Development of the ExoMol database

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Introduction

The desire to characterize and model the atmospheres of the many extrasolar planets that have been discovered over the last three decades is a major driver of current astronomy. This goal is impacted by the lack of spectroscopic data for the molecules in question since it requires significant quantities of spectroscopic data, to **accurately reproduce the spectroscopic features** of the atmospheres of hot exoplanets.

The ExoMol database provides **molecular data** for interpreting spectra and modelling atmospheres of hot exoplanets, cool stars, brown dwarfs, and other hot astronomical atmospheres and its molecules are selected because they are deemed to be important for **exoplanets and other studies of hot atmospheres**.

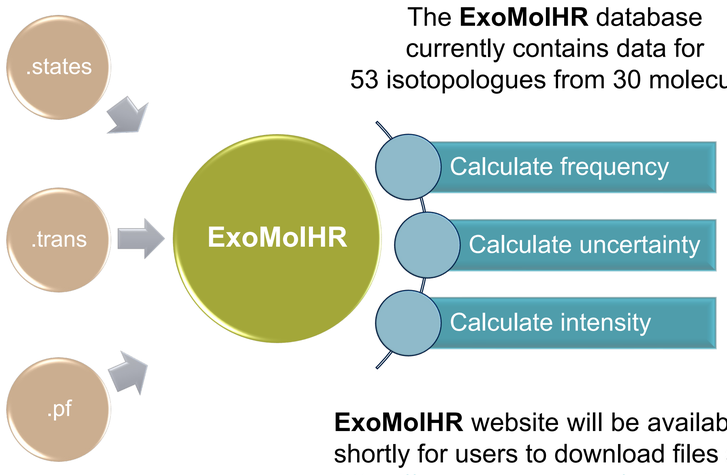
The core of the ExoMol database is **comprehensive high-temperature molecular line lists**; these are supplemented with **partition functions, state lifetimes, cooling functions, Landé g-factors, temperature-dependent cross sections, opacities, pressure broadening parameters, k-coefficients and dipoles**.

The ExoMol line lists are systematically published as a series in the journal Monthly Notices of the Royal Astronomical Society and summarised in release papers.

High-resolution line list database **ExoMolHR** [1]

The **ExoMolHR** database stores empirical high-resolution spectra extracted from the ExoMol with low uncertainty line positions.

ExoMolHR aims to precisely determine and characterize transition frequencies for high-resolution research, and this focus appears to be relevant for the updates of the ExoMol database.



The **ExoMolHR** database currently contains data for 53 isotopologues from 30 molecule.

ExoMolHR website will be available shortly for users to download files at https://www.exomol.com/exomolhr/.

Table 1. Sample ExoMolHR results for H_2O.

Frequency	Uncertainty	A	Intensity	Molecule	Isotopologue	Dataset	E"	g'	g"	J'	J"	QN'	QN"
0.400554	0.000002	9.35E-10	2.39E-28	H2O	1H2-16O	POKAZATEL	1907.61557	27	21	4	3	2 3 0 1 0 B1	3 0 0 1 0 B2
0.741682	0	1.96E-09	4.32E-25	H2O	1H2-16O	POKAZATEL	446.510665	39	33	6	5	1 6 0 0 0 B2	2 3 0 0 0 B1
0.895095	0.000003	7.93E-09	3.82E-28	H2O	1H2-16O	POKAZATEL	2129.59892	33	27	5	4	3 2 0 1 0 B2	4 1 0 1 0 B1
3.210931	0.000002	4.69E-07	1.74E-27	H2O	1H2-16O	POKAZATEL	2126.40758	9	11	4	5	4 0 0 1 0 A1	3 3 0 1 0 A2

Table 2. Summary of current ExoMolHR database.

Molecule	Isotopologue	Dataset	HR N Lines
AlCl	$^{27}Al^{35}Cl$	YNAT	101
	$^{27}Al^{37}Cl$	YNAT	121
AlH	$^{27}Al^{1}H$	AloHa	692
AlO	$^{26}Al^{16}O$	ATP	143197
	$^{27}Al^{16}O$	ATP	149577
	$^{27}Al^{17}O$	ATP	142905
	$^{27}Al^{18}O$	ATP	142976
C_2	$^{12}C_2$	8states	445682
C_2H_2	$^{12}C_2{}^{1}H_2$	aCeTY	473850
CH_4	$^{12}C^{1}H_4$	MM	
CN	$^{12}C^{14}N$	Trihybrid	244808
CO_2	$^{12}C^{16}O_2$	UCL-4000	2600218
CaH	$^{40}Ca^{1}H$	XAB	12341
CaOH	$^{40}Ca^{16}O^{1}H$	OYT6	
H_2CO	$^{1}H_2{}^{12}C^{16}O$	AYTY	317729
H_2CS	$^{1}H_2{}^{12}C^{32}S$	MOTY	
H_2O	$^{1}H_2{}^{16}O$	POKAZATEL	3520554
H_2S	$^{1}H_2{}^{32}S$	AYT2	63719
H_3O^+	$1H_3{}^{16}O^+$	eXeL	1785
H_3^+	$^{1}H_2{}^{2}H^+$	ST	646
	$^{1}H_3^+$	MiZATeP	13606
	$^{2}H_2{}^{1}H^+$	MiZo	683
	$^{2}H_3^+$	MiZo	225
LiOH	$^{6}Li^{16}O^{1}H$	OYT7	840
	$^{7}Li^{16}O^{1}H$	OYT7	749
MgH	$^{24}Mg^{1}H$	XAB	2462
	$^{25}Mg^{1}H$	XAB	5850
	$^{26}Mg^{1}H$	XAB	5339
NH	$^{14}N^{1}H$	kNigHt	26131
	$^{14}N^{2}H$	kNigHt	943
	$^{15}N^{1}H$	kNigHt	943
	$^{15}N^{2}H$	kNigHt	943
NH_3	$^{14}N^{1}H_3$	CoYuTe	412149
NO	$^{14}N^{16}O$	XABC	106711
NaOH	$^{23}Na^{16}O^{1}H$	OYT5	
SO	$^{32}S^{16}O$	SOLIS	2501
SO_2	$^{32}S^{16}O_2$	ExoAmes	1504495
SiN	$^{28}Si^{14}N$	SiNfull	670
	$^{28}Si^{15}N$	SiNfull	464
	$^{29}Si^{14}N$	SiNfull	464
	$^{30}Si^{14}N$	SiNfull	464
SiO	$^{28}Si^{16}O$	SiOUVenIR	8729
TiO	$^{48}Ti^{16}O$	Toto	499775
VO	$^{51}V^{16}O$	HyVO	
YO	$^{89}Y^{16}O$	BRYTS	25
	$^{89}Y^{17}O$	BRYTS	25
	$^{89}Y^{18}O$	BRYTS	25
ZrO	$^{90}Zr^{16}O$	ZorrO	145317
	$^{91}Zr^{16}O$	ZorrO	5164
	$^{92}Zr^{16}O$	ZorrO	5164
	$^{93}Zr^{16}O$	ZorrO	5164
	$^{94}Zr^{16}O$	ZorrO	5164
	$^{96}Zr^{16}O$	ZorrO	5164

Developments

Continuous updating of the ExoMol database is particularly important.

We present the recent developments of the ExoMol database (**https://www.exomol.com/**).

Ancillary database **LiDB** [2]

Molecular vibronic state radiative lifetimes for plasma processes

https://www.exomol.com/lidb/

Photodissociation cross sections and continuum absorption

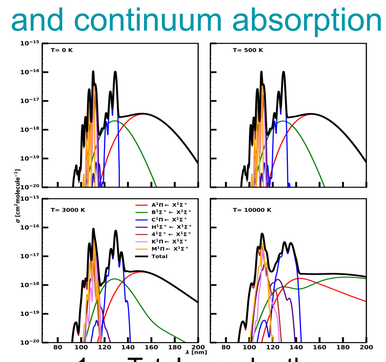


Figure 1. Total and the partial photodissociation cross-sections of $H^{35}Cl$ at 0, 500, 3000, and 10000 K [3]. We investigate the temperature dependence of the photodissociation cross-sections and rates for molecules of importance to exoplanetary.

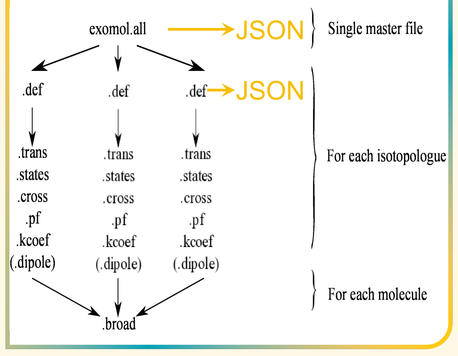
Adopting the IAEA standards for the atomic and molecular information

Table 3. Extract from the states file of the ^{27}AlH line list.

i	Ẽ (cm⁻¹)	g	J	unc (cm⁻¹)	τ (s)	+/−	e/f	State	v	|Λ|	|Σ|	|Ω|	Ecalc (cm⁻¹)	Source Label
1	0.000000	12	0	0.000001	inf	+	e	X(1Sigma+)	0	0	0	0	0.000000	Ma
2	1625.061501	12	0	0.000597	4.9288E-03	+	e	X(1Sigma+)	1	0	0	0	1625.069321	Ma
3	3194.213550	12	0	0.000365	2.6227E-03	+	e	X(1Sigma+)	2	0	0	0	3194.213685	MARVEL
4	4708.808866	12	0	0.000196	1.8633E-03	+	e	X(1Sigma+)	3	0	0	0	4708.817022	Ma
5	6170.189966	12	0	0.029900	1.4910E-03	+	e	X(1Sigma+)	4	0	0	0	6170.193041	Ma
6	7579.564189	12	0	0.250000	1.2740E-03	+	e	X(1Sigma+)	5	0	0	0	7579.564189	Ca
7	8938.046805	12	0	"Bad"	1.1350E-03	+	e	X(1Sigma+)	6	0	0	0	8938.046805	Ca
8	10246.644027	12	0	0.400000	1.0410E-03	+	e	X(1Sigma+)	7	0	0	0	10246.644027	Ca
9	11506.245734	12	0	0.400000	9.7520E-04	+	e	X(1Sigma+)	8	0	0	0	11506.245734	Ca
10	12717.633797	12	0	0.450000	9.2834E-04	+	e	X(1Sigma+)	9	0	0	0	12717.633797	Ca

We have updated our quantum number specifications to conform with the **PyValem** python package for parsing, validating, and manipulating quantum states labels of atoms, ions, and small molecules.

JSON format for line list APIs



High accuracy line lists with inclusion of uncertainties

I. BeH, MgH, CaH
II. SiO
III. HCN/HNC
IV. CH_4
V. NaCl, KCl
VI. PN
VII. PH_3
VIII. H_2CO
IX. AlO
X. NaH

High accuracy line lists

XI. HNO_3
XII. CS
XIII. CaO
XIV. SO_2
XV. HOOH
XVI. H_2S
XVII. SO_3
XVIII. VO
XIX. $H_2{}^{18}O$, $H_2{}^{17}O$
XX. H_3^+

High accuracy in progress

XXI. NO
XXII. SiH_4
XXIII. PO, PS
XXIV. SiH
XXV. SiS
XXVI. SN, SH
XXVII. C_2H_4
XXVIII. AlH
XXIX. CH_3Cl
XXX. $H_2{}^{16}O$

Old line lists

XXXI. C_2
XXXII. MgO
XXXIII. TiO
XXXIV. PH
XXXV. NH_3
XXXVI. SH (UV)
XXXVII. HCCH
XXXVIII. SiO_2
XXXIX. CO_2
XL. H_3O^+

In progress

O_2, NiH, CO, AlF, CH, HCO^+, OH^+

XLI. NaOH, KaOH
XLII. NO (UV)
XLIII. NaO
XLIV. SiO (UV)
XLV. MgH (UV), CaH (UV)
XLVI. SiN
XLVII. CaOH
XLVIII. H_2CS
XLIX. AlCl
L. H_3^+, H_2D^+, D_2H^+, D_3^+

LI. LiOH
LII. CH^+
LIII. YO
LIV. AlD
LV. VO (hyperfine)
LVI. SO
LVII. CH_4
LVIII. OCS
LIX. N_2O
LX. $^{15}NH_3$
LXI. OH
LXII. C_3
LXIII. HDO
LXIV. PN

A Python program **PyExoCross** [4] is designed to post process both ExoMol and HITRAN line lists

Figure 2. Calculation protocol.

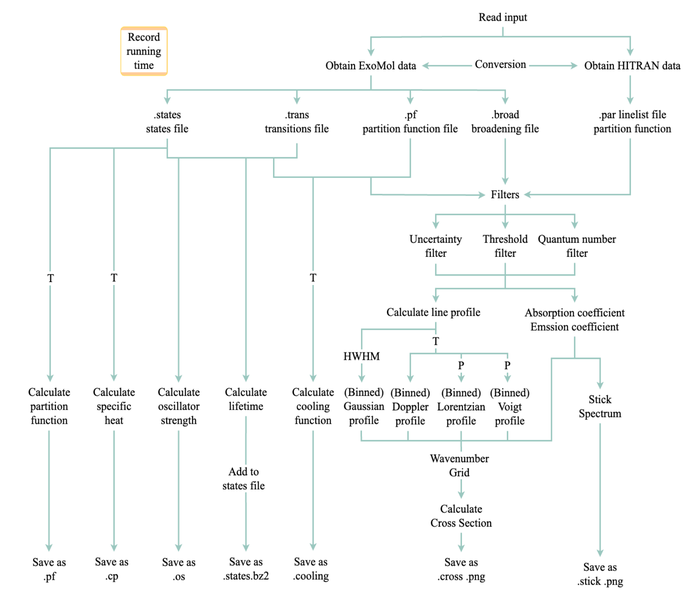


Figure 3(a). Partition functions.

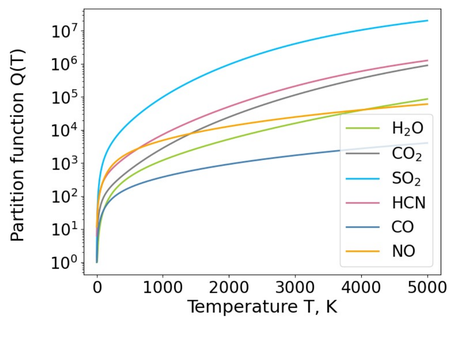


Figure 3(b). Specific heats.

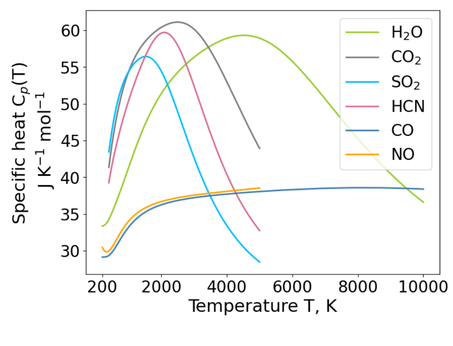


Figure 3(c). Cooling functions.

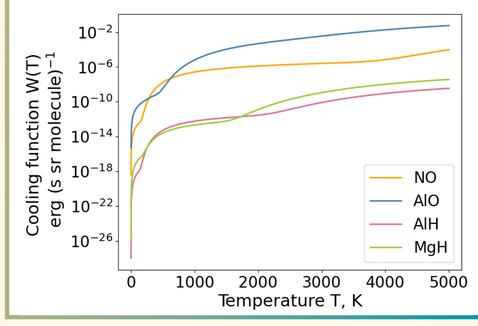


Figure 3(d). Lifetimes.

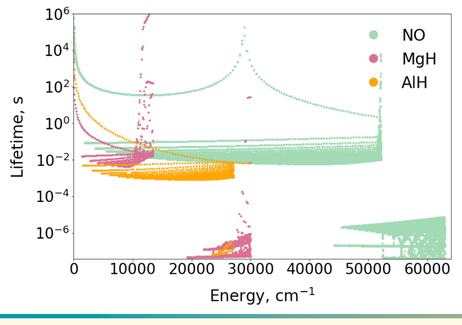


Figure 3(e). Oscillator strength.

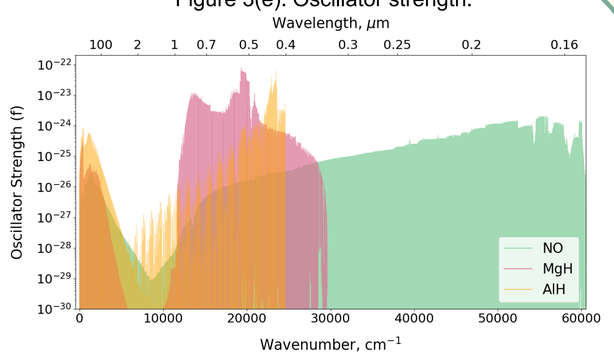


Figure 3(f). Stick spectra at different temperatures.

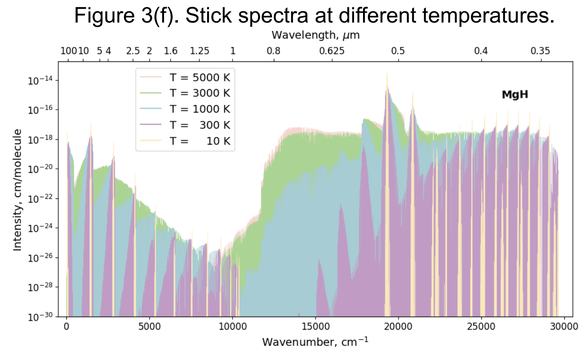


Figure 3(g). Stick spectra for different electronic states.

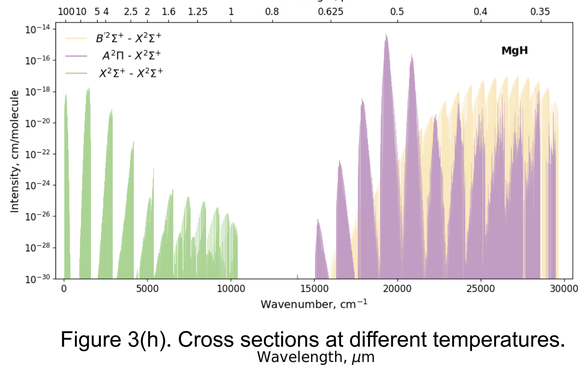
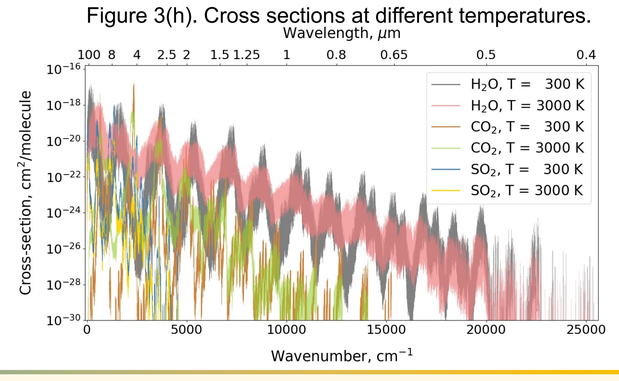


Figure 3(h). Cross sections at different temperatures.



Finding PostDoc Position

Interests:
Database, Molecular Spectroscopy, Exoplanet, Cross Sections
Programming Languages:
Python, Linux, Fortran, Django, HTML
Skills:
Scientific Computing, Data Mining, Machine Learning, Web Crawler Data Analysis, Data Visualization

LinkedIn CV GitHub

jingxin.zhang.19@ucl.ac.uk

https://github.com/Beryl-Jingxin

[1] Jingxin Zhang et al., "ExoMolHR: A Relational Database of Empirical High-Resolution Molecular Spectra", in preparation (2024).
[2] A. Owens et al., *Plasma Sources Sci. Tech.*, **32**, 085015 (2023).
[3] M. Pezzella et al., *Mon. Not. R. astr. Soc.*, **514**, 4413-4425 (2022).
[4] Jingxin Zhang et al., "PyExoCross: a Python program for generating spectra and cross sections from molecular line lists", *RAS Tech. Instr.*, (2024).