto](#)

ExoMol Database

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ExoMol Secondary databases

- [ExoMolOP: Opacities](#)
- [LIDB: Database of molecular radiative lifetimes for plasma processes](#)
- [ExoMolHR: High Resolution Database](#)
- [ExoPhoto: Photo-dissociation cross sections](#)

ExoMol is funded by the ERC under the Advanced Investigator Projects 267219 and 883830



ExoMol Opacities: available as a T/P grid for gas giants (ie H₂/He mix) only
Formats: TauRex, cross sections
ARCiS, NEMESIS, petitRADTRANS, k-tables

What else is needed?

K.L. Chubb, M. Rocchetto, S.N. Yurchenko, M. Min, I. Waldmann, J.K. Barstow, P. Molliere, A.F. Al-Refaie, M. Phillips and J. Tennyson, ExoMol cross-sections and k-tables for molecules of interest in high-temperature exoplanet atmospheres, *Astron. Astrophys.*, **646**, A21 (2021).



database with new features

www.exomol.com

1. Line lists
2. Cross-sections
3. Partition functions
4. Broadening parameters
(Barton et al, JQSRT **187**, 453 & 203, 490 (2017))
H₂ and He: J and T dependence (only)
5. k-tables
6. Lifetimes (Tennyson et al, J Phys B, 49, 044002 (2016))
7. Cooling functions
8. Lande g-factors (Semenov et al, J Mol Spectrosc (2016))
9. Dipoles for molecular control/orientation effects
A Yachmenev, RichMol project
(Owens et al, Sci Rep 7, 45068 (2017))
10. Application program interface (API) + data products

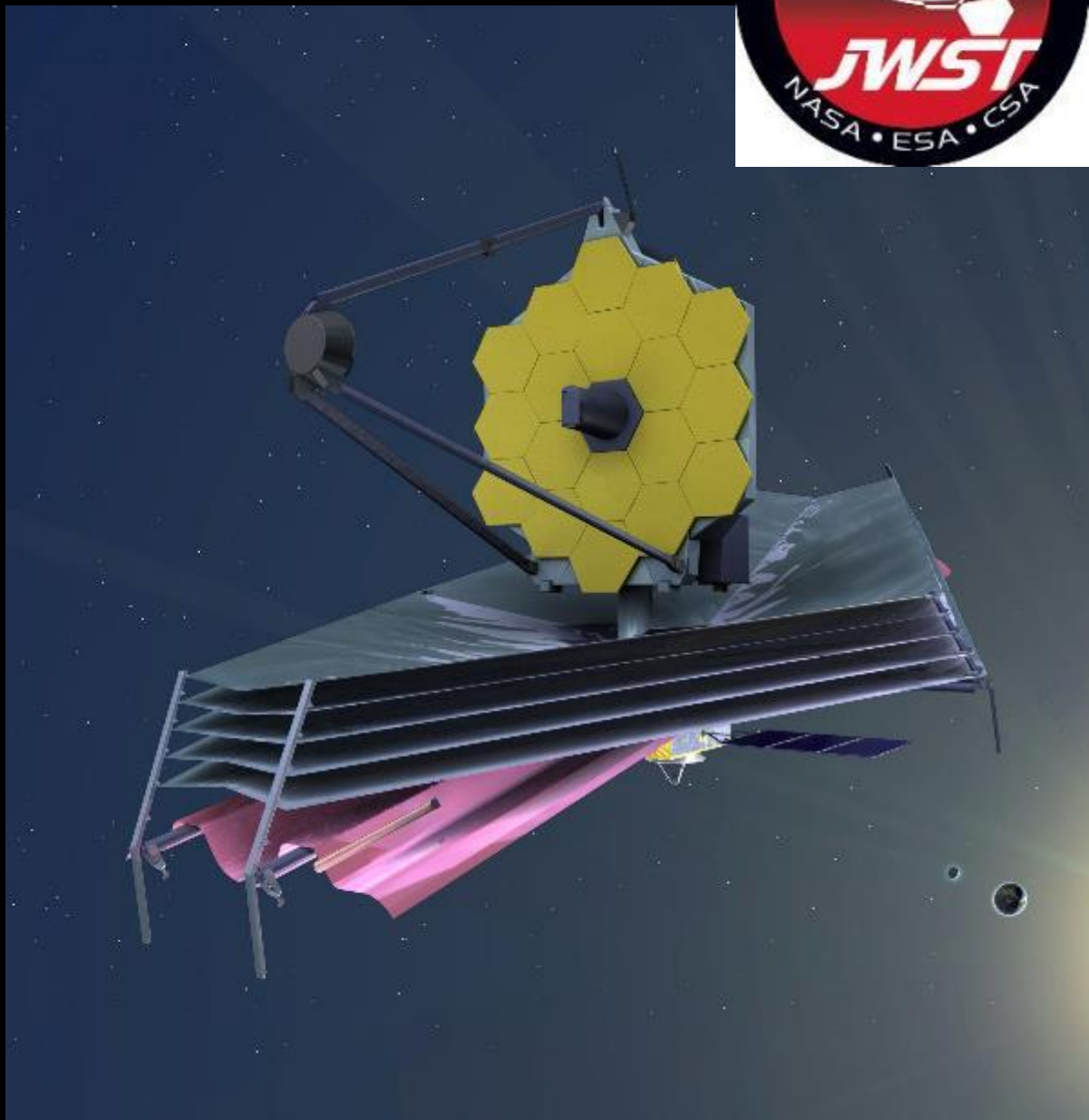
JWST: James Web Space Telescope



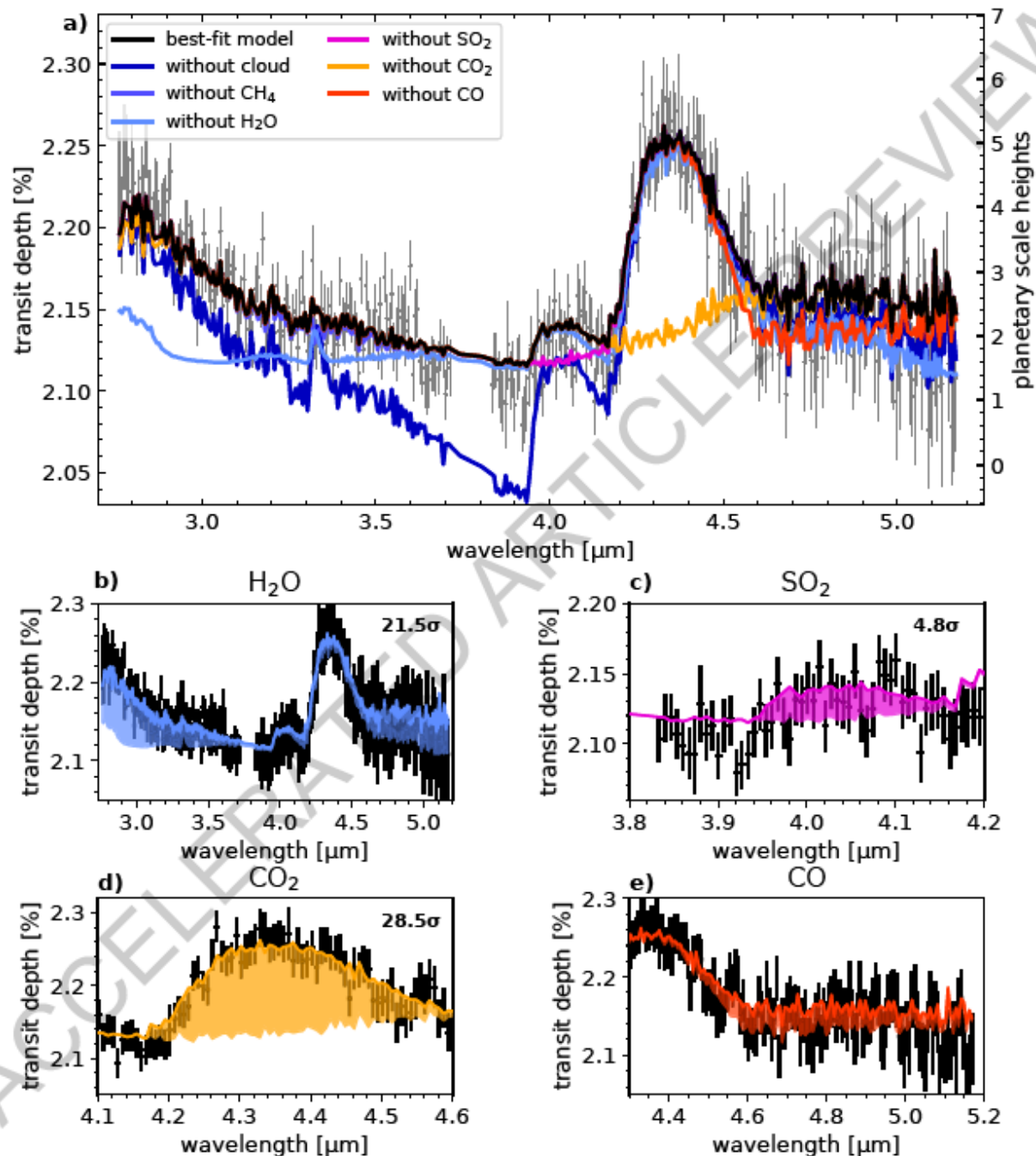
General purpose observatory
~25% time for exoplanets
Infrared capability
High resolution ($R \sim 3000$)

First data released

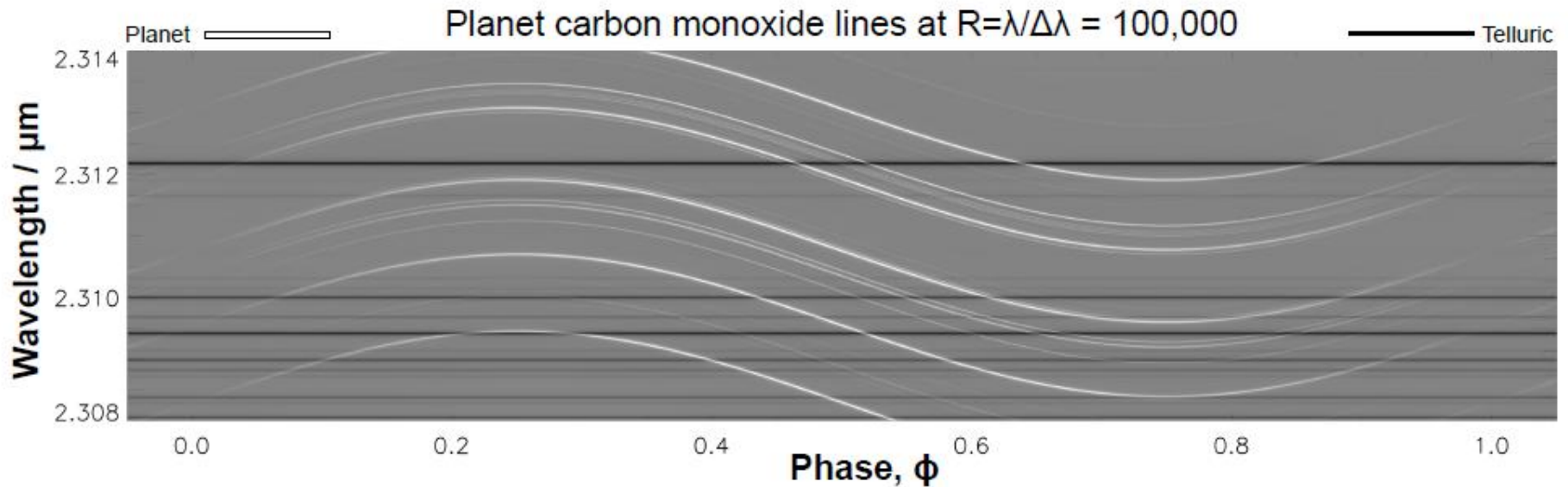
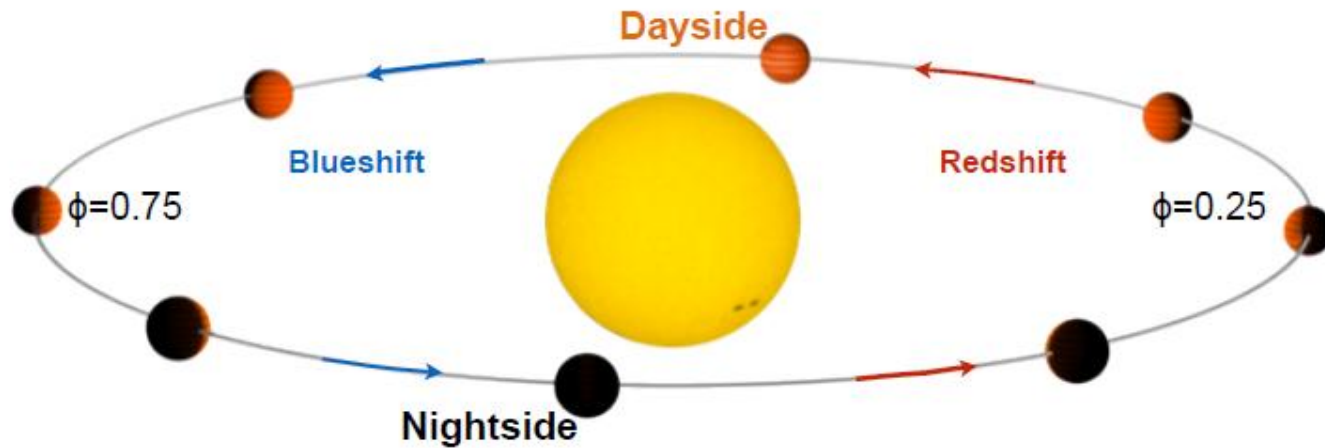
Transit spectroscopy
Direct imaging



Alderson+
Early Release Science of
the Exoplanet WASP-39b
with JWST NIRSpec G395H.
Nature 614, 664–669 (2023)



High resolution Doppler-shift spectroscopy



ExoMolHD

5 year project: 2020-25

Precision spectroscopic data for studies of exoplanets
and other hot atmospheres:

1. Line lists with spectroscopic accuracy
2. Spectroscopic line lists for isotopologues
3. Pressure broadening and pressure shifts
4. Photodissociation
5. The ExoMolHD Database



MARVEL (measured active rotation-vibration energy levels)

$$f = X E$$

frequency

energy

V1 T. Furtenbacher, A.G. Csaszar & J. Tennyson, *J. Molec. Spectrosc*, 245, 115 (2007).

V2 T. Furtenbacher & A.G. Csaszar , *JQSRT*, 115, 929 (2012).

V3 R. Tobias, T. Furtenbacher, A.G. Csaszar & J. Tennyson, *Phys. Chem. Chem. Phys.* (2019).

V4 J. Tennyson, T. Furtenbacher. S.N. Yurchenko & A.G. Csaszar, *JQSRT*, 316, 108902 (2024).

MARVEL (measured active rotation-vibration energy levels)

T. Furtenbacher, A.G. Csaszar & J. Tennyson, *J. Molec. Spectrosc.*, 245, 115 (2007).

T. Furtenbacher & A.G. Csaszar, *JQSRT*, 115, 929 (2012).

Completed studies:

1. Water, IUPAC task group, *JQSRT* (2009-14)
High accuracy, Furtenbacher et al. *PCCP* (2018)
Full update (W2020), Furtenbacher et al. *JPCRD* (2020)
2. H_3^+ , Furtenbacher *et al.*, *PCCP* (2013) & *J. Chem. Theory Comp.* (2013).
3. NH_3 , Al Derzi *et al.*, *JQSRT* (2015); update Furtenbacher et al. *JQSRT* (2020)
4. C_2 , Furtenbacher *et al.*, *ApJS* (2016).
5. TiO , McKemmish *et al.*, *ApJS* (2017).
6. HCCH , Chubb *et al.*, *JQSRT* (2018).
7. SO_2 , Tobias *et al.*, *JQSRT* (2018).
8. H_2S , Chubb et al., *JQSRT* (2018).
9. ZrO , McKemmish *et al.*, *ApJS* (2018).
10. O_2 , Furtebacher *et al.*, *J. Phys. Chem. Ref. Data* (2019).
11. NH , Darby-Lewis *et al.*, *J. Mol. Spectrosc.* (2019).
12. CaOH , Wang et al., *Astrophys. J. Suppl.* (2020).
13. H_2CO , Al-Derzi *et al.*, *JQSRT* (2021).
14. AlO , Bowesman et al., *MNRAS* (2021).
15. HOCl , Racsai et al., *J. Mol. Spectrosc.* (2022).
16. VO , Bowesman et al., *JQSRT* (2022).
17. CH & OH , Furtenbacher *et al.*, *PCCP* (2022).
18. N_2O , Xu & Tennyson, *JQSRT* (2023).

MARVEL (measured active rotation-vibration energy levels)

T. Furtenbacher, A.G. Csaszar & J. Tennyson, *J. Molec. Spectrosc.*, 245, 115 (2007).

T. Furtenbacher & A.G. Csaszar, *JQSRT*, 115, 929 (2012).

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12. $CaOH$, Wang *et al.*, *Astrophys. J. Suppl.* (2020).
13. H_2CO , Al-Derzi *et al.*, *JQSRT* (2021).
14. AlO , Bowesman *et al.*, *MNRAS* (2021).
15. $HOCl$, Racsai *et al.*, *J. Mol. Spectrosc.* (2022).
16. VO , Bowesman *et al.*, *JQSRT* (2022).
17. CH & OH , Furtenbacher *et al.*, *PCCP* (2022).
18. N_2O , Xu & Tennyson, *JQSRT* (2023).

ORBYTS

(original research by young Twinkle scientists)

C. Sousa-Silva *et al.*,

When can students start performing original research?

Phys. Educ., 53, 015020 (2018).

2021 UK



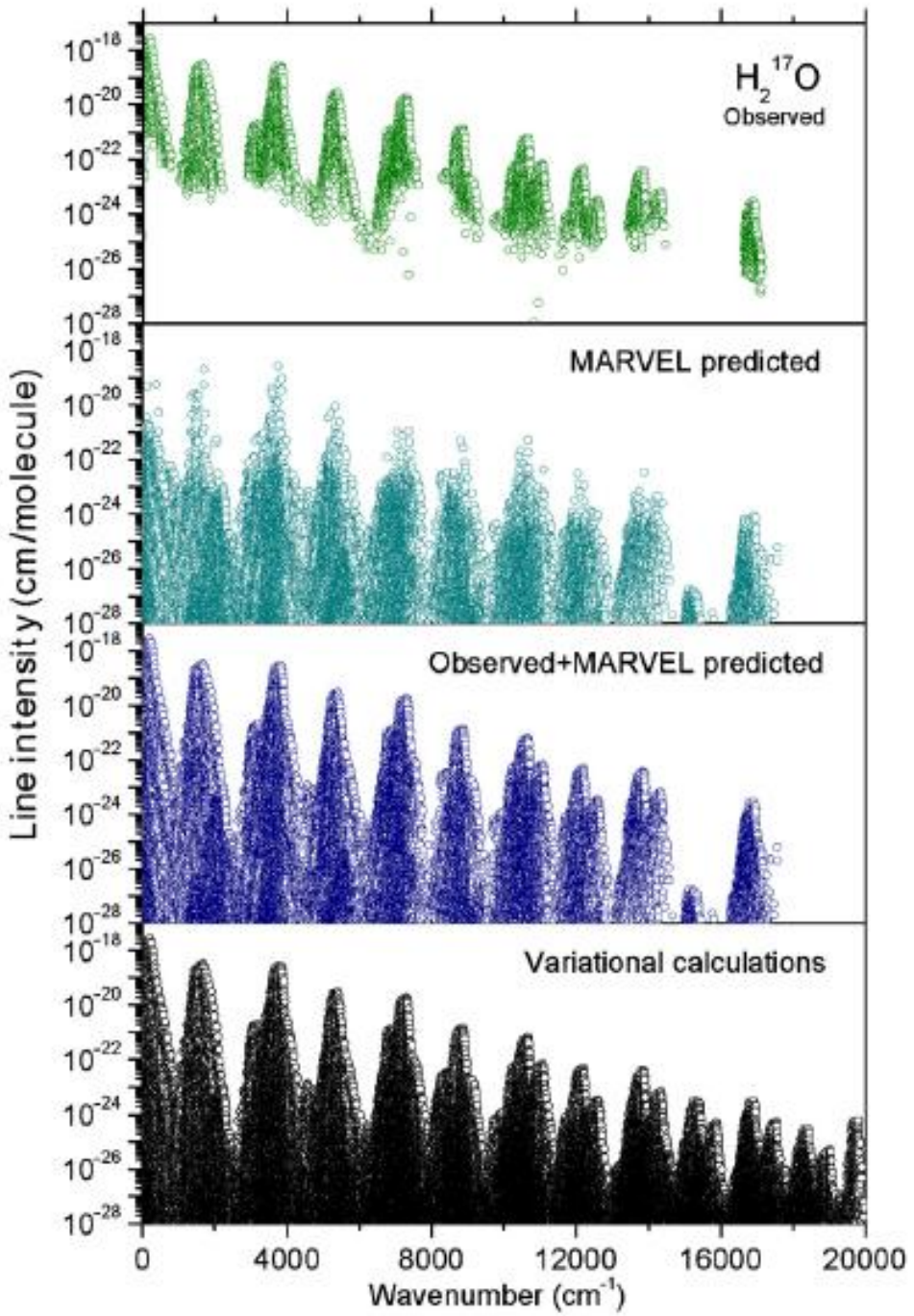
award for

National Education Opportunities Network

Widening Access Initiative (Outreach)



2022 INSPIRE award



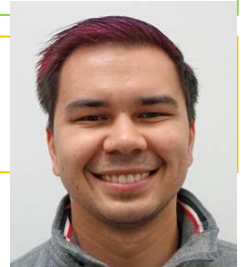
Tennyson+ IUPAC Critical Evaluation of the Rotational-Vibrational Spectra of Water Vapor. Part I. Energy Levels and Transition Wavenumbers for H_2^{17}O and H_2^{18}O , *J. Quant. Spectrosc. Rad. Transf.*, **110**, 573 (2009).

Improve line position for high-res exoplanet observations

For isotopologues can generate “pseudo-experimental levels using Obs-Calc shifts from the parent species
Polyansky+ *MNRAS* **466**, 1363 (2017).

Isotope Extrapolation (IE)
L.K. McKemmish+ *RAS Tech. Instr.*, **3**, 565 (2024)

M/L for isotopologue? See Poster by Marco Barnfield



ExoMol

Hot line lists; Published in MNRAS

MARVELised

MARVEL in progress

I. BeH, MgH, CaH

II. SiO

III. HCN/HNC

IV. CH₄

V. NaCl, KCl

VI. PN

VII. PH₃

VIII. H₂CO

IX. AlO

X. NaH

XI. HNO₃

XII. CS

XIII. CaO

XIV. SO₂

XV. HOOH

XVI. H₂S

XVII. SO₃

XVIII. VO

XIX. H₂¹⁸O, H₂¹⁷O

XX. H₃⁺

XXI. NO

XXII. SiH₄

XXIII. PO, PS

XXIV. SiH

XXV. SiS

XXVI. SN, SH

XXVII. AlH

XXVIII. C₂H₄

XXIX. CH₃Cl

XXX. H₂¹⁶O

XXXI. C₂

XXXII. TiO

XXXIII. MgO

XXXIV. PH

XXXV. NH₃

XXXVI. SH (UV)

XXXVII. HCCH

XXXVIII. SiO₂

XXXIX. CO₂

XL. H₃O⁺

XLI. NaOH, KOH

XLII. NO (UV)

XLIII. SiO (UV)

XLIV. NaO

XLV. MgH (UV), CaH (UV)

XLVI. SiN

XLVII. CaOH

XLVIII. AlCl

XLVIII. H₂CS

L. H₃⁺, H₂D⁺, D₂H⁺, D₃⁺

Li. LiOH

LII. CH⁺

LIII. YO

LIV. VO (hyperfine)

LV. AlH (predissociation)

LVI. SO

LVII. CH₄

LVIII. OCS

LIX. N₂O

LX. ¹⁵NH₃

LXI. OH

LXII. C₃

LXIII. HDO

LXIV. PN

LXV. NiH

2024 data releases:

J. Tennyson *et al.*, *MNRAS* **326**, 109083 (2024)

ExoMol

Hot line lists; Published in MNRAS
MARVELised
MARVEL in progress

I. BeH, MgH, CaH
II. SiO
III. HCN/HNC
IV. CH₄
V. NaCl, KCl
VI. PN
VII. PH₃
VIII. H₂CO
IX. AlO
X. NaH
XI. HNO₃
XII. CS
XIII. CaO
XIV. SO₂
XV. HOOH
XVI. H₂S
XVII. SO₃
XVIII. VO

XIX. H₂¹⁸O, H₂¹⁷O
XX. H₃⁺
XXI. NO
XXII. SiH₄
XXIII. PO, PS
XXIV. SiH
XXV. SiS
XXVI. SN, SH
XXVII. AlH
XXVIII. C₂H₄
XXIX. CH₃Cl
XXX. H₂¹⁶O
XXXI. C₂
XXXII. TiO
XXXIII. MgO
XXXIV. PH
XXXV. NH₃
XXXVI. SH (UV)

XXXVII. HCCH
XXXVIII. SiO₂
XXXIX. CO₂
XL. H₃O⁺
XLI. NaOH, KOH
XLII. NO (UV)
XLIII. SiO (UV)
XLIV. NaO
XLV. MgH (UV), CaH (UV)
XLVI. SiN
XLVII. CaOH
XLVIII. AlCl
XLVIII. H₂CS
L. H₃⁺, H₂D⁺, D₂H⁺, D₃⁺
Li. LiOH
LII. CH⁺
LIII. YO
LIV. VO (hyperfine)
LV. AlH (predissociation)



LVI. SO
LVII. CH₄
LVIII. OCS
LIX. N₂O
LX. ¹⁵NH₃
LXI. OH
LXII. C₃
LXIII. HDO
LXIV. PN
LXV. NiH

Need for other MARVEL projects?

2024 data releases:

J. Tennyson *et al.*, *JQSRT* **326**, 109083 (2024)

Databases

[ExoMol](#)

[ExoMolOP](#)

[LIDB](#)

[ExoMolHR](#)

[ExoPhoto](#)

ExoMol Database

ExoMol is the main database of molecular line lists for exoplanets and other hot atmospheres.

ExoMol Secondary databases

- [ExoMolOP: Opacities](#)
- [LIDB: Database of molecular radiative lifetimes for plasma processes](#)
- [ExoMolHR: High Resolution Database](#)
- [ExoPhoto: Photo-dissociation cross sections](#)



ExoMol is funded by the ERC under the Advanced Investigator Projects 267219 and 883830



Jingxin Zhang

ExoMolHR: extracts only high res lines ($R > 100000$)

Jingxin Zhang, C. Hill, J. Tennyson & S.N. Yurchenko, ExoMolHR:
A Relational Database of Empirical High-Resolution Molecular Spectra,
Astrophys. J. Suppl., **276**, 67 (2025).

ExoMolHR

High Resolution Database

@NASA+ESA, and The Hubble Heritage Team STScI/AURA

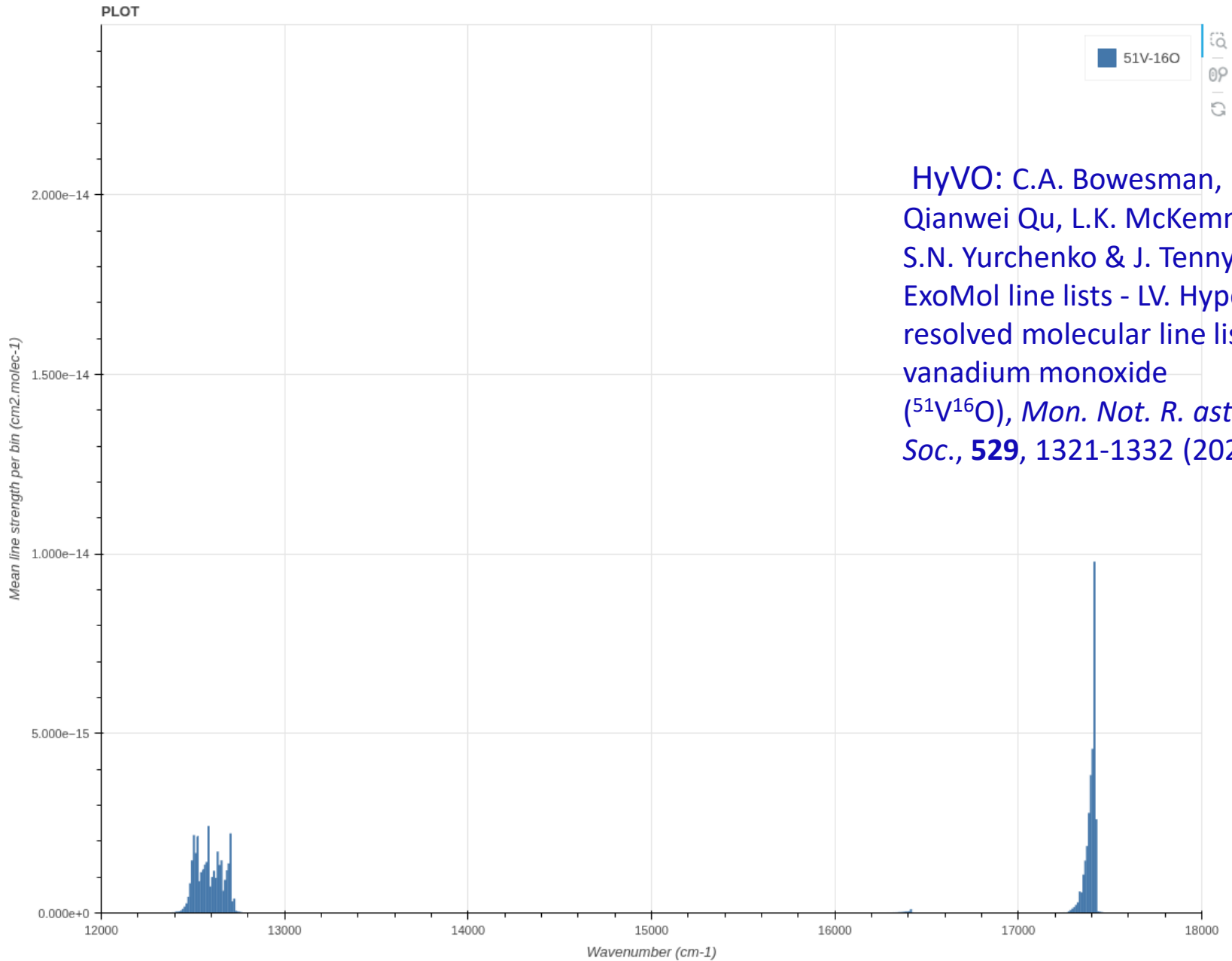
[Home](#)

Molecules

Step 1: Choose molecules

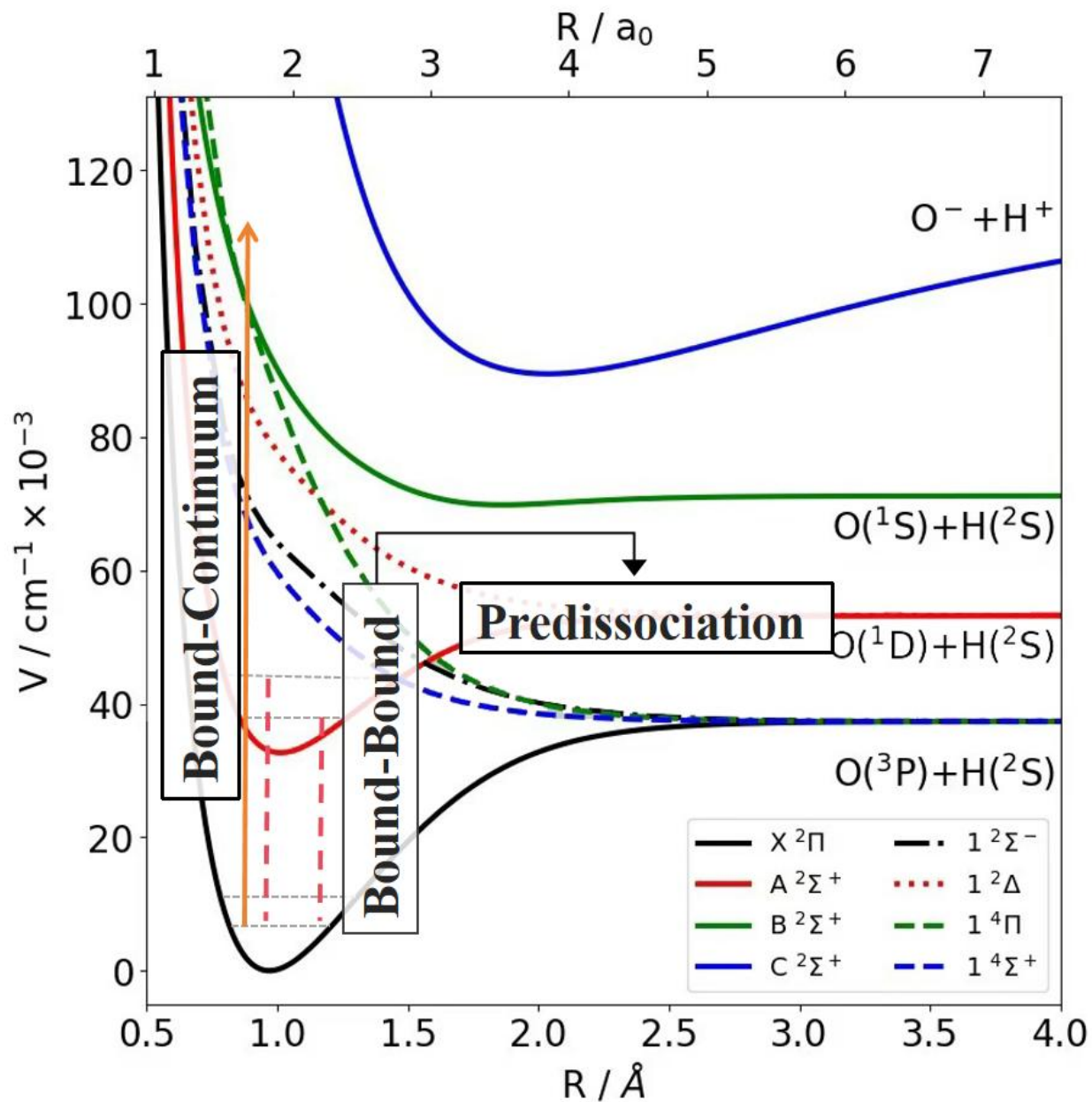
Selected Molecules:

Molecule	Molecule Name	Mass (Da)	Choose
AlCl	Aluminum monochloride	62.432	<input type="checkbox"/>
AlH	Aluminum hydride	27.990	<input type="checkbox"/>
AlO	Aluminum monoxide	42.981	<input type="checkbox"/>
C ₂	Dicarbon	24.022	<input type="checkbox"/>
C ₂ H ₂	Acetylene	26.038	<input type="checkbox"/>
CaH	Calcium monohydride	41.086	<input type="checkbox"/>
CH ₄	Methane	16.043	<input type="checkbox"/>
CN	Cyano radical	26.018	<input type="checkbox"/>



HyVO: C.A. Bowesman,
Qianwei Qu, L.K. McKemmish,
S.N. Yurchenko & J. Tennyson,
ExoMol line lists - LV. Hyperfine-
resolved molecular line list for
vanadium monoxide
($^{51}\text{V}^{16}\text{O}$), *Mon. Not. R. astr.*
Soc., **529**, 1321-1332 (2024).

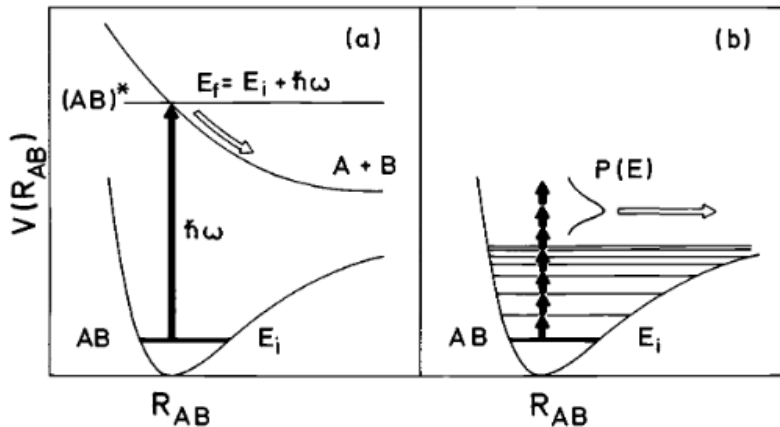
Into the deep blue yonder...



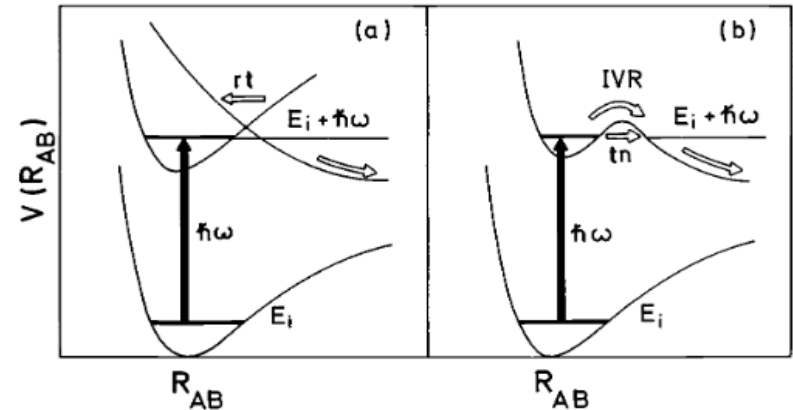
photodissociation

Fragmentation of a molecule after absorption one or more photons.

Direct photodissociation:



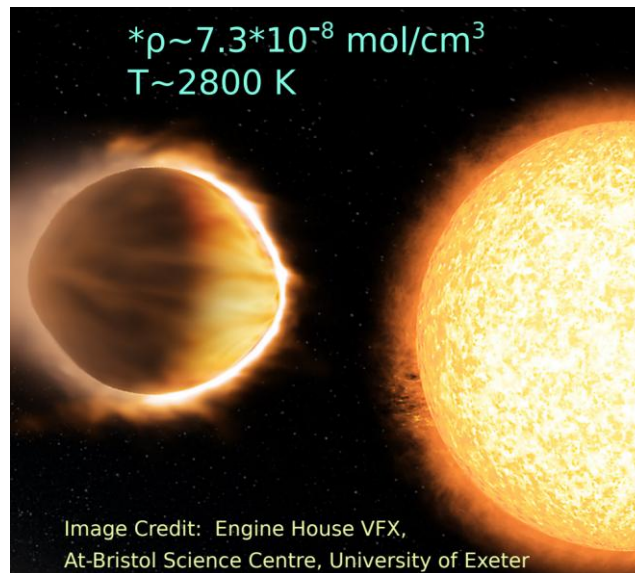
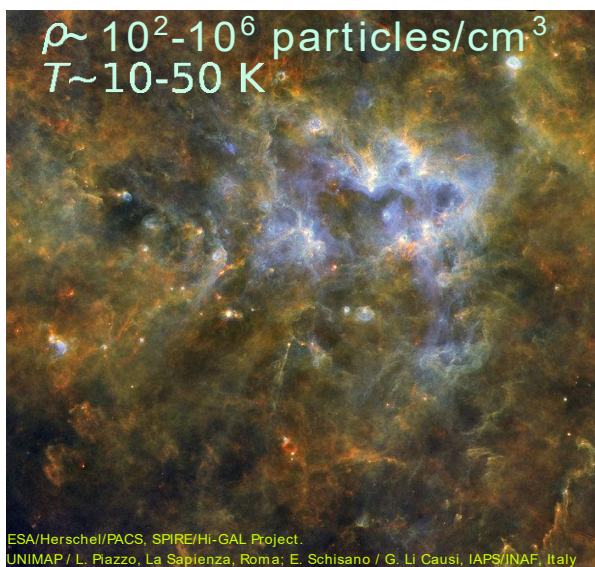
Indirect photodissociation:



Reinhard Schinke, *Photodissociation Dynamics Spectroscopy and Fragmentation of Small Polyatomic Molecules*, Cambridge University Press (1993).

Photodissociation impacts atmospheres of exoplanets in UV-rich environments.

Temperature-dependent models required; currently state-of-the-art photodissociation calculations based on the interstellar medium (ie $T=0$ K).



Measurements:

O. Venot *et al*, *ApJ*, 2016, **830**, 77; B. Fleury *et al*, *ApJ*, 2019, **871**, 158; N. K. Lewis *et al*, *ApJL*, 2020, **902**, L19.

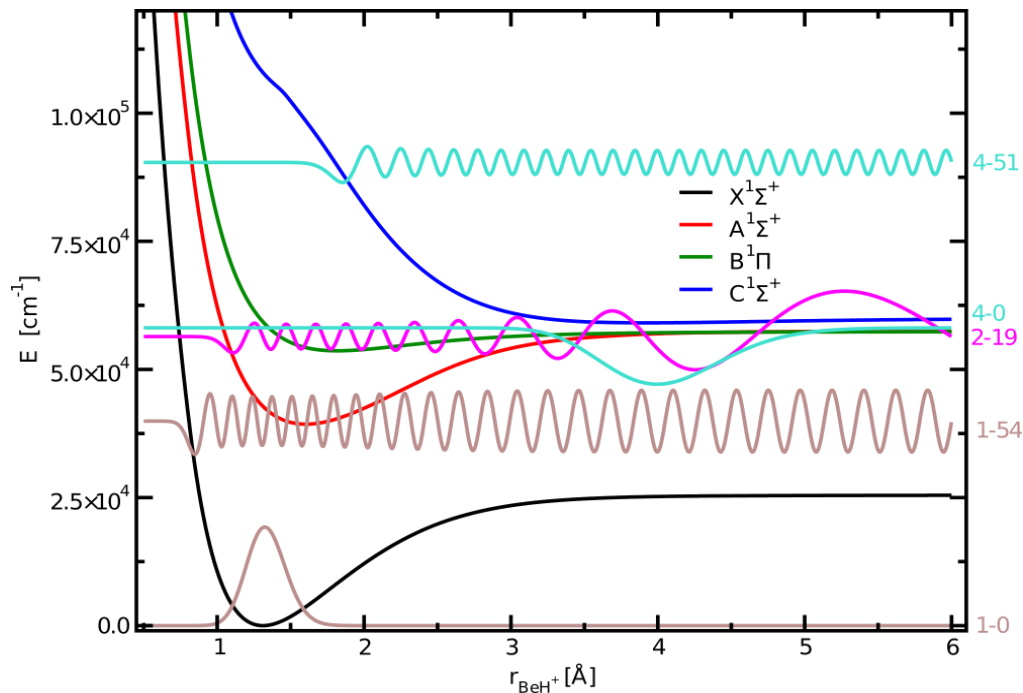
Leiden database:

A.N. Heays *et al*, *A&A*, 2017 **602**, A105.
H.R. Hrodmarsson & E.F. van Dishoeck, *A&A*, 2023, 675, A25

+ Atmospheric density from Jupiter,
temperature from WASP-121b stratosphere.

Our Approach

Given the **potential energy curves** and **transition dipole moments** between them, program **Duo** solves the 1-D Schrödinger equation and calculates intensities.



σ recovered with **ExoCross**, applying a line profile to the intensity:

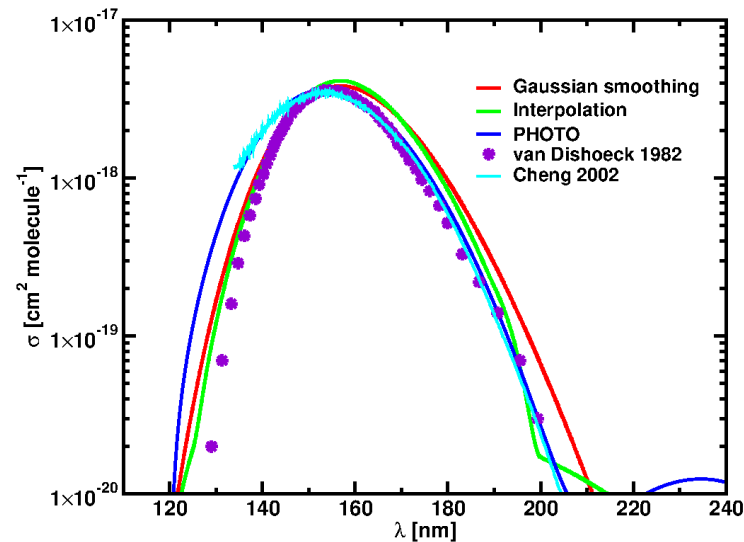
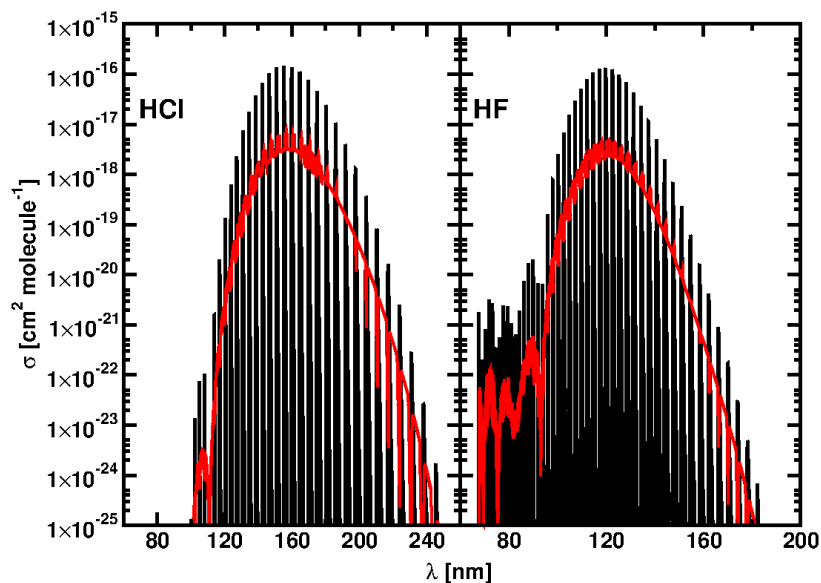
$$\sigma_{fi}(\nu) = I(f \leftarrow i) f_{\nu fi}(\nu)$$

Duo: [S.N. Yurchenko *et al*, CPC, 2016, 202, 262](https://github.com/Trovemaster/Duo); <https://github.com/Trovemaster/Duo>

ExoCross [S.N. Yurchenko *et al*, A&A, 2018, 614, A131](https://github.com/Trovemaster/exocross/); <https://github.com/Trovemaster/exocross/>

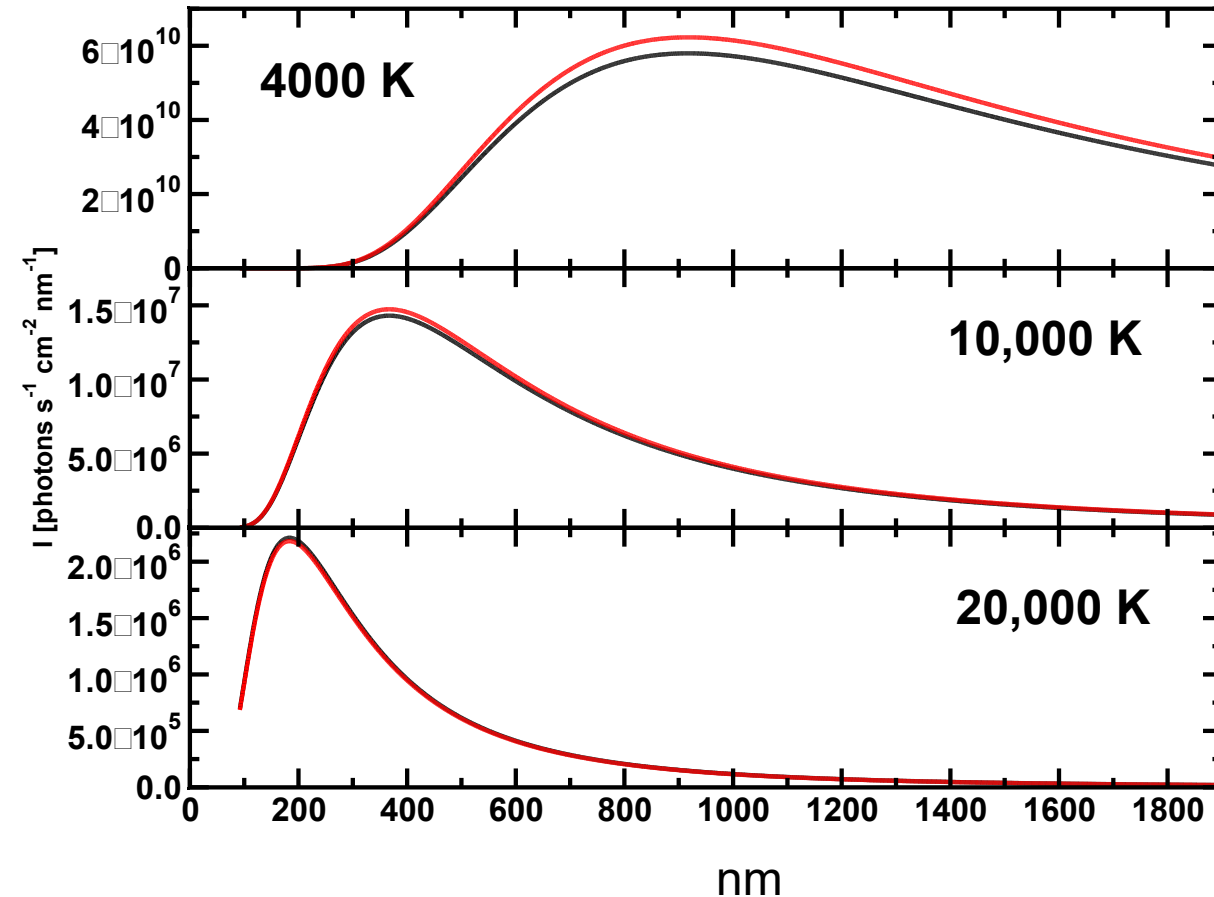
Our Approach

- Discretized continuum spectrum
- Gaussian smoothing function
- Full rovibrational treatment to allow for T-dependence



M. Pezzella, S.N. Yurchenko & J. Tennyson, A method for calculating temperature-dependent photodissociation cross sections and rates, *Phys. Chem. Chem. Phys.*, **23**, 16390-16400 (2021).

Black Body flux

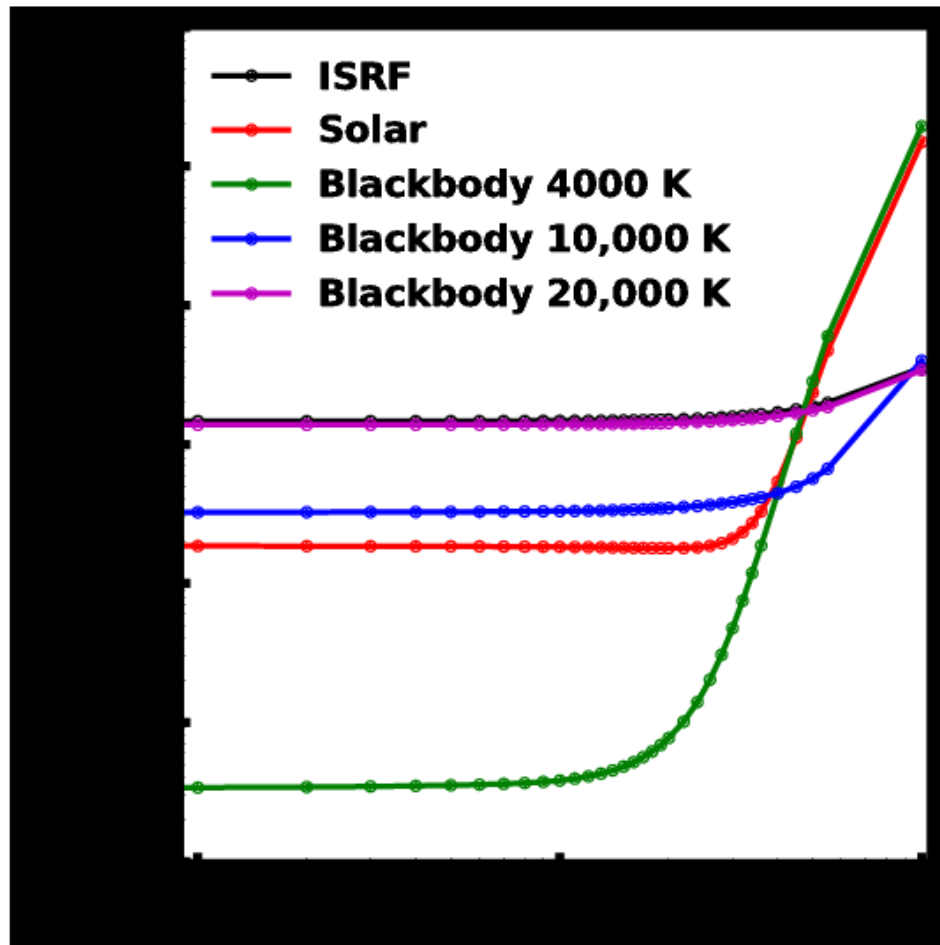


T Tauri stars: young stars moving towards the main sequence.

Herbig Ae stars: young A stars. They are still embedded in gas dust envelope.

B-type star: very luminous and blue stars. They are energetic and short lived.

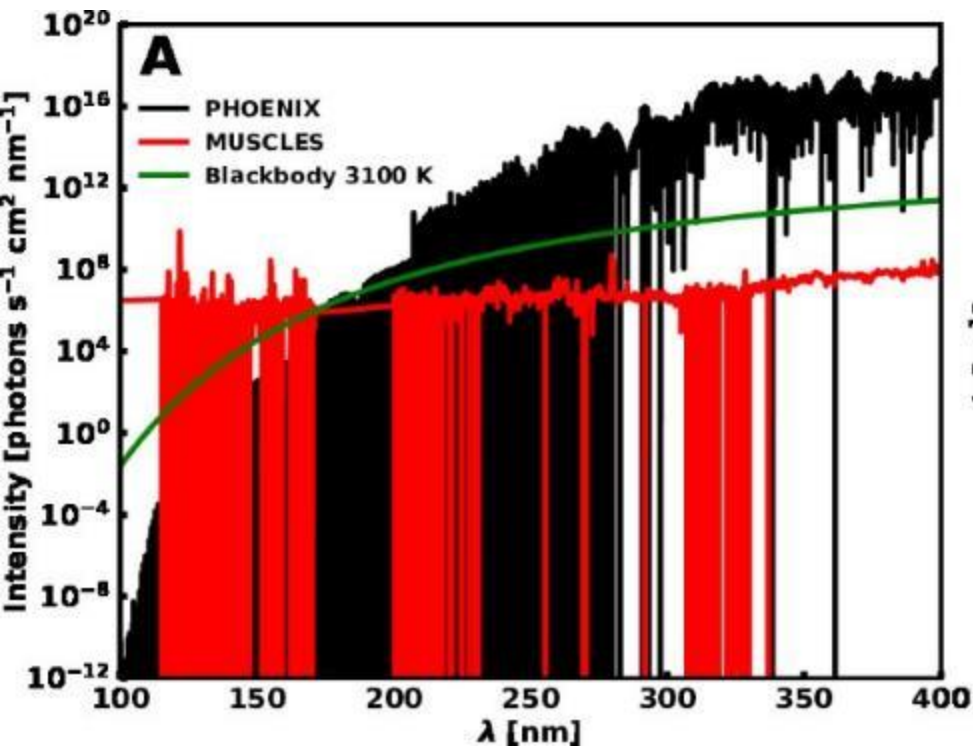
Computed rate of photodissociation of HCl in different radiation fields



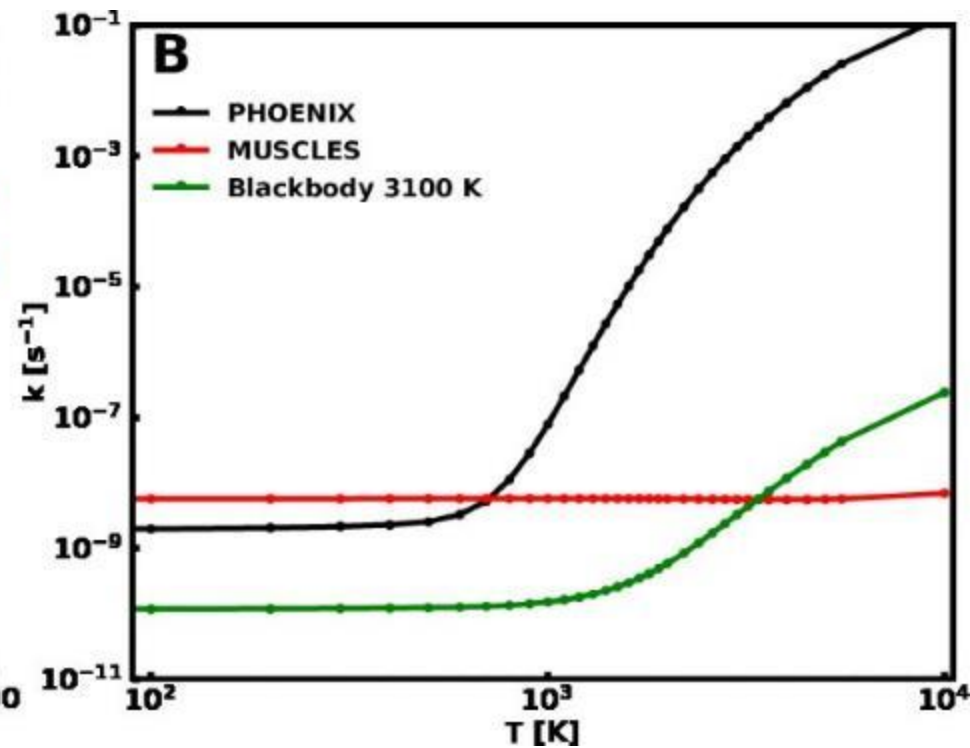
Marco Pezzella

- temperature of the molecule

HCl photodissociation rates in radiation fields of Proxima Centauri



Radiation fields



photodissociation rates

Urgent need to understand stellar radiation fields in the UV for cool stars



MAUVE

UV spectroscopy to monitor stars

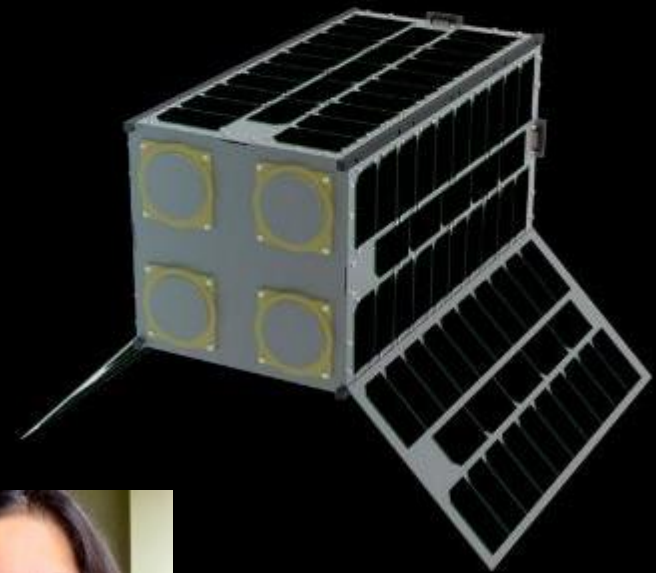
Launch in Q4 2025

15cm class telescope - 50kg in LEO

Construction started November 2022

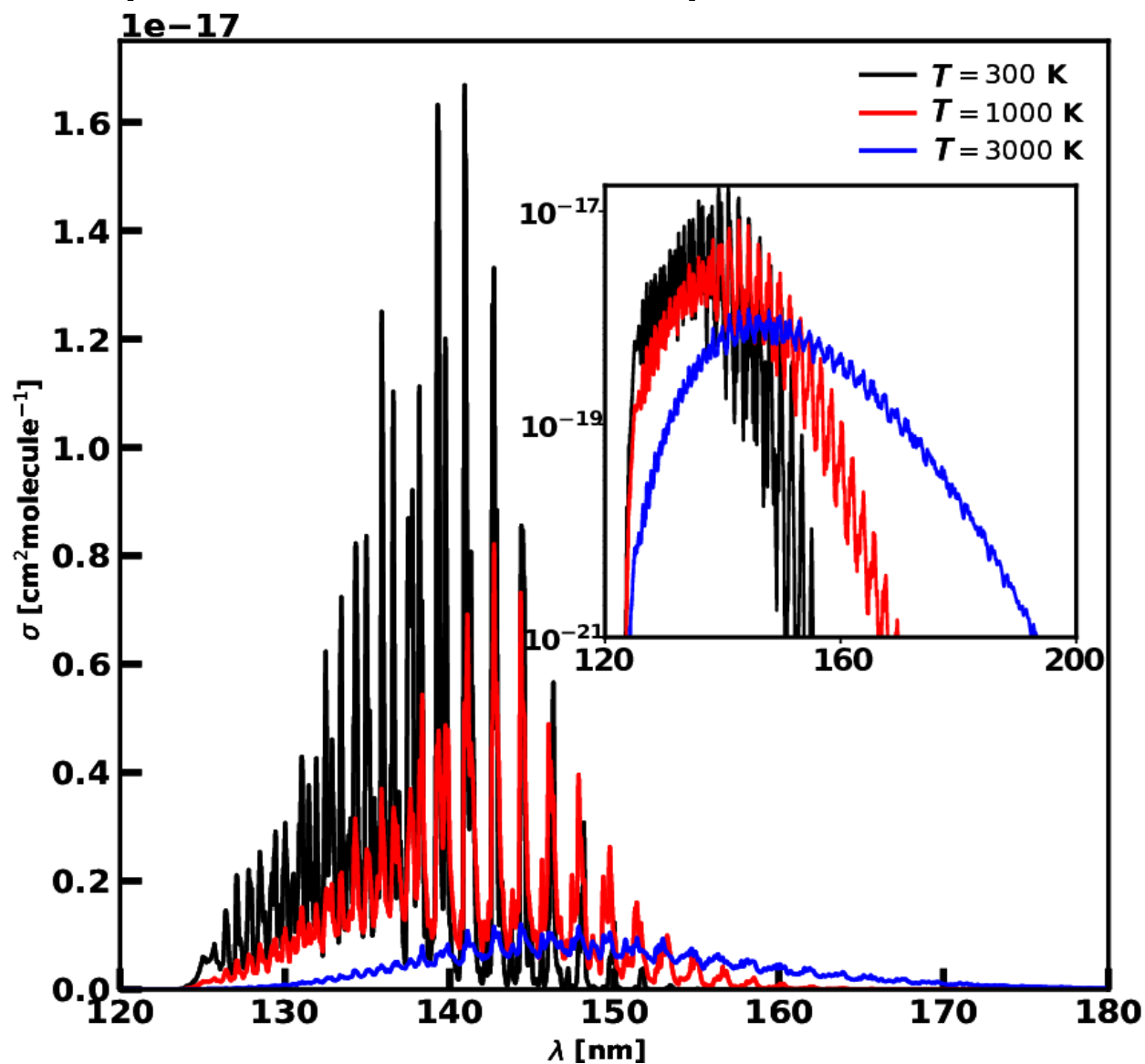
Built by C3S LLC & ISISPACE Group

Funded by European Commission



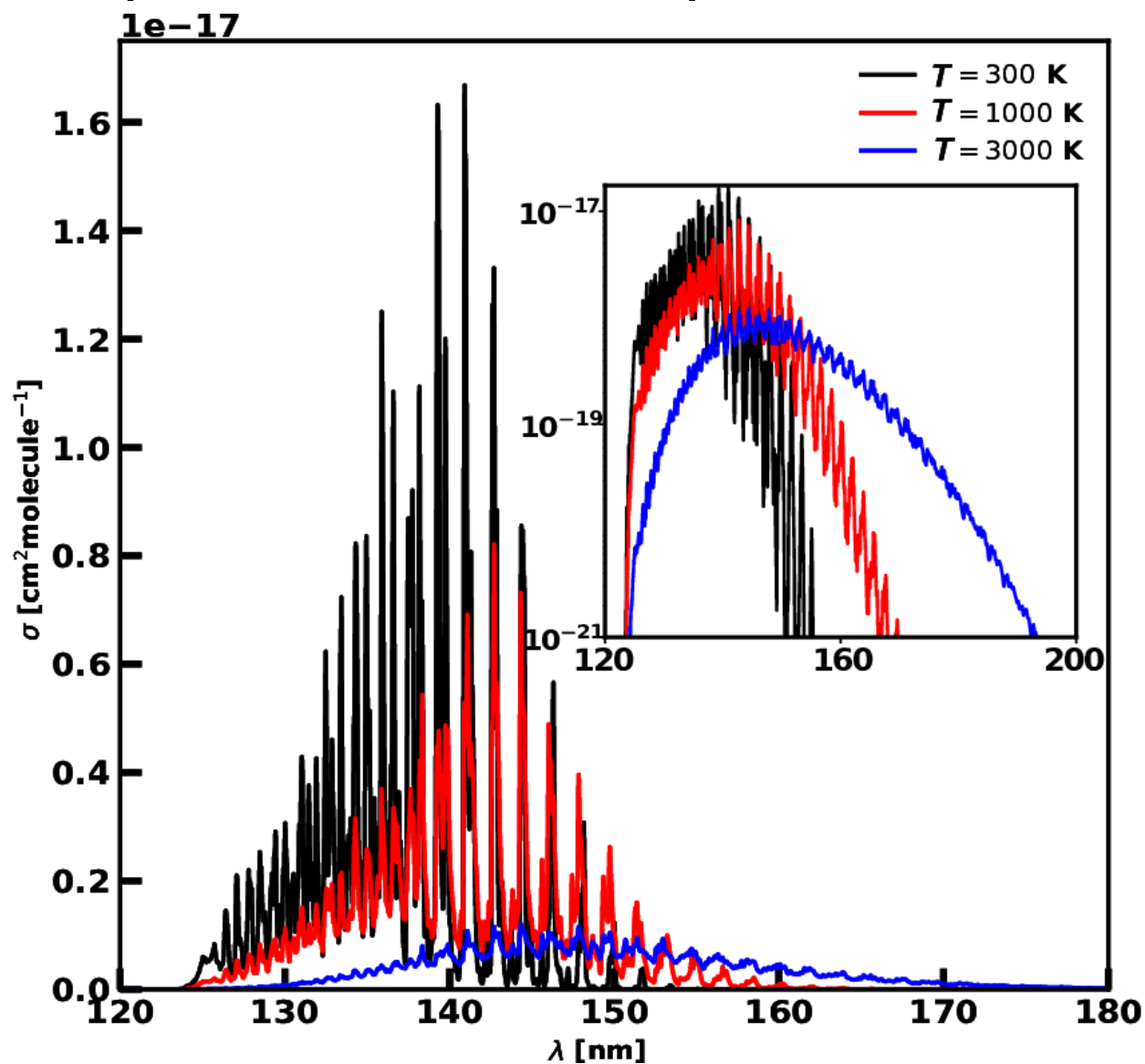
Parul Janagal (BSSL)
Friday pm

T-dependence of HCN photodissociation



M. Pezzella, S.N. Yurchenko, J. Tennyson & A. Mitrushchenkov,
Phys. Chem. Chem. Phys., **26**, 27519-27529 (2024).

T-dependence of HCN photodissociation

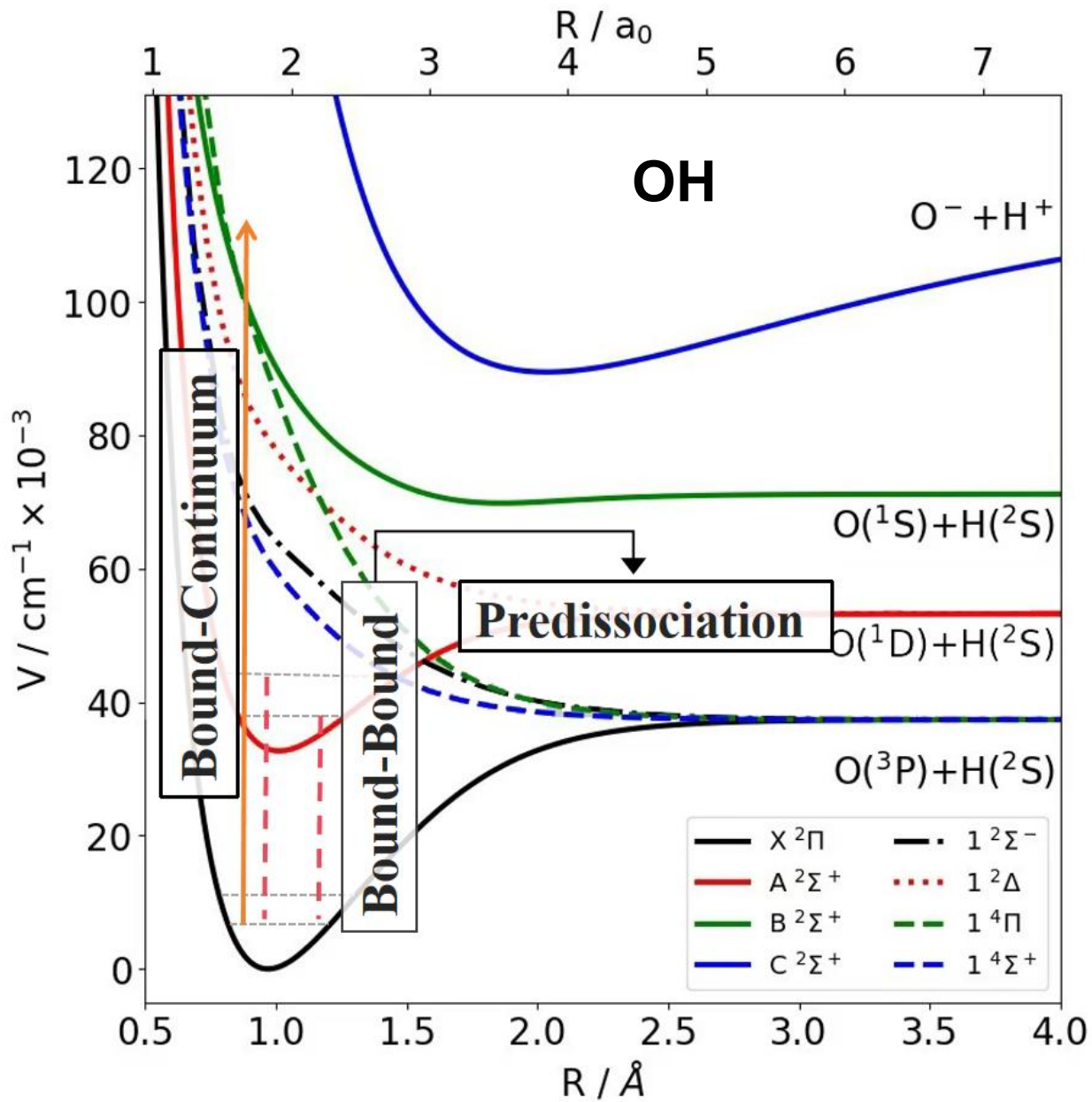


H₂S and H₂O
photodissociation



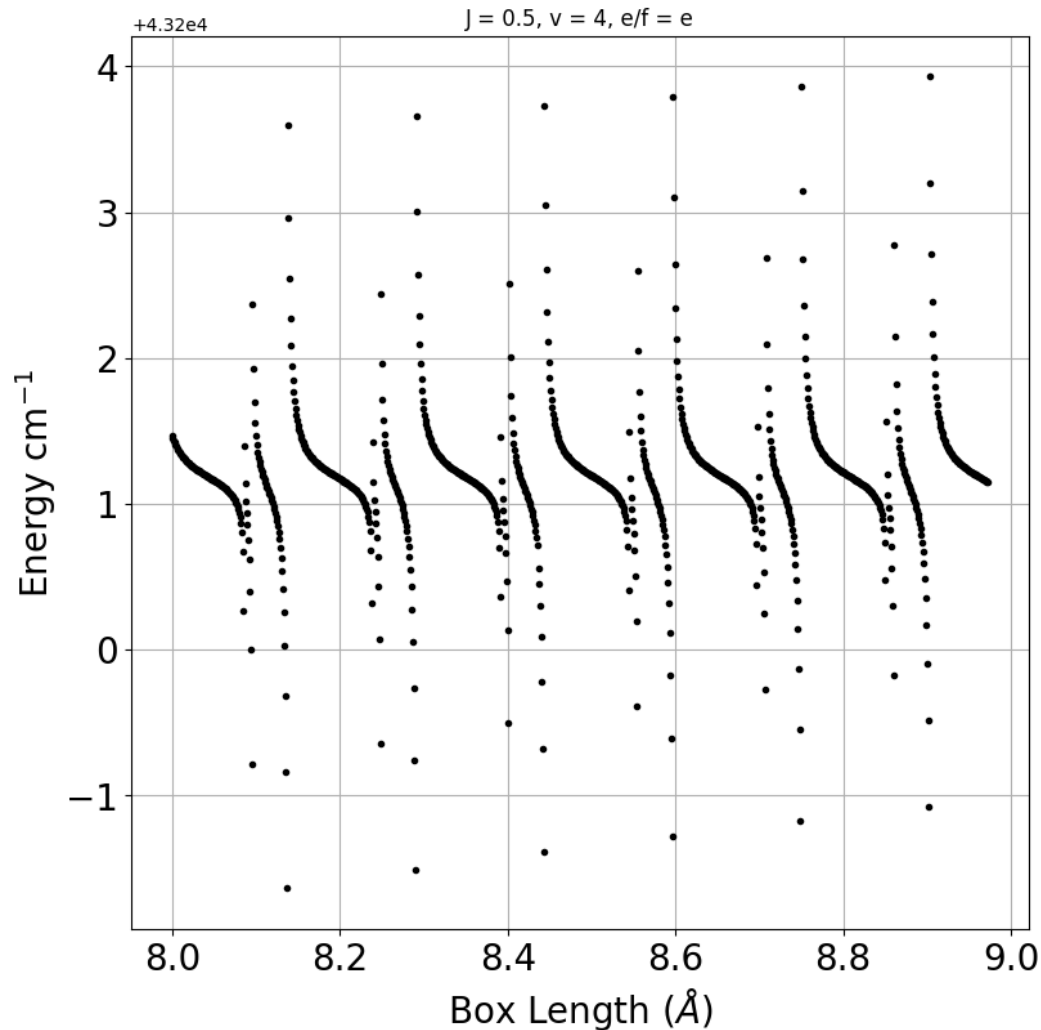
Armando Perri
Friday pm

M. Pezzella, S.N. Yurchenko, J. Tennyson & A. Mitrushchenkov,
Phys. Chem. Chem. Phys., **26**, 27519-27529 (2024).



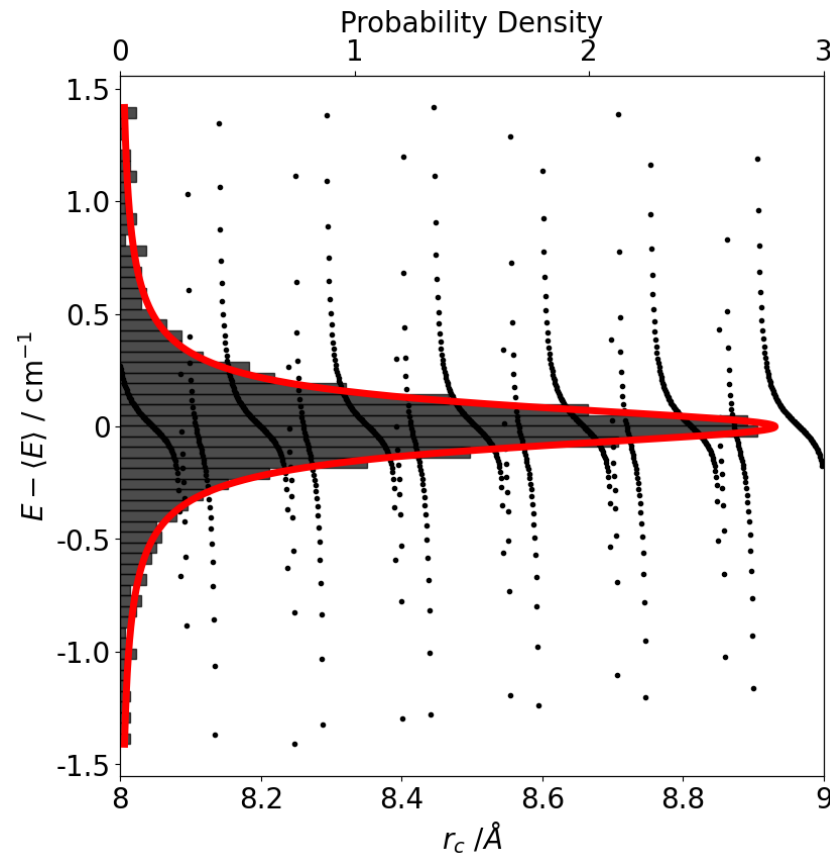
Georgi Mitev

OH Predissociation: Stabilisation method

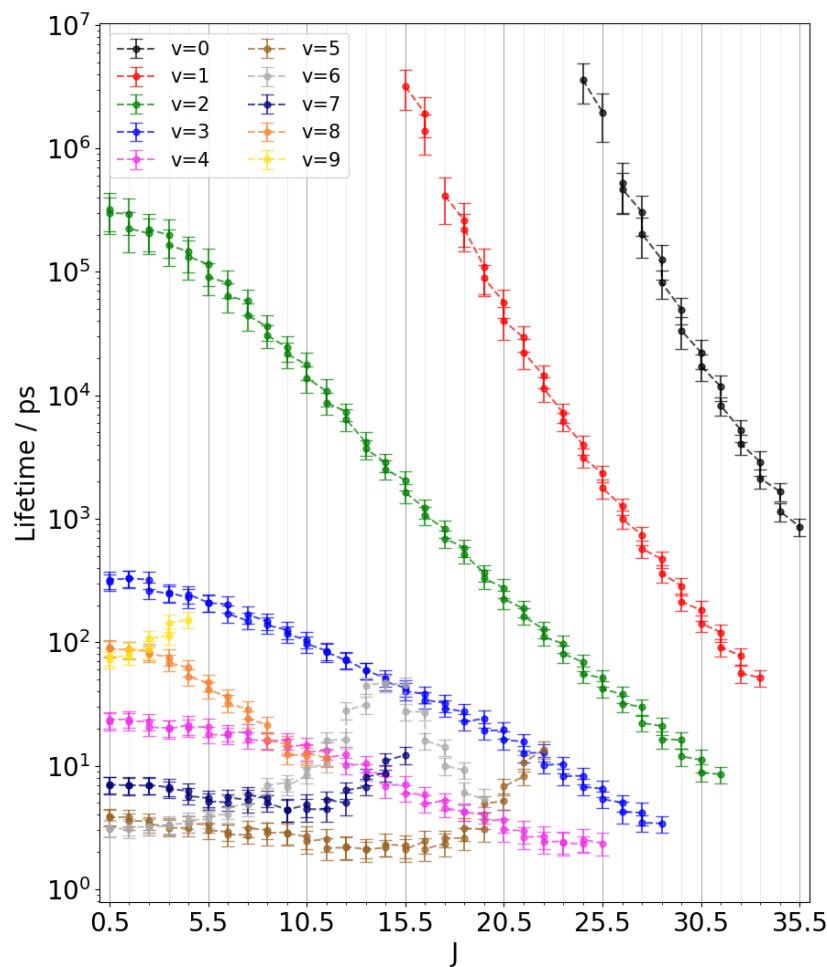


G.B. Mitev, S.N. Yurchenko & J. Tennyson, Predissociation dynamics of the hydroxyl radical (OH) based on a five-state spectroscopic model, *J. Chem. Phys.*, **160**, 144110 (2024).

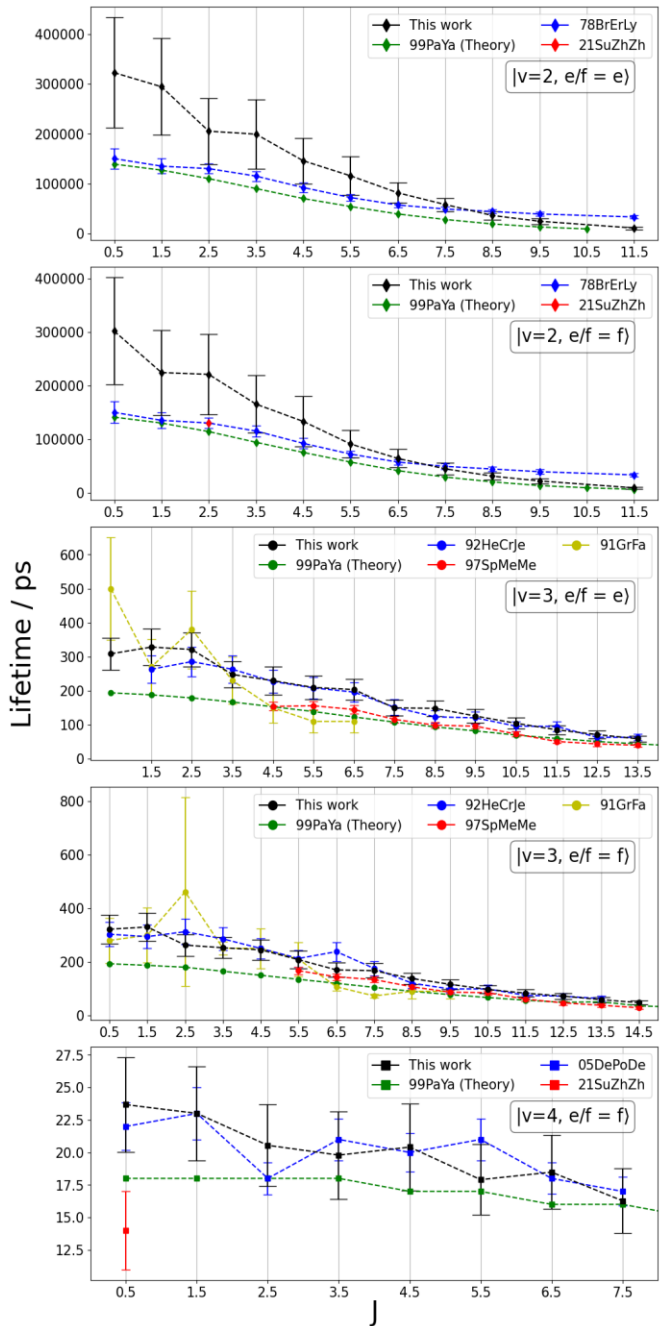
Aggregating data gives position and width of the predissociative states



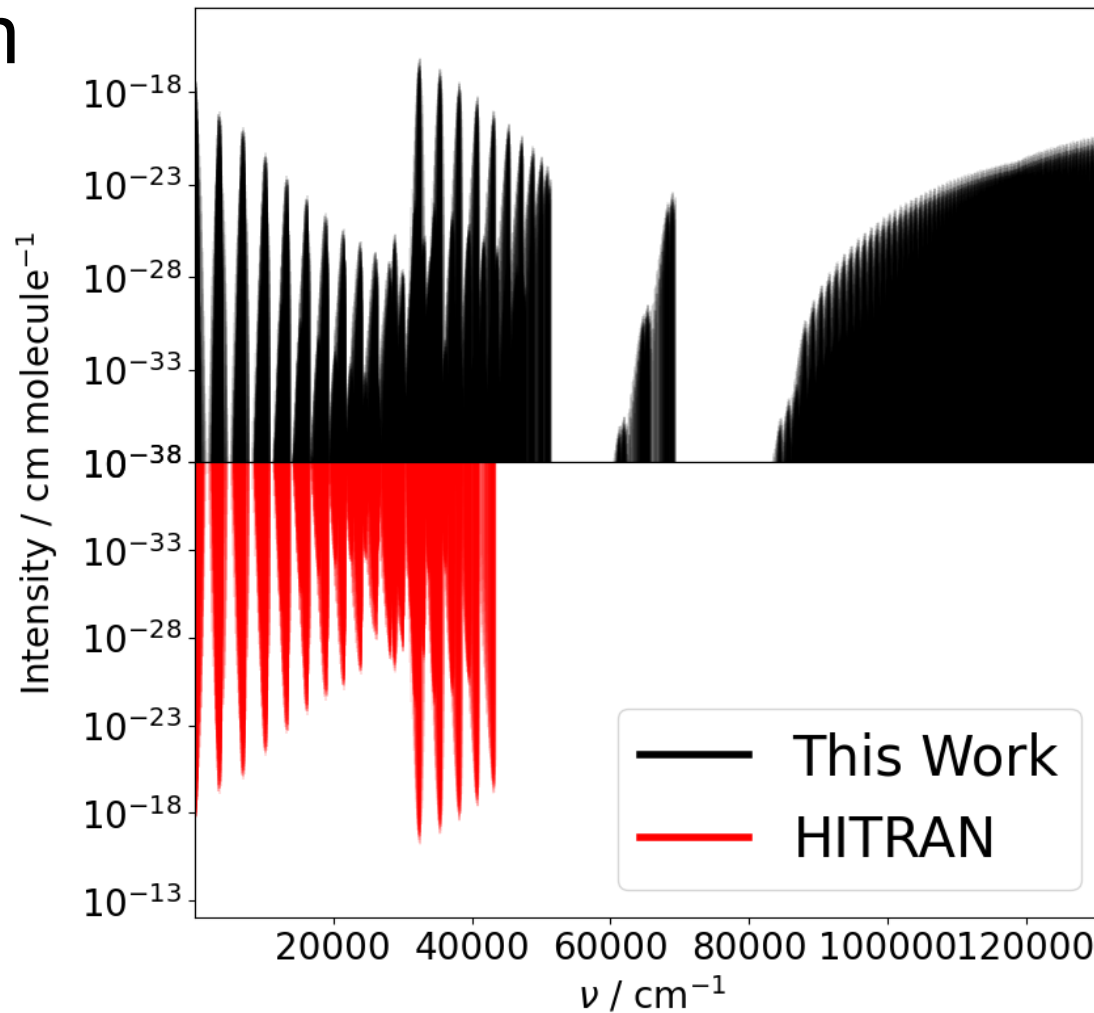
Computed predissociative lifetimes



G.B. Mitev, S.N. Yurchenko & J. Tennyson,
 Predissociation dynamics of the hydroxyl radical (OH)
 based on a five-state spectroscopic model,
J. Chem. Phys., **160**, 144110 (2024).

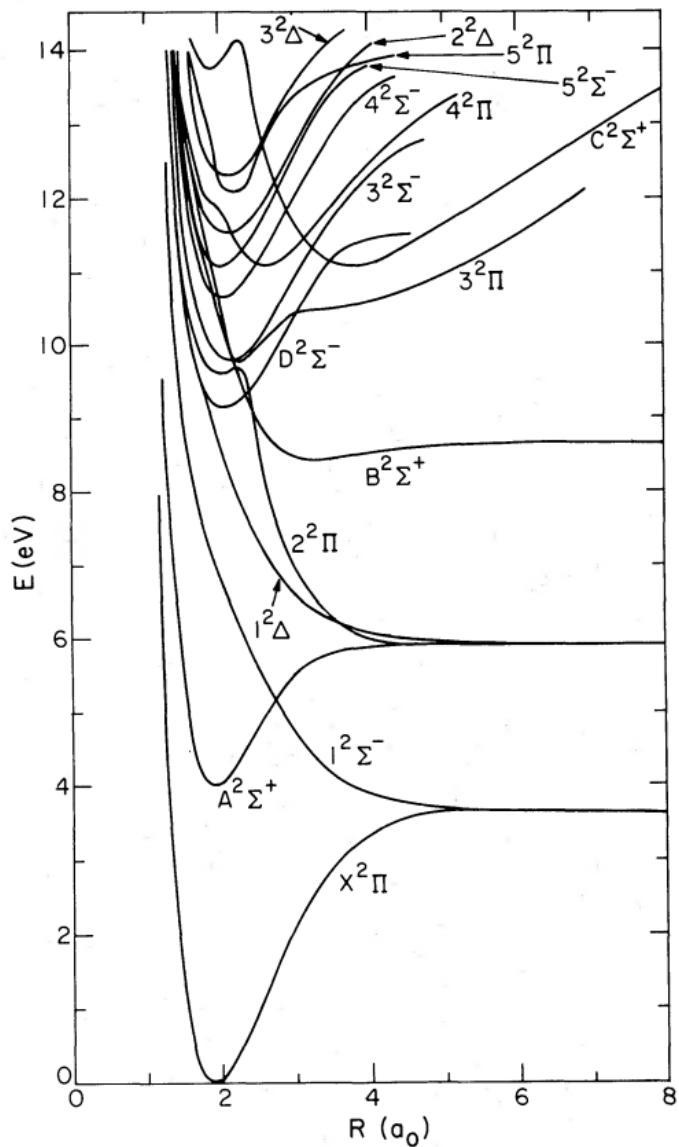


OH photoabsorption: Line list, predissociation + continuum



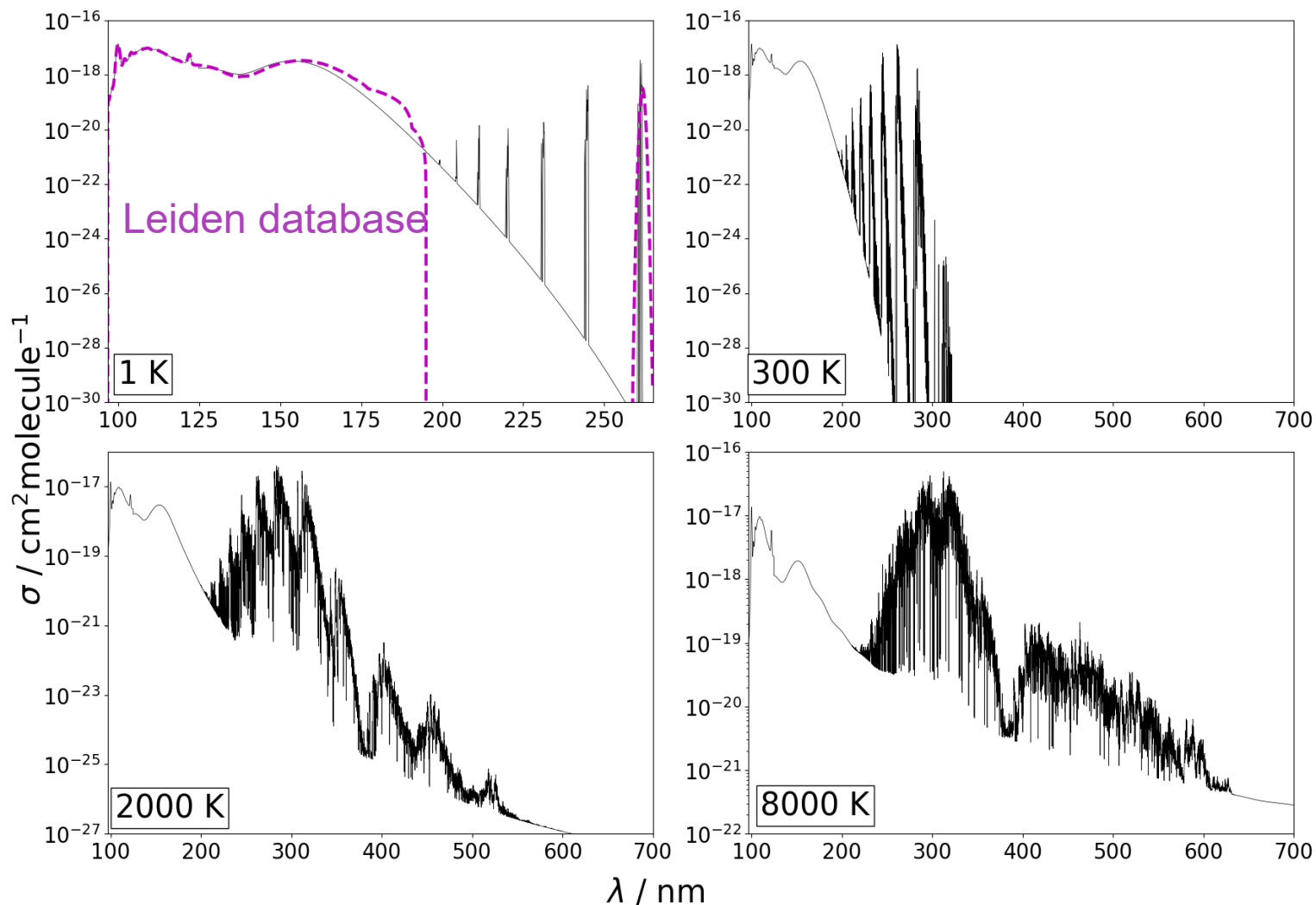
G.B. Mitev, C.A. Bowsman, S.N. Yurchenko & J. Tennyson, ExoMol Line Lists - LXI: A trihybrid linelist for rovibronic transitions of the hydroxyl radical (OH), *Mon. Not. R. astr. Soc.*, **536**, 3401-3420 (2025)

Photodissociation: requires more curves!



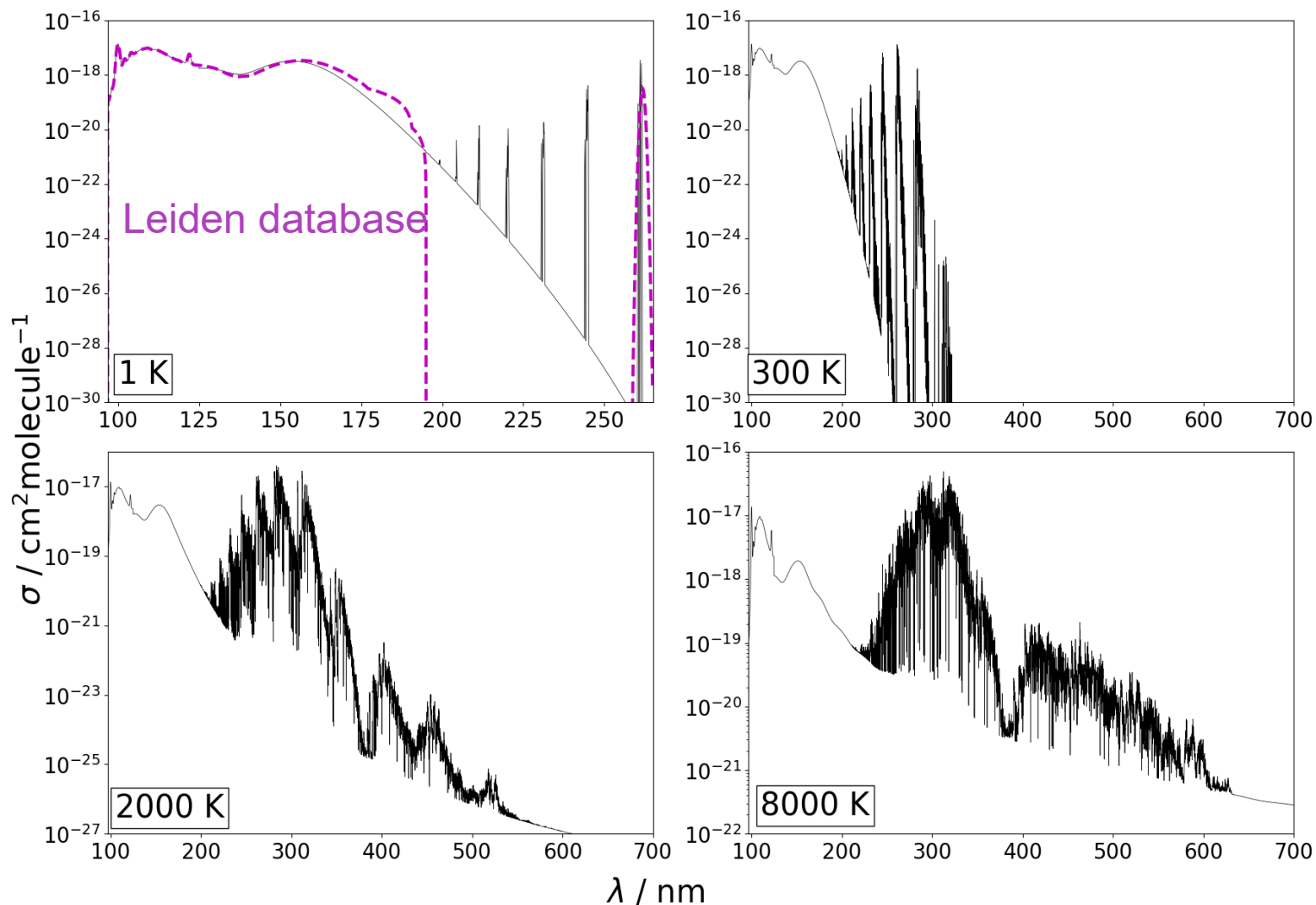
van Dishoeck E. F., Dalgarno A., 1984,
Astrophys. J., 277, 576

Computed photodissociation cross sections: T-dependent



G.B. Mitev, M Pezzella, C.A. Bowsman, Jingxin Zhang, S.N. Yurchenko & J. Tennyson, ExoMol Photodissociation Cross Sections – II: Continuum Absorption and Predissociation Spectra for the Hydroxyl Radical, *Mon. Not. R. astr. Soc.*, **539**, 3732 (2025)

Computed photodissociation cross sections: T-dependent



G.B. Mitev, M Pezzella, C.A. Bowsman, Jingxin Zhang, S.N. Yurchenko & J. Tennyson, ExoMol Photodissociation Cross Sections – II: Continuum Absorption and Predissociation Spectra for the Hydroxyl Radical, *Mon. Not. R. astr. Soc.*, **539**, 3732 (2025)



CH photodissociation

Andrei Sokolov
Saturday pm

Non-LTE photodissociation of OH

Charles Bowesman
Friday am



Databases

[ExoMol](#)

[ExoMolOP](#)

[LIDB](#)

[ExoMolHR](#)

[ExoPhoto](#)

ExoMol Database

[ExoMol](#) is the main database of molecular line lists for exoplanets and other hot atmospheres.

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- [ExoMolHR: High Resolution Database](#)
- [ExoPhoto: Photo-dissociation cross sections](#)

ExoMol is funded by the ERC under the Advanced Investigator Projects 267219 and 883830



ExoPhoto: photodissociation cross sections

Qing-He Ni: Friday am



Qing-He Ni, C. Hill, S.N. Yurchenko, M. Pezzella, A.Z. Fateev, Zhi Qin, O. Venot & J. Tennyson, ExoPhoto: A database of temperature dependent photodissociation cross sections, *RAS Tech. Instr.* (2025)

Data / By Data Type

Search

Molecules

Atoms

By Data Type

Bibliography

Licence

ExoMolHR

Databases

ExoPhoto: Species with Photo-dissociation cross sections

Search species:

metal hydrides

MgH

AlH

other hydrides

OH

HCl

HF

metal oxides

MgO

NaO

other oxides

CO

O₂

triatomic molecules

H₂O

CO₂

SO₂

other diatomics

CS

AlCl

AlF

larger molecules

NH₃

H₂CO

C₂H₄

C₂H₂

ions

HeH⁺

**Only 20 species: which others are needed?
Are state-resolved cross sections for NLTE studies needed?**

This is the development version of ExoAtom.

Search for species using terms such as 'Al', 'Cr+' or 'W+', or select an element from the periodic table below.

Species All ionization stages?

1 H																	2 He									
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne									
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar									
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr									
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe									
55 Cs	56 Ba											72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra											104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og
		57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu										
		89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr										



Qing-He Ni: Friday am

Qing-He Ni, Rujia Wang, Tianyang Xie, Jingxin Zhang, C. Hill, S.N. Yurchenko & J. Tennyson, ExoPhoto: A database of temperature dependent photodissociation cross sections, *RAS Tech. Instr.*, (submitted).

Pressure broadening

Contributions to line profiles:

1. Natural broadening: lifetime effect

Lorentzian

2. Doppler broadening: thermal motion

Gaussian, T-dependent

3. Pressure broadening: collisional effect

Lorentzian (approx.), P-dependent

Also: line mixing

4. T and P: Voigt profile

Beyond Voigt:

speed-dependence, hard/soft collisions, correlation etc

J. Tennyson et al, Pure Appl. Chem., 86 1931-1943 (2014)

Line broadening: essential

Fortney+ 2019 The need for laboratory measurements and ab initio studies to aid understanding of exoplanetary atmospheres, Astro2020: Decadal Survey on Astronomy and Astrophysics, arXiv:1905.07064

- For ExoMol:
- Need to consider $\sim 10^{13}$ lines
 - About 12 key broadeners
 - High temperatures

Solution:

- Detailed semi-classical calculations with ab initio potential
HCCH – (H₂, He, N₂, HCCH, CO, and CO₂)
A. Sokolov, S.N. Yurchenko, J. Tennyson, R.R. Gamache and B. Vispoel, *JQSRT*, 330, 109225 (2024).

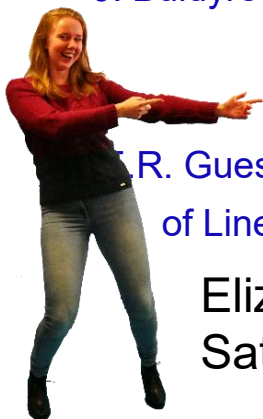
- Approximate semi-classical formulae
J. Buldyreva, S.N. Yurchenko and J. Tennyson, Simple semi-classical model of pressure-broadened infrared/microwave linewidths in the temperature range 200--3000 K, *RAS Tech. Instr.*, 1, 43 (2024)
J. Buldyreva+ *JQSRT*, 313 108843 (2024), and *ApJS* 276, 23 (2025)

Jeanna Buldyreva
Thursday pm

Machine learning

E.R. Guest, J. Tennyson and S.N. Yurchenko, Modelling the Rotational Dependence of Line Broadening using Machine Learning, *J. Mol. Spectrosc.*, **401**, 111901 (2024).

Elizabeth Guest
Saturday am





database with new features
+ data products

www.exomol.com

Coming soon: Atomic line lists
Cooling functions

1. Molecular line lists
2. Cross-sections
3. Partition functions
4. Broadening parameters
5. k-tables and opacities (Chubb+ MNRAS 2021)
6. Lifetimes (Tennyson+ J Phys B, 2016)
7. Cooling functions
8. Lande g-factors (Semenov+, J Mol Spectrosc 2016)
9. Dipoles for molecular control/orientation effects
A Yachmenev, RichMol project (Owens+ Sci Rep 2017)
10. Specific heats (NASA polynomials) (Wang+ JQSRT 2023)
11. LiDB Lifetimes database (Owens+ PSST 2023, JQSRT 2025)
12. ExoMolHR: high res spectra (Zhang+ ApJS 2025)
13. ExoPhoto Photodissociation (Ni+ RASTI 2025)
14. Application program interface (API)

J. Tennyson, S.N. Yurchenko, J. Zhang and others, The 2024 release of the ExoMol database: molecular line lists for exoplanet and other hot atmospheres, *J. Quant. Spectrosc. Rad. Transf.*, **326**, 109083 (2024)

← → ↻ exomol.com/databases/

ExoMol *High temperature molecular line lists for modelling exoplanet atmospheres* Search Everyth

Data ▾ Software Activities ▾ Outreach ▾ About ▾ Contact Databases ▾

Databases

- ExoMol
- ExoMolOP
- LIDB
- ExoMolHR
- ExoPhoto

ExoMol Database


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- ExoMolHR: High Resolution Database
- ExoPhoto: Photo-dissociation cross sections

?

ExoMol is funded by the ERC under the Advanced Investigator Projects 267219 and 883830



What else?

- T-dependent Continuum Induced Absorption (CIA)
- Opacity data for atmospheres other than gas giants
- Something else

With huge thanks to

Sergey Yurchenko

Oleg Polyansky



ExoMolIHD (2020-25)

HiRes Line lists

Charles Bowesman

Kyriaki Kefala

Qianwei Qu

Mikhail Semenov

Apoorva Uphadyay

Alex Smola

Tony Tao

Photodissociation

Marco Pezzella

Georgi Mitev

Armando Perri

Ryan Brady

Pressure broadening

Elizabeth Guest

Andrei Sokolov

Jeanna Buldyreva (Bourgogne)

Bob Gamache (UMass)

Database

Jingxin Zhang

Qing-He Ni

Terrance Corey

Christian Hill (IAEA)

ExoMol (2011-16)

Ahmed Al-Refaie (UCL)

Ala'a Azzam (Univ Jordan)

Emma Barton

Bob Barber

Katy Chubb

Philip Coles

Maire Gordan (Sussex)

Christian Hill (IAEA)

Lorenzo Lodi

Laura McKemmish (UNSW)

Alec Owens

Andrei Patrascu (ELI-NP, Romania)

Clara Sousa-Silva (Bard College)

Tom Rivlin

Dan Underwood

Andrey Yachmenev (DESY)

Emil Zak


Advanced Textbooks in Physics

Astronomical Spectroscopy

An Introduction to the Atomic and
Molecular Physics of Astronomical Spectroscopy

Third Edition

Jonathan Tennyson

 World Scientific

About the first edition

“The best book for anyone who is embarking on research in astronomical spectroscopy”

Contemporary Physics (2006)

About the third edition:

“Makes an ideal companion ... for observational aspects of spectroscopy”

The Observatory Magazine (2019)

3rd edition published 2019

www.worldscientific.com/worldscibooks/10.1142/q0207