What you need to know to use the ExoMol Line Lists for Studying Exoplanetary Atmospheres

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University College London

July 14th, 2015

Molecules in Space

Observations

ExoMol Theory

Result!

Problems?

Vanadium Monoxide

Cool stars

Molecules in Space
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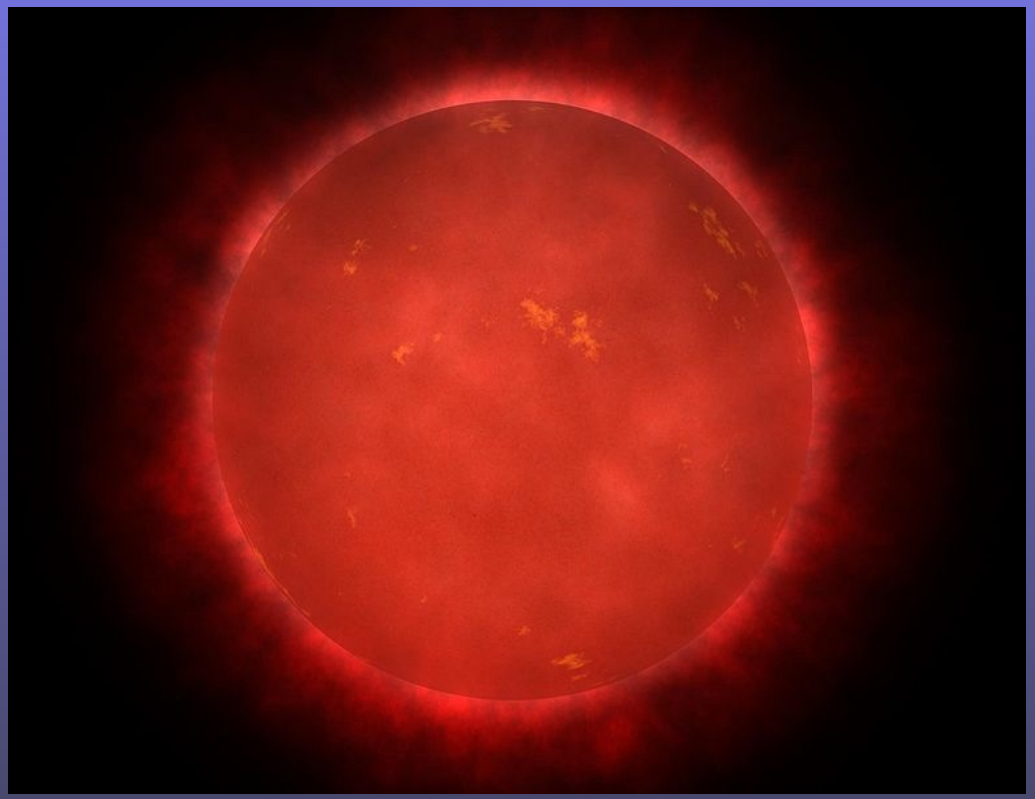

- TiO, VO
- H_2O

Brown Dwarfs

- CH_4
- CrH, TiH

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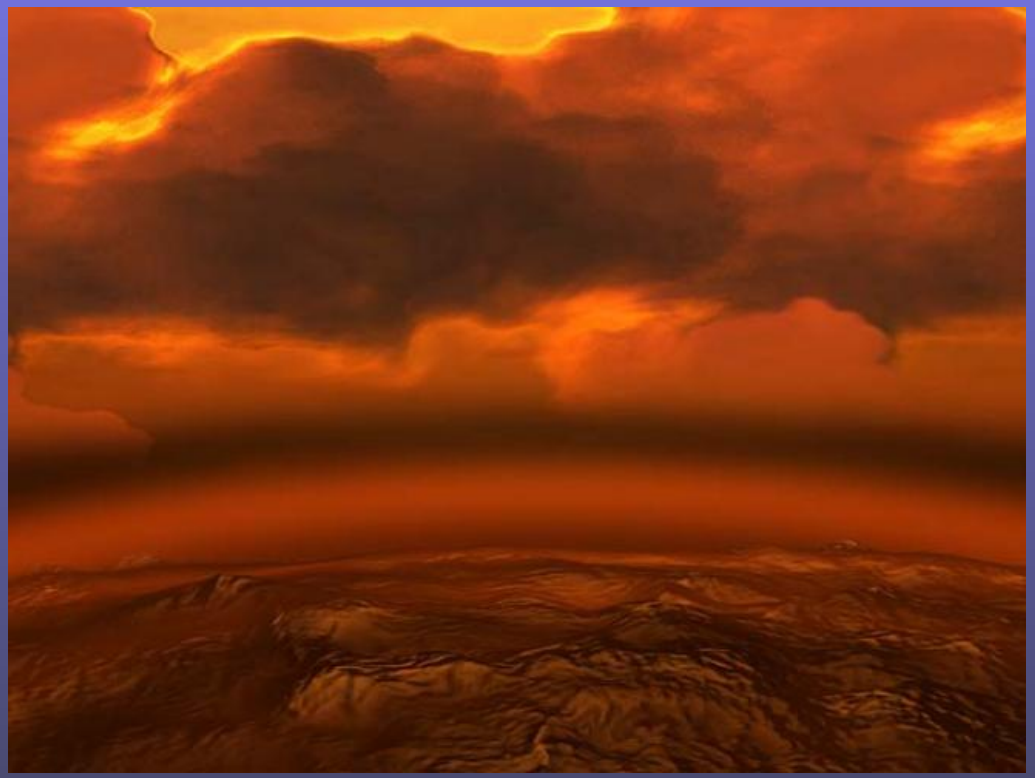
Hot "Jupiter" ExoPlanets



- TiO, VO
- H_2O, CO

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Earth-like ExoPlanets

- CO_2
- H_2O
- O_2, N_2
- O_3
- HNO

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Ultimate Goal

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Astronomers Methodology

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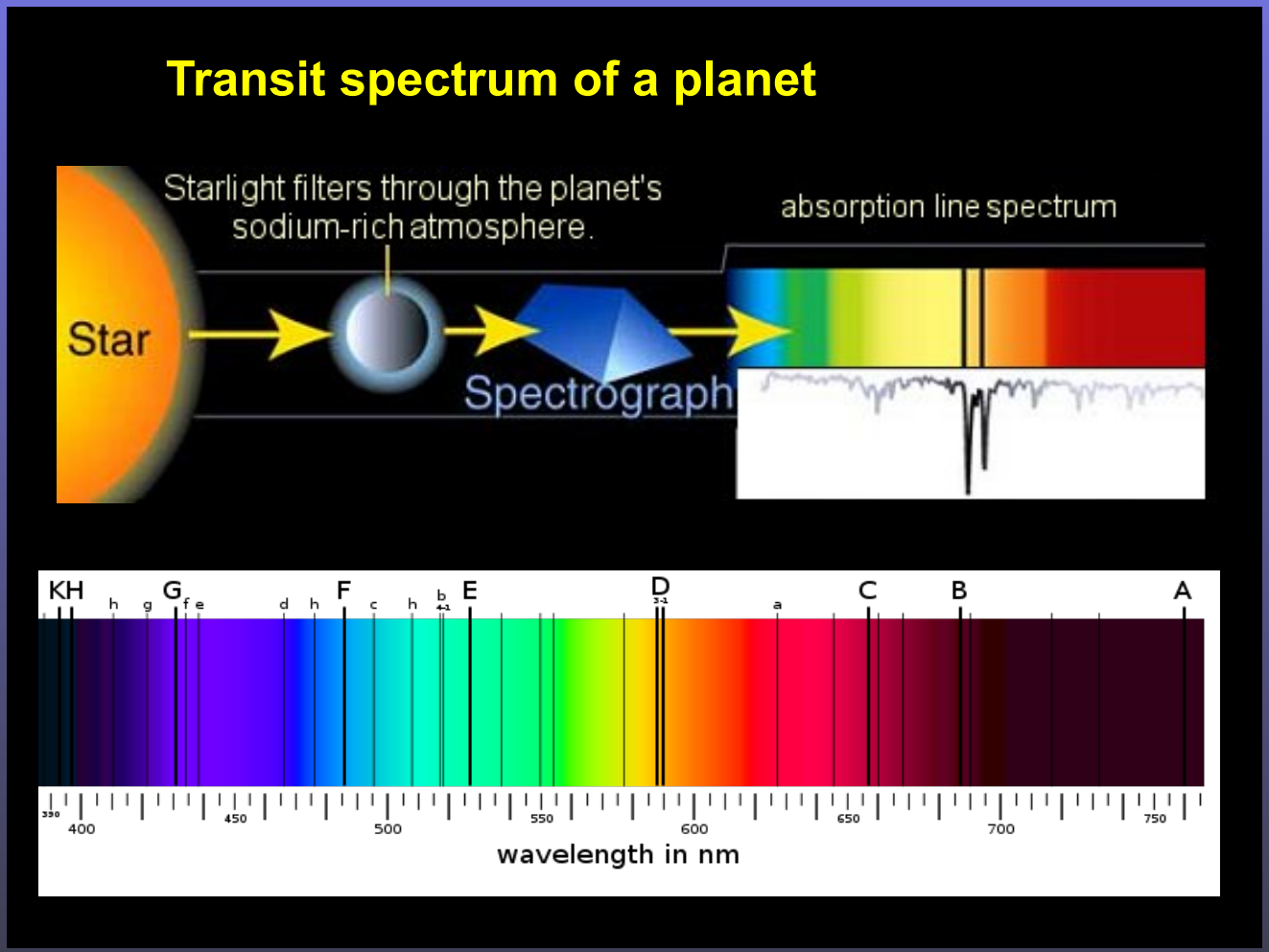

What next?

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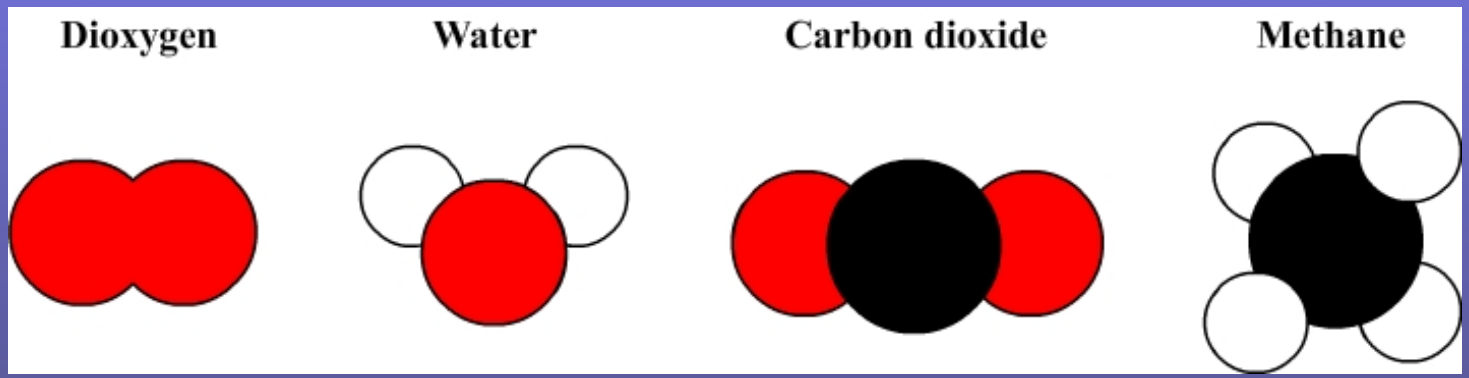
Which Molecule?



What frequencies of light?

How much light is absorbed?

Goal

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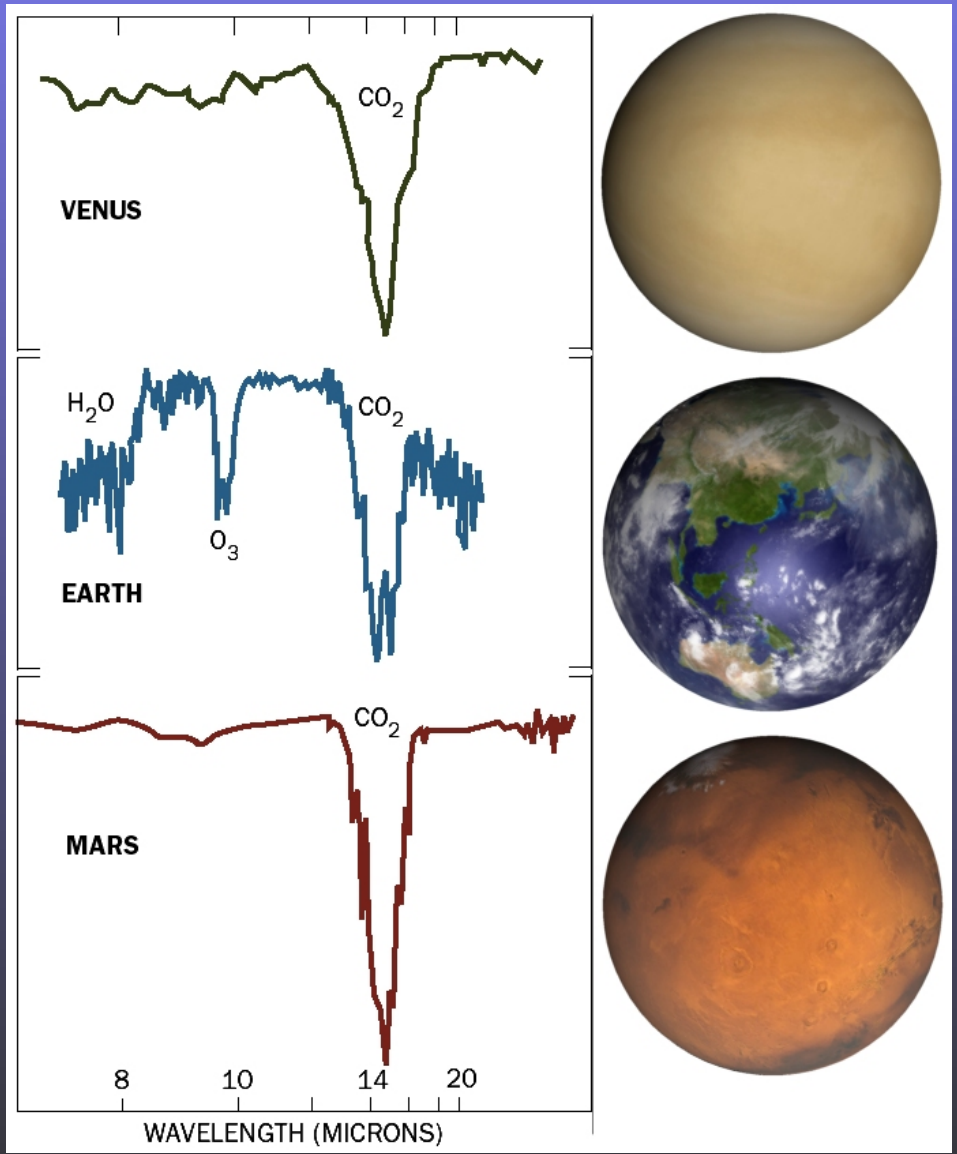
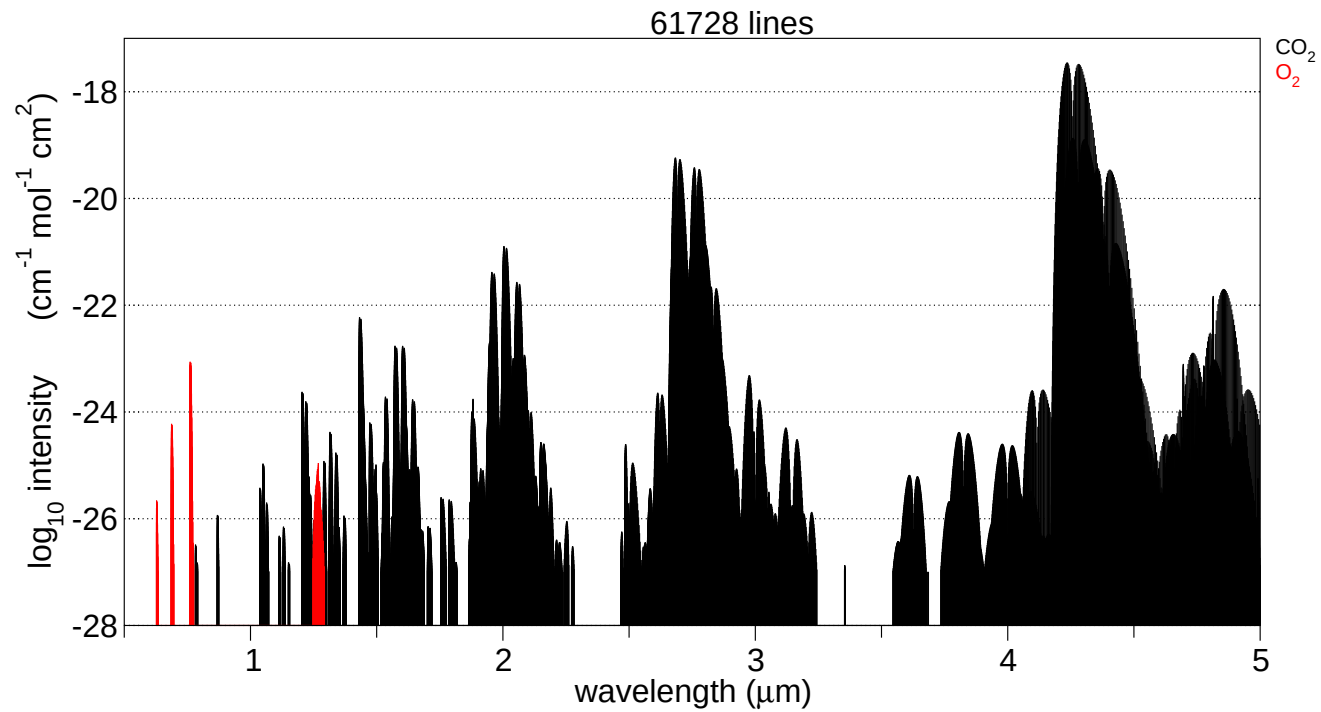


A note on O_2

O_2 is a weak absorber of infrared and visible light (this is why it is not a greenhouse gas)!



spectralcalc.com

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ExoMol Methodology

Finding the **frequency** and **intensity** of the transitions of small hot molecules in astrophysical environments using:

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ExoMol Methodology

Finding the **frequency** and **intensity** of the transitions of small hot molecules in astrophysical environments using:

- Lots of PhD students
- Some Masters students
- Post-docs
- Supervisors

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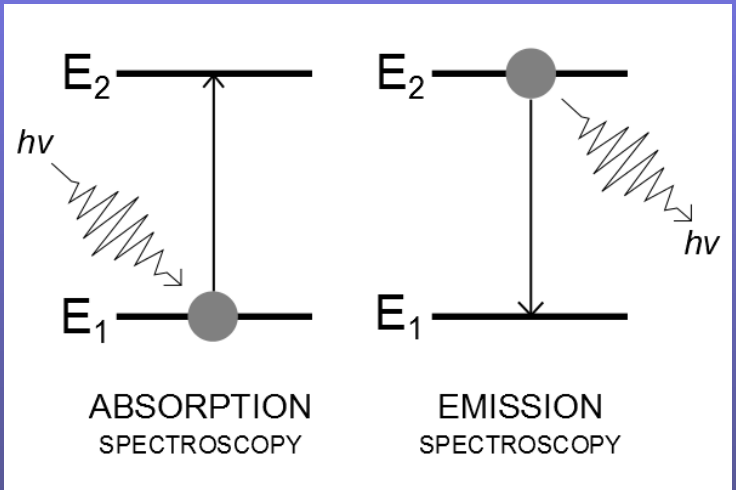
The Core of All Spectroscopy



- Initial Energy Level
- Final Energy Level
- Transitions Between Them

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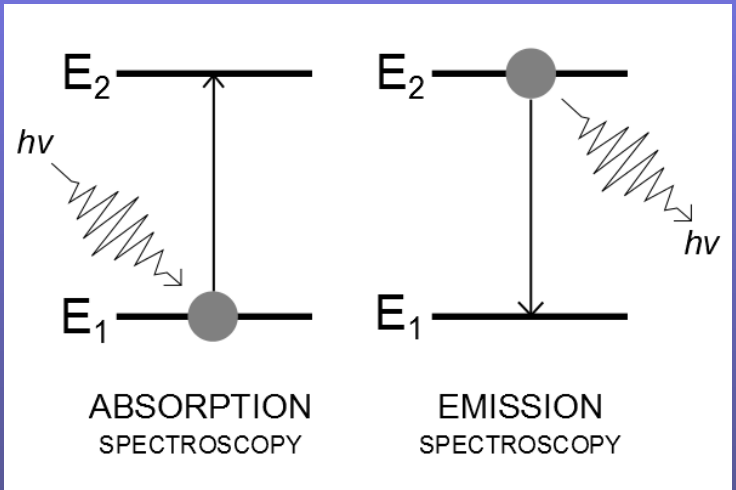
The Core of All Spectroscopy



- Initial Energy Level
- Final Energy Level
- Transitions Between Them

Energy levels: Need **Potential Energy Curves**.

Transitions: Need **Dipole Moment Curves**.

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Two sources of information

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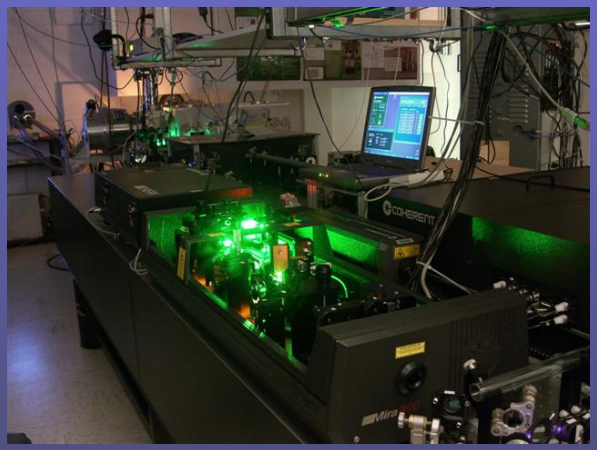
Theory

Experiment



Neither is good enough by themselves, so we use both!

ExoMol Methodology

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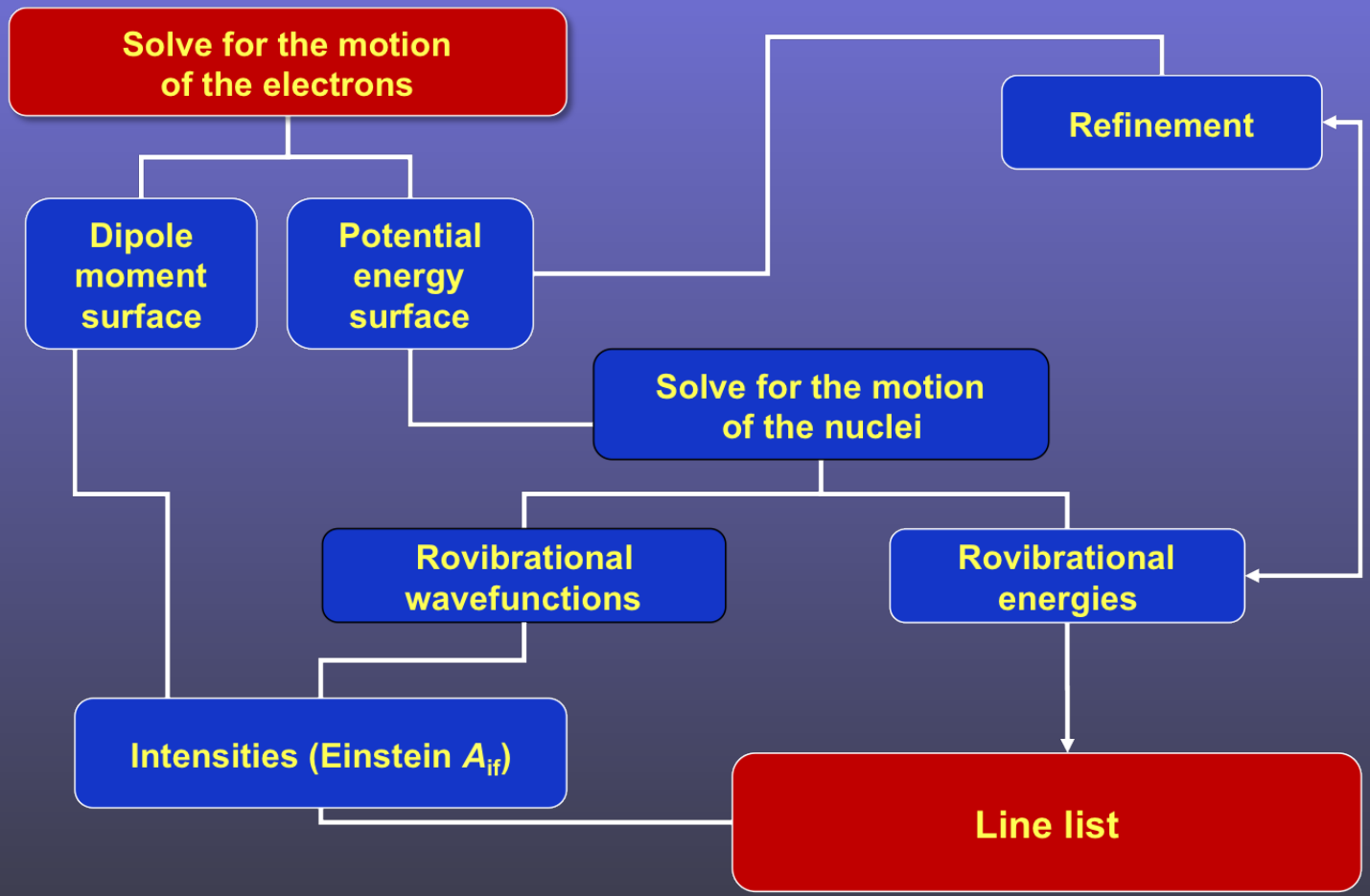

The Result: Line Lists

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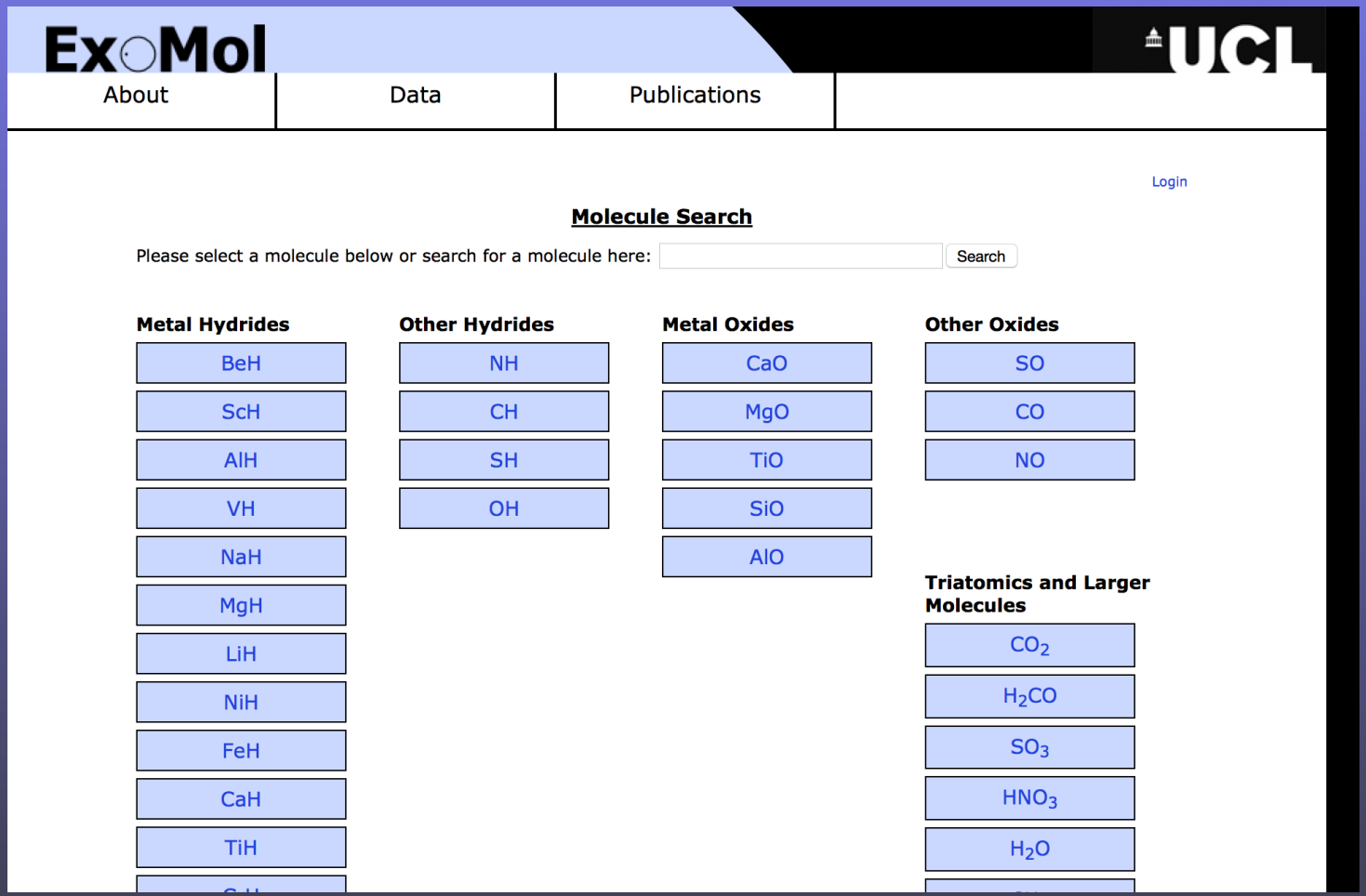
Vanadium Monoxide



ExoMol Output: Line Lists

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Login

Data for ^{9}BeH

Yadin: line list

Rovibrational line lists for BeH, MgH and CaH

9Be-1H__Yadin.states [48.3 KB]

9Be-1H__Yadin.trans [1.9 KB]

README.txt [1.9 KB]

References

1. B. Yadin, T. Veness, P. Conti, C. Hill, S. N. Yurchenko, J. Tennyson, "ExoMol line lists – I. The rovibrational spectrum of BeH, MgH and CaH in the $X\,^2\Sigma^+$ state", *Monthly Notices of the Royal Astronomical Society* **425**, 34-43 (2012). [link to article][12YaVeCo.XH]

Yadin: partition function

Rovibrational line lists for BeH, MgH and CaH

9Be-1H__Yadin.pf

References

1. B. Yadin, T. Veness, P. Conti, C. Hill, S. N. Yurchenko, J. Tennyson, "ExoMol line lists – I. The rovibrational spectrum of BeH, MgH and CaH in the $X\,^2\Sigma^+$ state", *Monthly Notices of the Royal Astronomical Society* **425**, 34-43 (2012). [link to article][12YaVeCo.XH]

The Result: Line Lists

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1	16410.168800	32	1.5	-	11	1 e
2	16402.093900	16	0.5	+	11	0 e
3	15721.783500	32	1.5	-	10	1 e
4	15710.467200	16	0.5	+	10	0 e
5	14731.961100	32	1.5	-	9	1 e
6	14718.826200	16	0.5	+	9	0 e
7	13541.079500	32	1.5	-	8	1 e
8	13526.656400	16	0.5	+	8	0 e
9	12198.490600	32	1.5	-	7	1 e
10	12183.050600	16	0.5	+	7	0 e
11	16426.182400	48	2.5	+	11	2 e
12	16426.182400	32	1.5	+	11	2 f
13	16410.168800	16	0.5	-	11	1 f
14	10732.929200	32	1.5	-	6	1 e
15	10716.629200	16	0.5	+	6	0 e
16	9162.317600	32	1.5	-	5	1 e
17	9145.253300	16	0.5	+	5	0 e
18	7498.109100	32	1.5	-	4	1 e
19	7480.340100	16	0.5	+	4	0 e
20	5747.698100	32	1.5	-	3	1 e
21	5729.261900	16	0.5	+	3	0 e
22	3915.950700	32	1.5	-	2	1 e
23	3896.871500	16	0.5	+	2	0 e
24	2006.125100	32	1.5	-	1	1 e

*.states file contains all energy levels, with quantum numbers.

There are often millions of energy levels!

ExoMol Output: Line Lists

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*.trans file

1	2	9.0173e-06
3	4	6.4289e-05
5	6	1.3058e-04
7	8	1.8319e-04
9	10	2.1458e-04
11	1	8.2197e-05
12	13	8.2197e-05
14	15	2.2387e-04
16	17	2.1512e-04
18	19	1.9373e-04
20	21	1.6431e-04
22	23	1.3067e-04
24	25	9.6070e-05
26	27	6.3375e-05
28	3	6.0976e-04
29	30	6.0976e-04
31	11	2.7140e-04
32	12	2.7140e-04
33	5	1.2468e-03
34	35	1.2468e-03
36	7	1.7535e-03
37	38	1.7535e-03
39	9	2.0567e-03
40	41	2.0567e-03
42	31	5.8075e-04
43	32	5.8075e-04
44	14	2.1477e-03
45	46	2.1477e-03
47	28	2.1603e-03

Three columns

- Initial energy level (ID)
- Final energy level (ID)
- Strength of transition (Einstein coefficient)

Billions of transitions are common!

Simpler ExoMol Output

Sometimes (often?) billions of lines is too much. We aim to help here too.

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- Cross-sections of absorption at different temperatures - Available now on ExoMol website!

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- Currently developing k coefficient tables

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- Currently developing k coefficient tables
- We can 'trim' the line list for particular applications quite easily; just tell us what temperature, what frequency range etc.

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Sometimes (often?) billions of lines is too much. We aim to help here too.

- Cross-sections of absorption at different temperatures - Available now on ExoMol website!
- Currently developing k coefficient tables
- We can 'trim' the line list for particular applications quite easily; just tell us what temperature, what frequency range etc.
- Ask us for anything else that will be useful

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Simpler ExoMol Output

Take home message:

- These line lists often take PhDs.
- They are useless if they are not used.
- So anything we can do to maximise their usefulness to you - let us know!

laura.mckemmish@gmail.com
www.exomol.com/

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ExoMol Periodic Table

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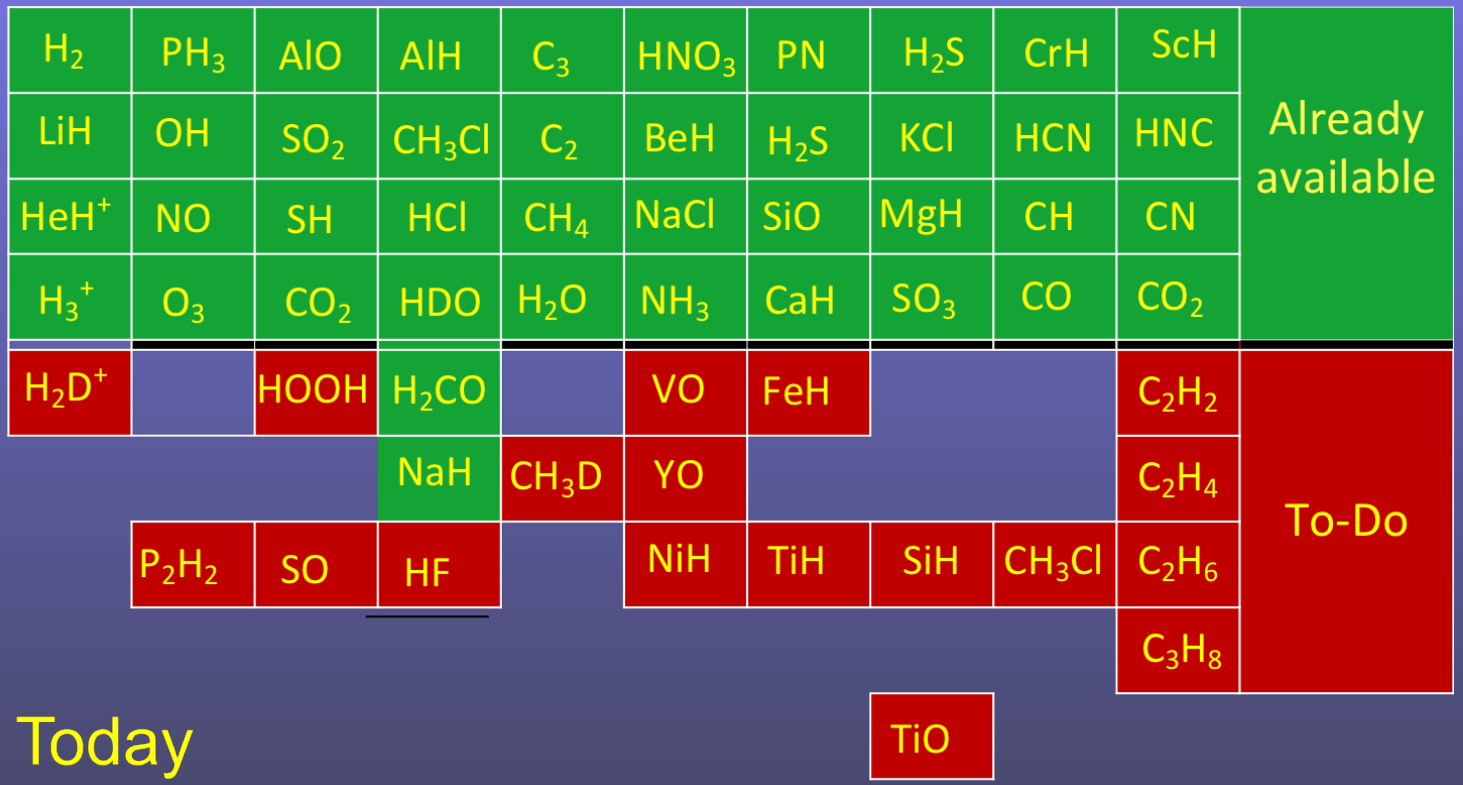

Input Data: Line Lists, Physics

Molecules in Space

Observations

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Result!

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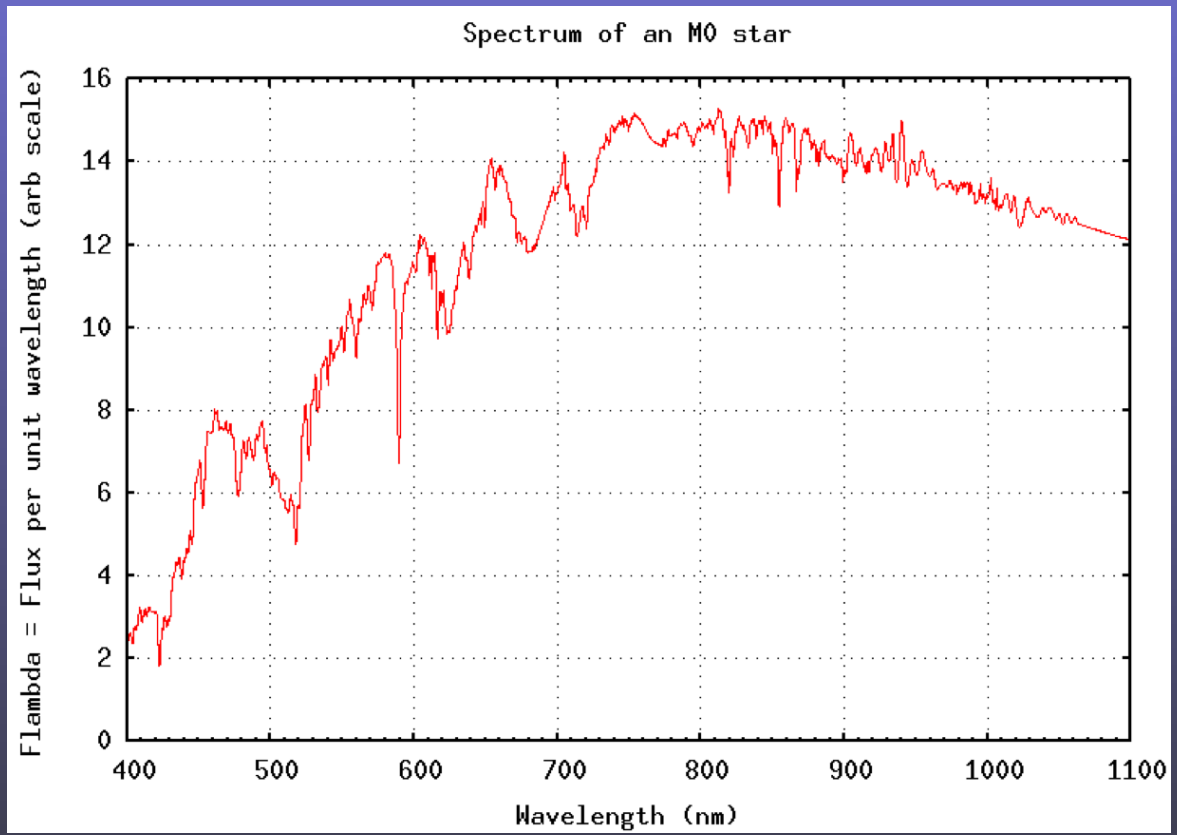
Astronomy Modellers Methodology

Input Data: Line Lists, Physics
Input Observation: Spectrum from star/ exoplanet



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Astronomy Modellers Methodology

Input Data: Line Lists, Physics
Input Observation: Spectrum from star/ exoplanet

Method: Computational Models of Atmosphere

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Astronomy Modellers Methodology

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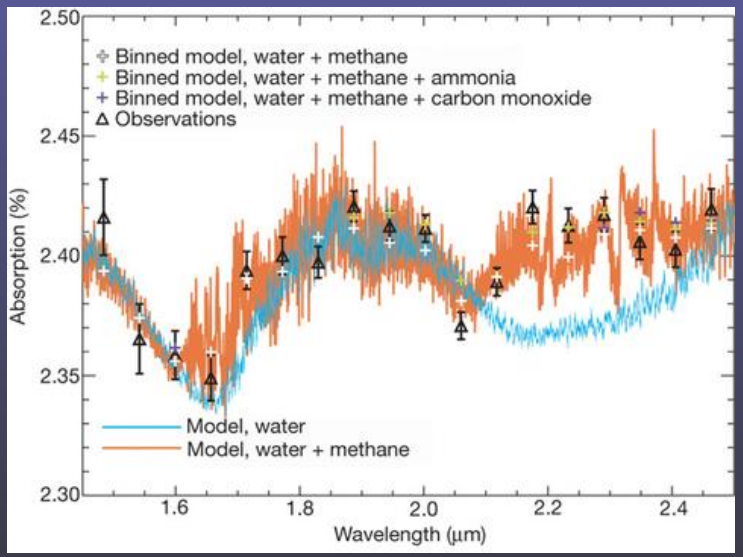
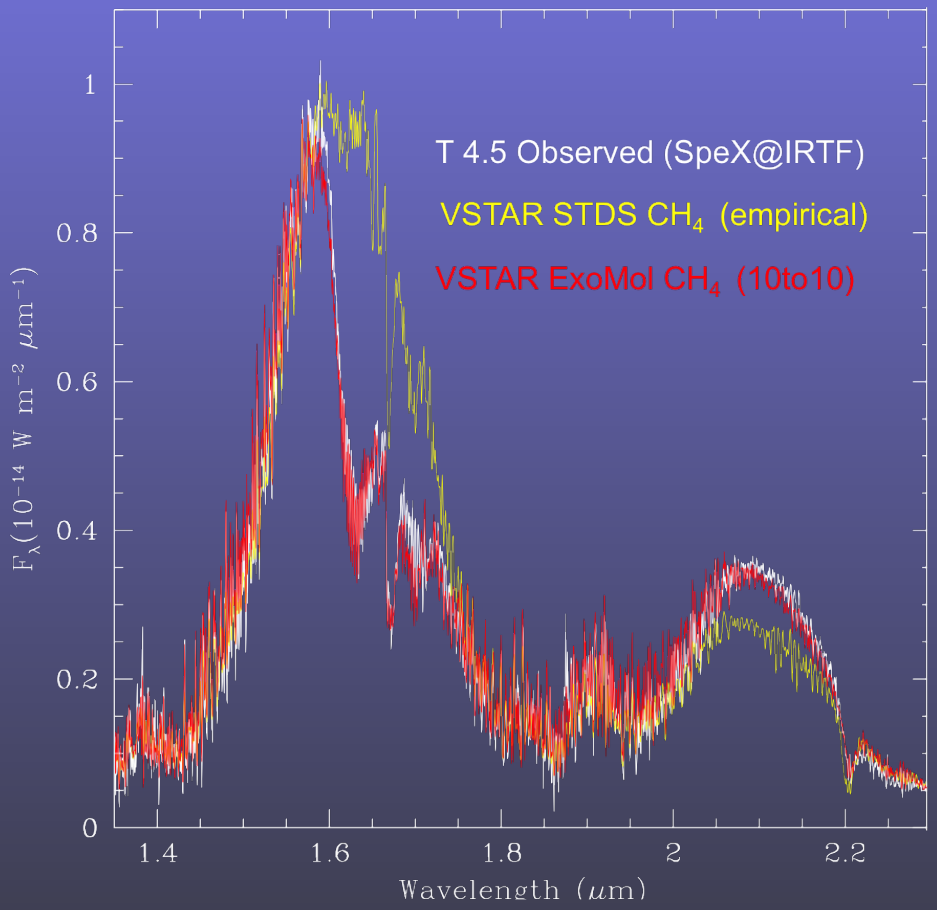
Input Data: Line Lists, Physics
Input Observation: Spectrum from star/ exoplanet

Method: Computational Models of Atmosphere

Output: Characteristics of atmosphere; pressure, temperature, molecular composition and more!



Some Output So Far



2MASS 0559-14

Yurchenko et al PNAS, 111, 9379 (2014)

Cushing Rayner, Vacca (2005)

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Output Hopefully

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If there are problems

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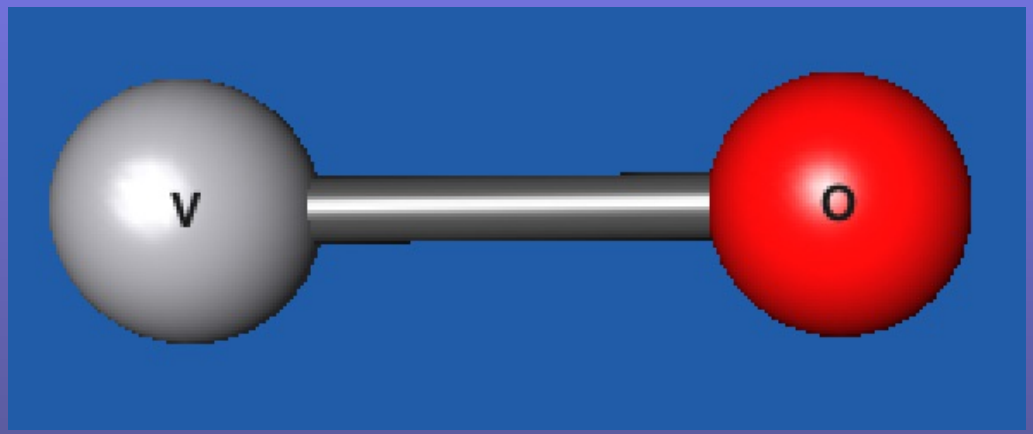
Are they caused by the ExoMol Line Lists?

Questions to ask:

1. Is it a big molecule?
2. Is there little experimental data?
3. Does the molecule contain a transition metal?
4. Is it an electronic transition?
5. Is it a high energy transition?
6. Is your error at high resolution?
7. Is the initial state very high in energy?
8. Is your line list not from the ExoMol project?

If **Yes**, then it could be the line list.
If **No**, then it is probably the astrophysical model.

My Molecule



Innoculous?

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My Molecule

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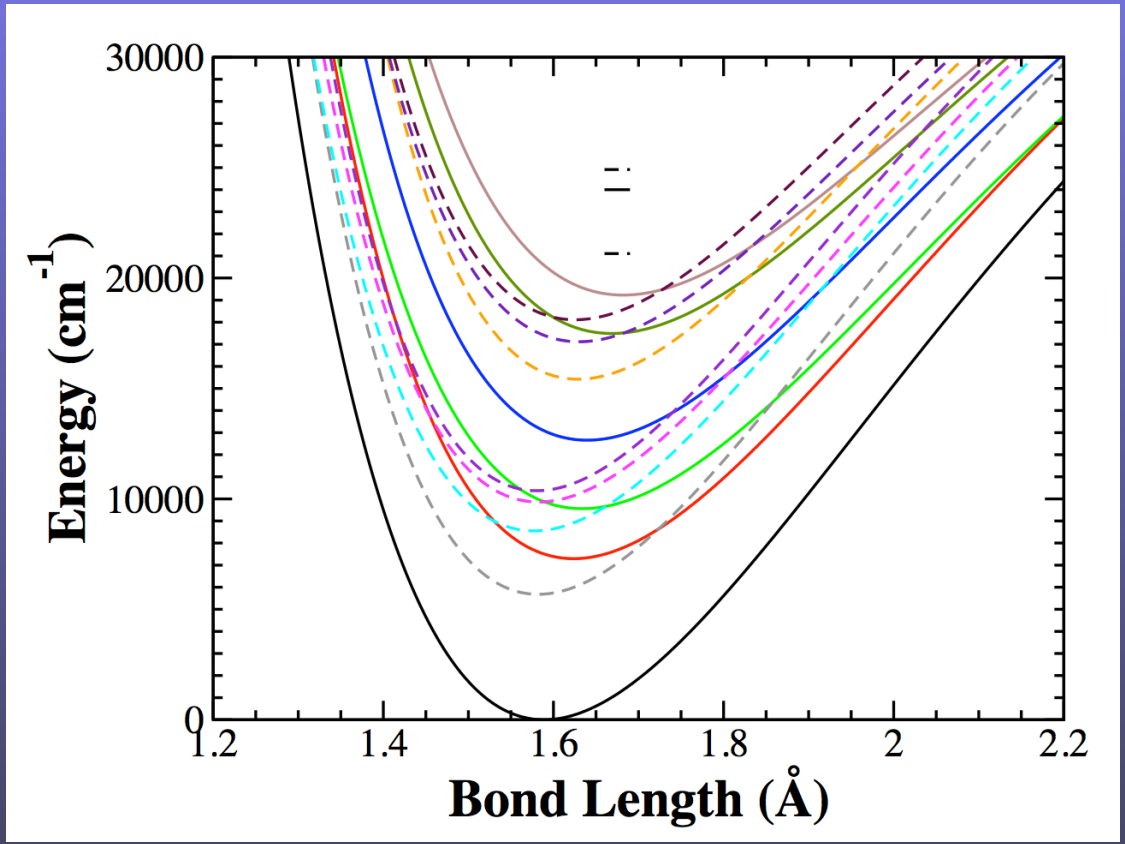

Umm... No!

Current Spectra

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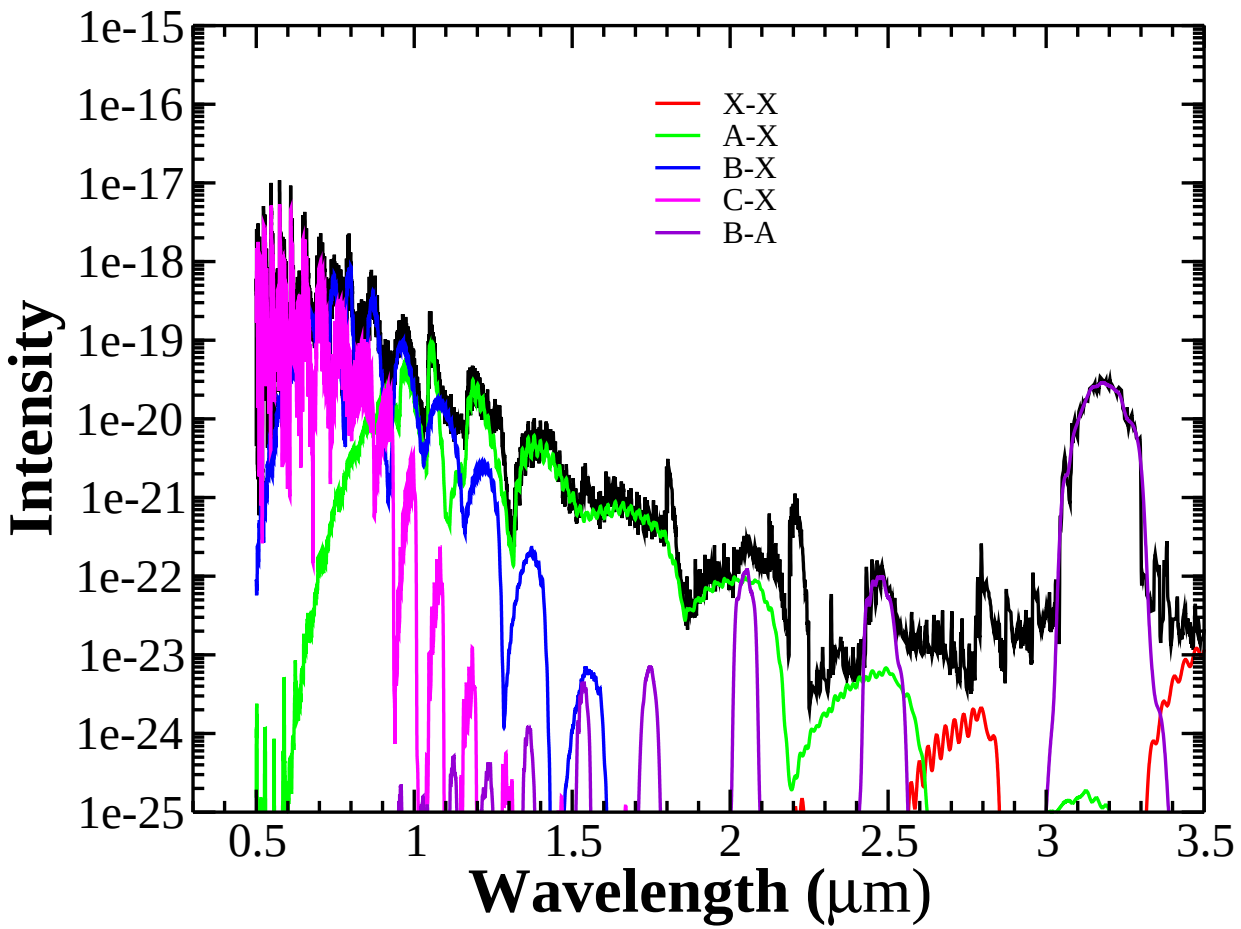
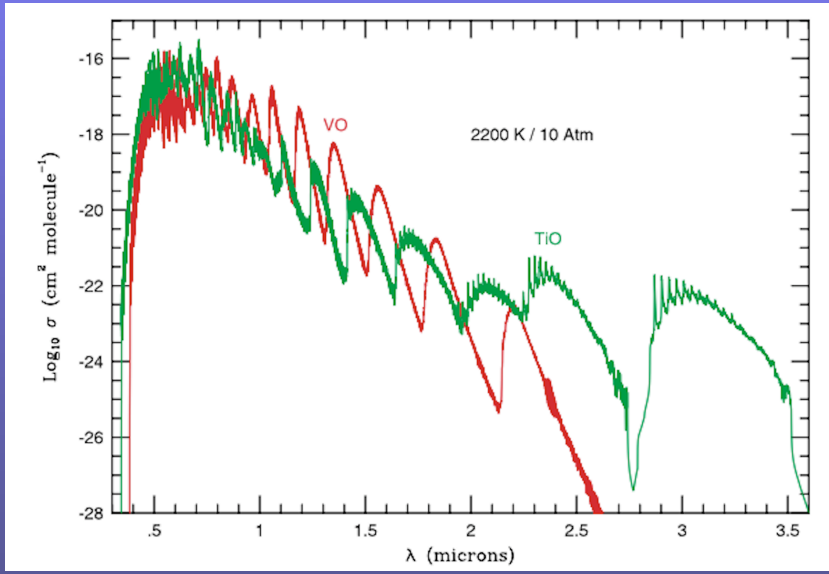
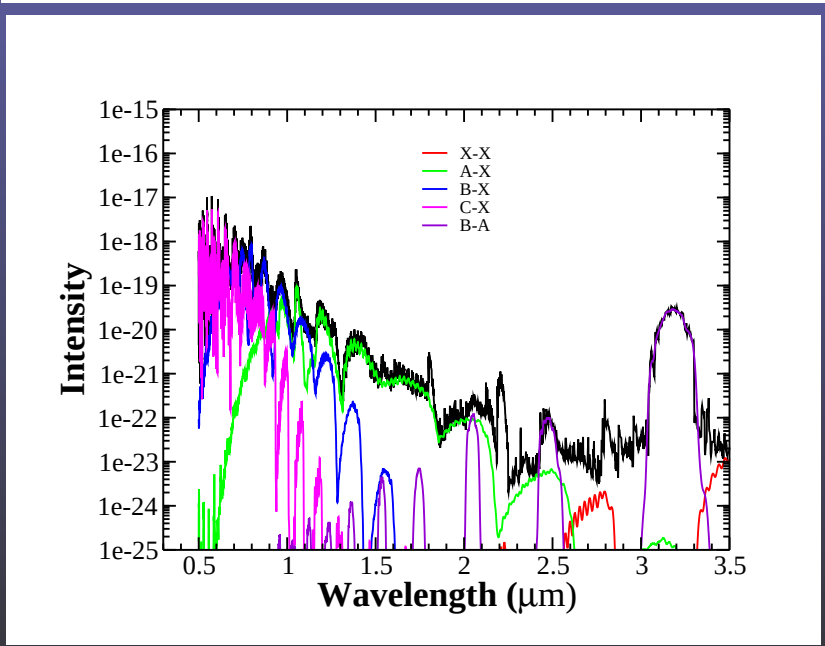


Compared to Previous Spectra

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