ExoMol:

Molecular Line Lists for Modelling Atmospheres

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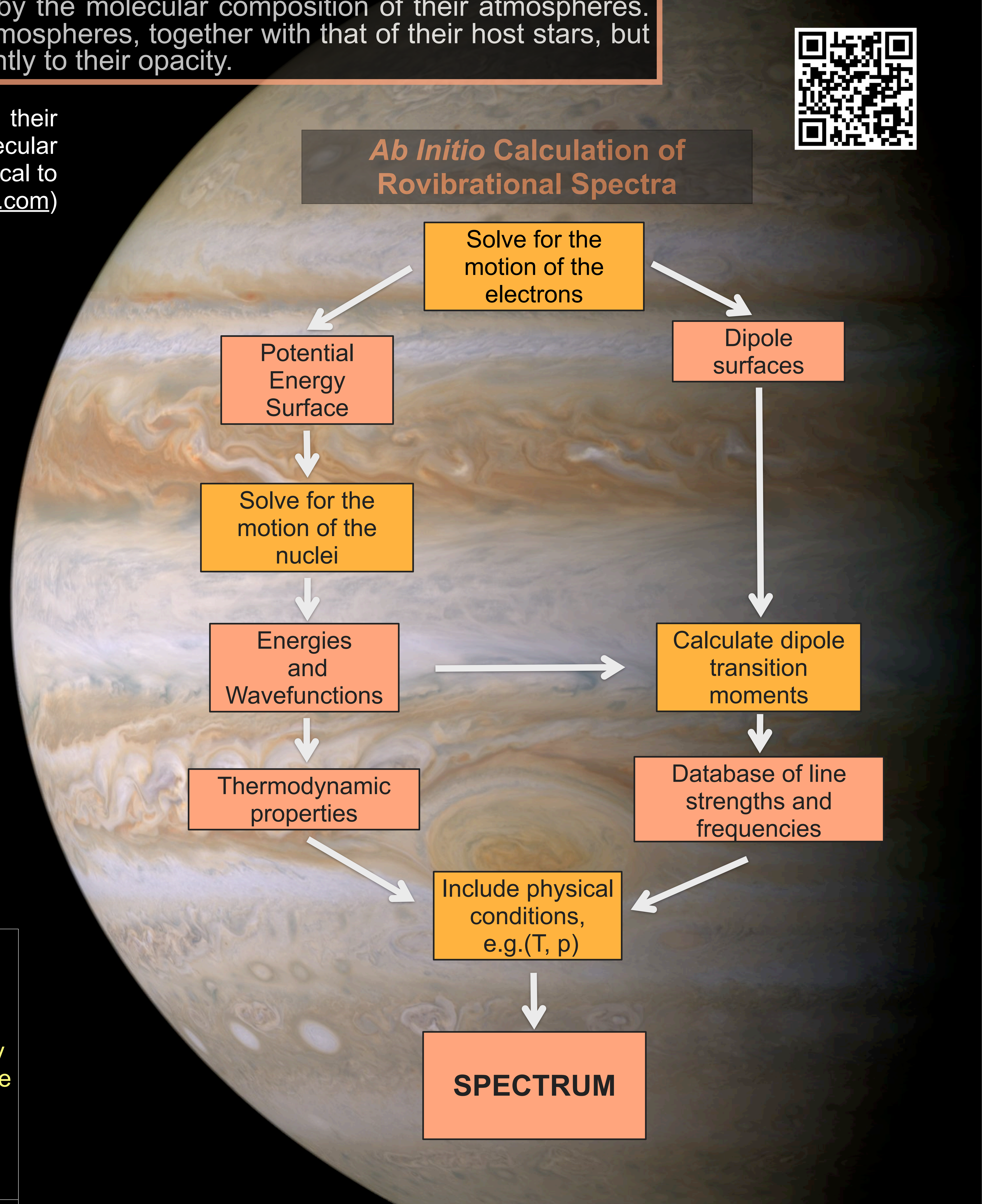
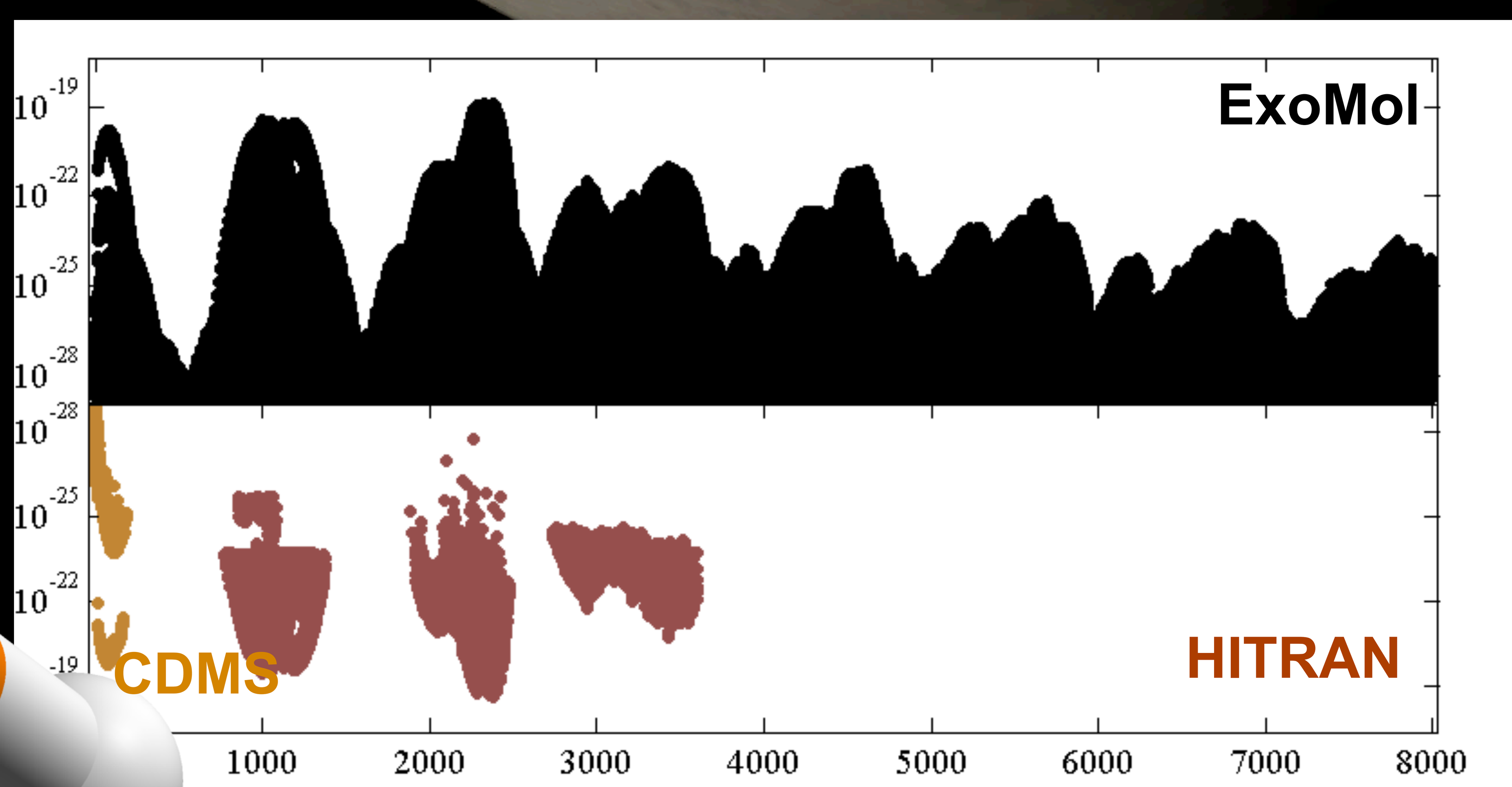
As many as 889 exoplanets have been detected to date and attention has begun to focus on characterising their physical and chemical properties : What is their temperature? What is the composition of their atmospheres? Could they sustain life? Furthermore, there are objects like Brown Dwarfs, which are classified by the molecular composition of their atmospheres. This analysis can be done by interpreting the spectra of these bodies' atmospheres, together with that of their host stars, but this requires fundamental data for all the species that contribute significantly to their opacity.

Analysing and modelling planetary and stellar atmospheres is difficult because their spectra are extremely rich in structure and their opacity is dominated by molecular absorbers, each with hundreds of thousands to trillions of spectral lines. It is not practical to determine line lists of this size experimentally, so the ExoMol project[1] (www.exomol.com) will use very high-accuracy, *ab initio* theoretical tools to calculate them.



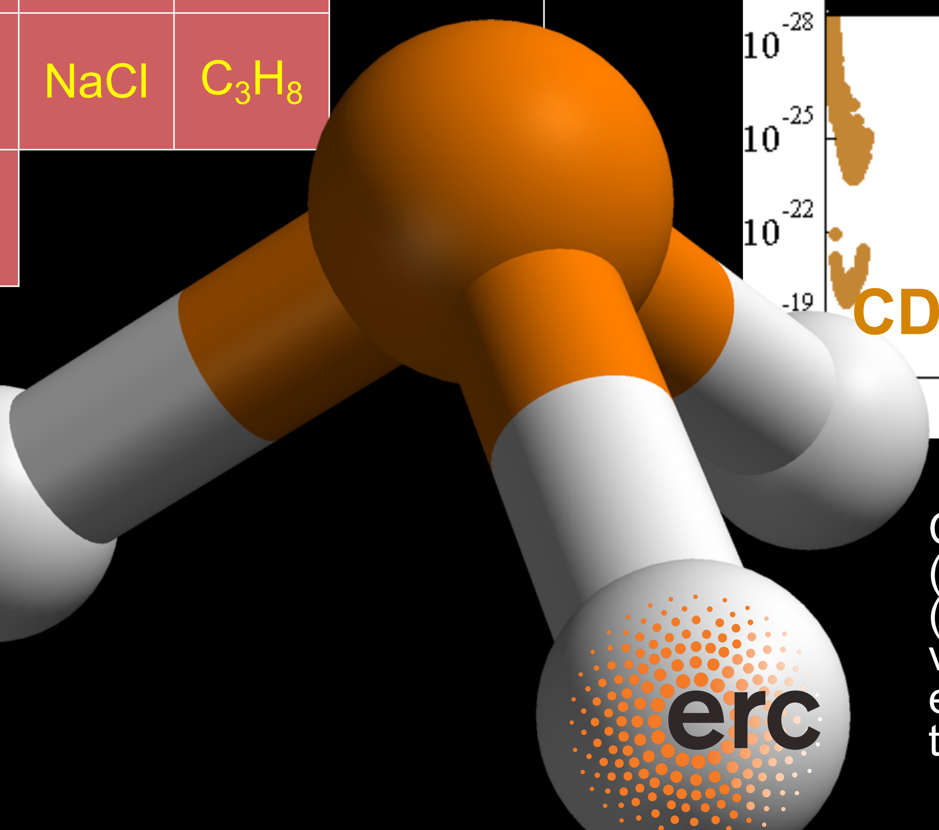
Primordial	Terrestrial Planets (Oxidising)			Giant-Planets & Cool Stars						
H_2									H_2	Already available
UCL LiH	OH HITEMP						TiO Schwenke	CO HITEMP	CO_2 HITEMP	
UCL HeH^+	NO HITEMP						CN SCAN	CH Kurucz	UCL HCN	
UCL H_3^+	O_3 Reims	CO_2 HITEMP	UCL HDO	UCL H_2O HITEMP	UCL NH_3	UCL CaH UGAMOP	UCL BeH	UCL MgH UGAMOP	UCL HNC	
H_2D^+	O_2	HOOH	HNO_3	H_2S	VO	FeH Kurucz	AlH	C_3 SCAN	C_2H_2	ExoMol
	SO_3	H_2CO	PH_3	SO_2	YO	AlO	SiH	HCl	C_2H_4	
				CH_4	NiH	TiH	SiH Kurucz	KCl	C_2H_6	
					CrH	SiO	HF	NaCl	C_3H_8	
					C_2 SCAN	SO	SH SCAN			

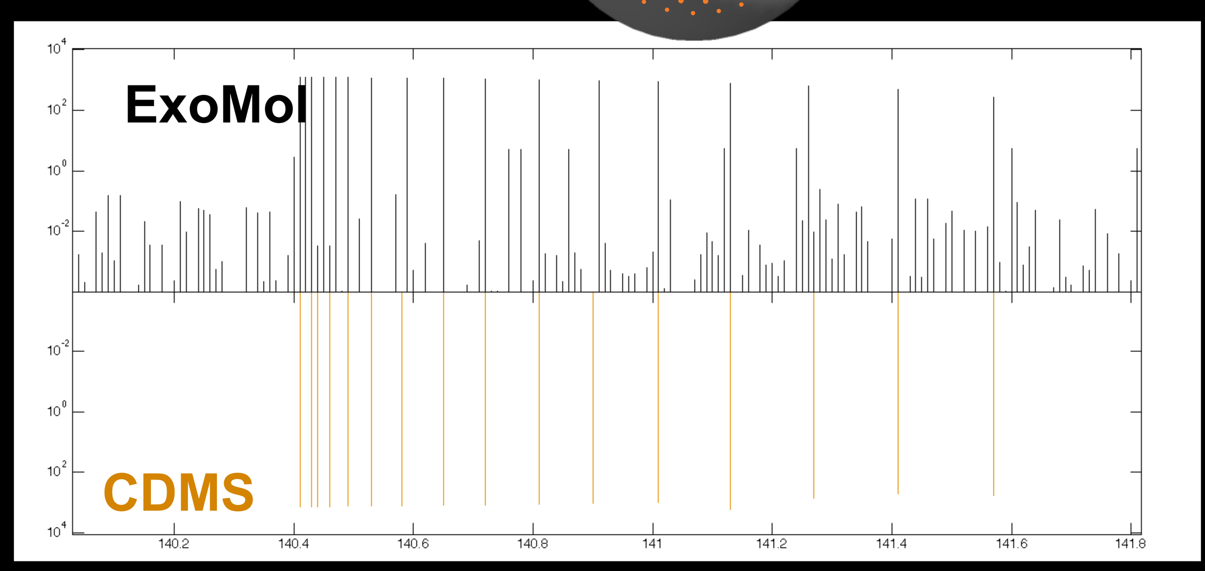


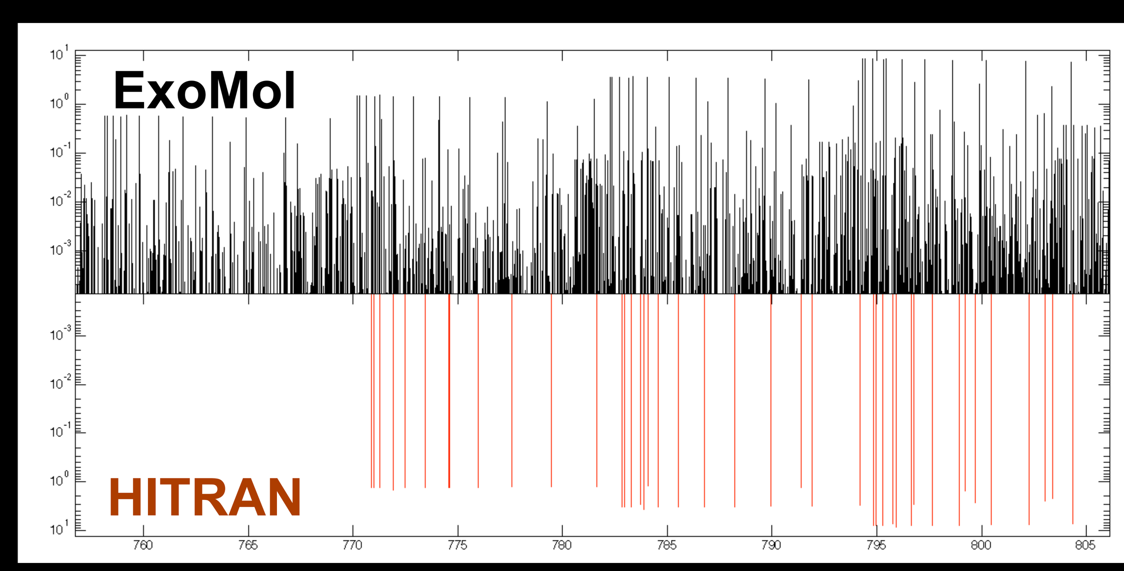
Comparison of the intensities (cm/molecule, log scale) and wavenumber (cm^{-1}) of transitions values between TROVE and experimental data (HITRAN[6] and CDMS[7]). The full range of calculations (137 million lines versus the ~20,000 experimental lines) can be seen on the left with two enlargements on the right giving line-by-line comparisons of a section of the rotational spectrum (above) and the 700 - 800 cm^{-1} region (below).

Phosphine (PH_3) is an equilateral pyramidal molecule (it is the phosphorus analogue to ammonia) and it is known to be important for the atmospheres of giant-planets, cool stars and many other astronomical bodies. Rotational transition features of phosphine have been found in the far-infrared spectra of Saturn and Jupiter[2,3], where it is a marker for vertical convection zones.

A computed room temperature line list of phosphine is presented here[4] as a precursor to a high temperature equivalent to be produced in the near future, necessary for the analysis of cool stars and brown dwarfs. All the transitions' energy levels and Einstein A-coefficients were computed using the program TROVE[5].







[1] J. Tennyson, S. Yurchenko, Mon. Not. R. Astr. Soc. 425 (2012) 21–33.
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[3] L.N. Fletcher et al. - Icarus 202, 543–564 (2009).
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[6] L. S. Rothman, et al. - J. Quan. Spectrosc. Rad. Transfer 110, 533 (2009).
[7] H.S.P. Müller, et al. - J. Molec. Struct. THEOCHEM 742 (2005), 215–227.