ExoMol

High temperature molecular line lists for modelling exoplanet atmospheres

Sergei N. Yurchenko, Jonathan Tennyson, Katy L. Chubb, Victoria H.J. Clark, Alec Owens, Samuel Wright, *et al*.

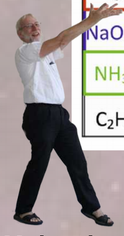
University College London, Gower Street, London, WC1E 6BT, UK

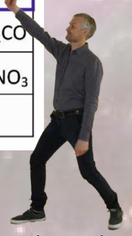
EXOMOL :

The ExoMol database (www.exomol.com) provides molecular data for spectroscopic studies of hot atmospheres. The basic form of the database is extensive line lists; these are supplemented with partition functions, state lifetimes, cooling functions, Landé g-factors, temperature-dependent cross sections, opacities, pressure broadening parameters, k -coefficients and dipoles. Currently containing 80 molecules and 190 isotopologues totaling over 700 billion transitions, the database is concentrated at infrared and visible wavelengths. The core of the database comes from the ExoMol project which primarily uses theoretical methods, albeit usually fine-tuned to reproduce laboratory spectra, to generate very extensive line lists for studies of hot bodies.

THE EXOMOL PERiODiC TABLE :

AlH	AlCl	AlO	BeH	C_2	CaO	CaF	CaH	CH	CN	CO	CP
CrH	CS	FeH	FeO	H_2	H_3^+	H_3O^+	HCl	HF	LiCl	LiF	LiH
LiH^+	KCl	KF	MgF	MgH	MgO	N_2	NaCl	NaF	NaH	NaF	NiH
NH	NS	NO	OH	O_2	PH	PN	PO	PS	ScH	SiC	SiH
SiS	SH	SiO	SiS	SO	TiO	TiH	TiF	VO	VN	YO	ZnS
C_3	CaOH	CO_2	CH_2	H_3^+	H_2D^+	HCN	HNC	H_2O	HDO	H_2S	KOH
NaOH	N_2O	OCS	PO_2	SiH_2	SiO_2	SO_2	AsH_3	CH_3	C_2H_2	HOOH	H_2CO
NH_3	SiH_3	PH_3	P_2H_2	PF_3	SO_3	CH_4	CH_3D	CH_3Cl	CH_3F	SiH_4	HNO_3
C_2H_4	C_2H_6	C_3H_8									





Molecular line lists: Red indicates line lists in progress, blue corresponds to the line lists suggested for molecules specific for hot rocky exoplanets and green indicates line lists which contain data applicable for high resolution.

PUBLiCATiONS :

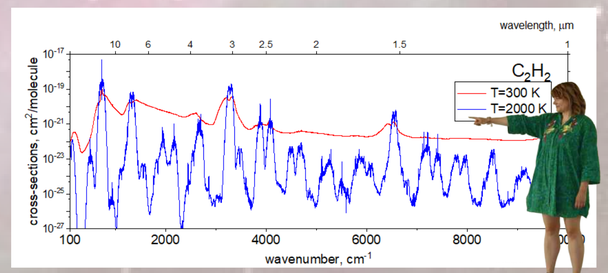
ExoMol2020 - https://doi.org/10.1016/j.jqsrt.2020.107228
aCeTy - https://doi.org/10.1093/mnras/staa229
CATS - https://doi.org/10.1016/j.jqsrt.2020.106929
OYT3 - https://doi.org/10.1093/mnras/staa1287
UCL-4000 - https://doi.org/10.1093/mnras/staa1874

Background image: NASA Hubble Space Telescope Flickr

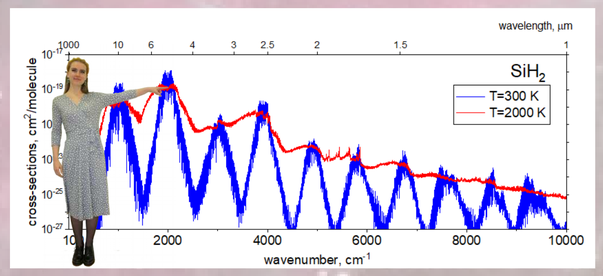
RECENT WORK PERFORMED WiTH DiRAC :

C_2H_2

aCeTY, a ro-vibrational line list for the ground electronic state of $^{12}C_2H_2$ covers the transition wavenumbers up to 10 000 cm^{-1} ($\lambda > 1$ μm), with lower and upper energy levels up to 12 000 and 22 000 cm^{-1} considered, respectively. The calculations are performed up to a maximum value for the vibrational angular momentum, $K_{max} = L_{max} = 16$, and maximum rotational angular momentum, $J = 99$. Einstein-A coefficients, which can directly be used to calculate intensities at a particular temperature, are computed for 4.3 billion (4 347 381 911) transitions between 5 million (5 160 803) energy levels. The aCeTY line list is considered to be complete up to 2200 K



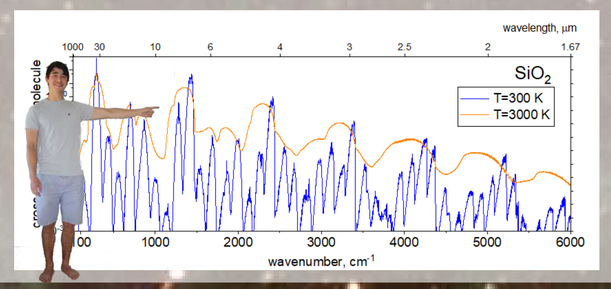
SiH_2



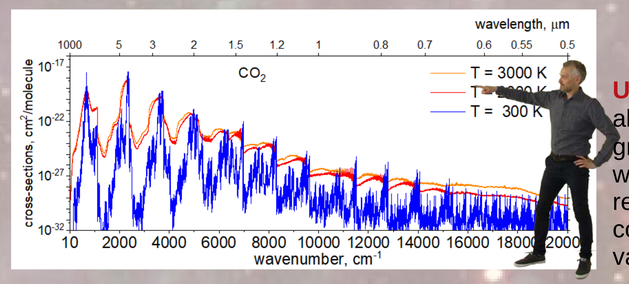
CATS, a ro-vibration line list for the electronic ground state of SiH_2, is suitable for temperatures up to 2000 K and covers the wavenumber range 0–10 000 cm ($\lambda > 1.0$ μm) for states with rotational excitation up to $J = 52$. Over 310 million transitions between 593 804 energy levels were computed variationally with a new empirically refined potential energy surface, determined by refining to 75 empirical term values with $J \leq 5$ and a newly computed high-level ab initio dipole moment surface. This work was the first, comprehensive high-temperature line list to be reported for SiH_2.

SiO_2

OYT3, the first, comprehensive molecular line list for SiO_2, covers the wavenumber range 0 – 6000 cm^{-1} ($\lambda > 1.67$ μm) and is suitable for temperatures up to T = 3000 K. Almost 33 billion transitions involving 5.69 million rotation–vibration states with rotational excitation up to $J = 255$ have been computed using robust first-principles methodologies. Silicon dioxide is expected to occur in the atmospheres of hot rocky super-Earth exoplanets but a lack of spectroscopic data is hampering its possible detection.



CO_2



UCL-4000, a new hot line list for $^{12}C^{16}O_2$ has been calculated. The line list consists of almost 2.5 billion transitions between 3.5 million rotation-vibration states of CO_2 in its ground electronic state, covering the wavenumber range 0–20 000 cm^{-1} ($\lambda > 0.5$ μm) with the upper and lower energy thresholds of 36 000 cm^{-1} and 16 000 cm^{-1}, respectively. The ro-vibrational transition probabilities in the form of Einstein coefficients were computed using an accurate ab initio dipole moment surface with variational program TROVE.