Spectroscopic Databases for Astronomical Applications

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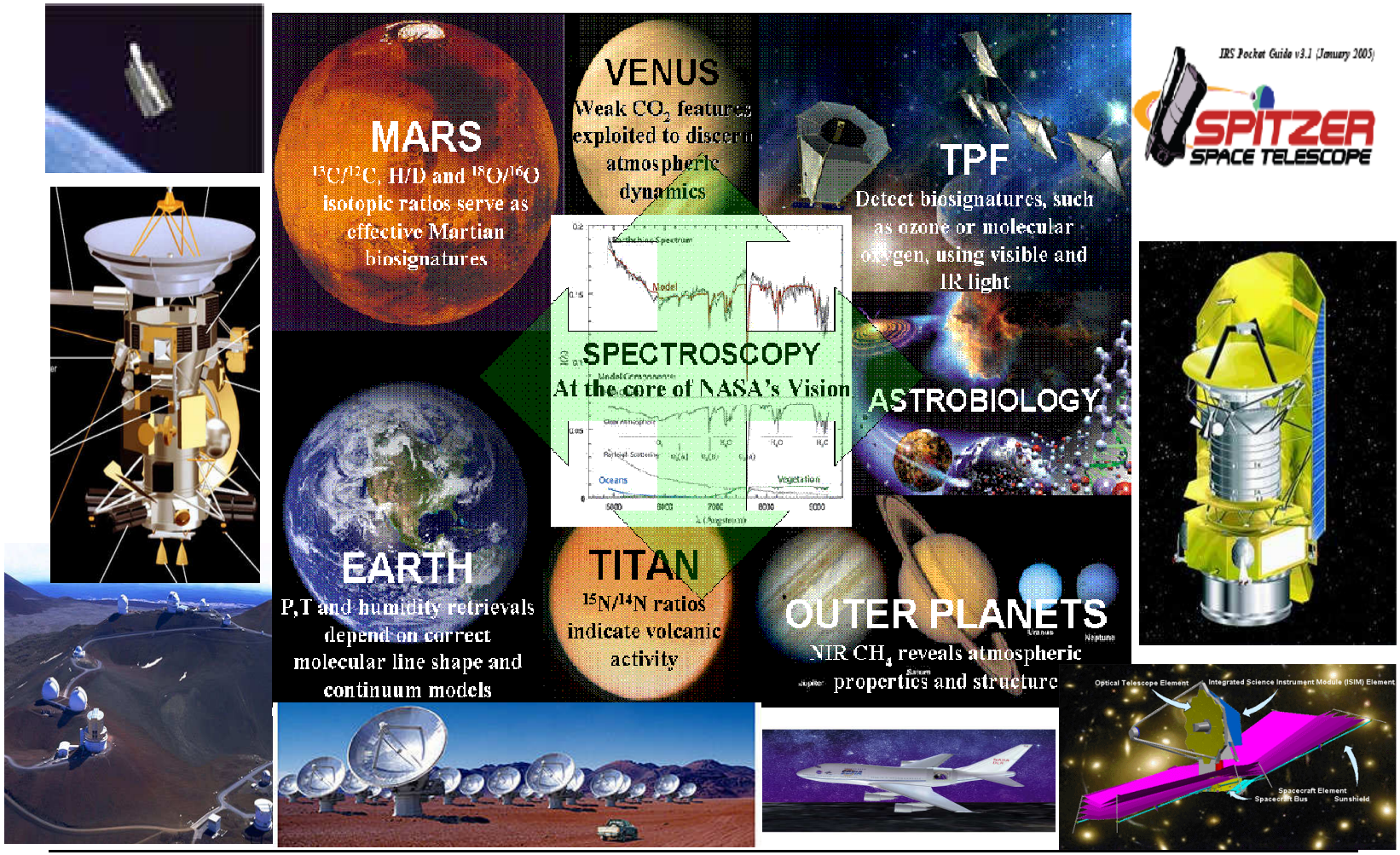
ASTRONOMICAL REMOTE SENSING



Basic transition *line* parameters:

- **Line position** (or center frequency)
- **Line intensity @ 296 K**
- **Lower state energy**
- **Vib - rotational quantum assignment**

Line shape parameters (Voigt)

- Pressure-broadened **widths** & temperature depend.
- Pressure-induced **frequency shifts**
- **Line mixing: H_2 + (CO_2, CO, CH_4, H_2O, NH_3 ….)**
- **Continua: collision-induced absorption (CIA)**

(given as *absorption cross sections*)

METHODS TO OBTAIN SPECTROSCOPIC PARAMETERS

- **Calculations based on successful theoretical modeling** ***(good positions and intensities, but not shapes)***
- **Predictions based on limited data and/or poorer theoretical modeling** ***(extrapolations very poor!)***

- **Empirical data retrieved line-by-line with some known assignments** ***(many weak lines omitted!)***
- **Absorption cross sections from lab spectra at different temperatures and broadeners** ***(for unresolved heavy species and continua)***
- **Raw laboratory spectra!**

Current Public Databases (from Web)

Standardized formats, documentation **Quality control** and **FUNDED!!**

Database	Websites (http://)	cm^{-1}	#Species	#Transitions
HITRAN 2008 HITEMP	cfa - www.harvard.edu (/hitran) H_2O,CO_2, CO,OH,NO	0.0 to 26000 *(385 nm)*	39 + 32 xsec	2,713,968 ~ 113 M
GEISA 2009	ara.lmd.polytechnique.fr molecules planetary → terrestrial	0.0 to 35877 *(279 nm)*	50 (111 iso)	3,807,997
JPL 2010 CMSD (Cologne)	spec.jpl.nasa.gov www.ph1.uni-koeln.de molecules, radicals, atoms for astrophysics	0. to ~500. ++ (one species up to 5600 cm^{-1})	~580	1,530,000 *at long wavelengths*
NIST	www.nist.gov			
at short wavelengths ??? INDIVIDUAL COLLECTIONS				

HITRAN: Bi-annual meetings

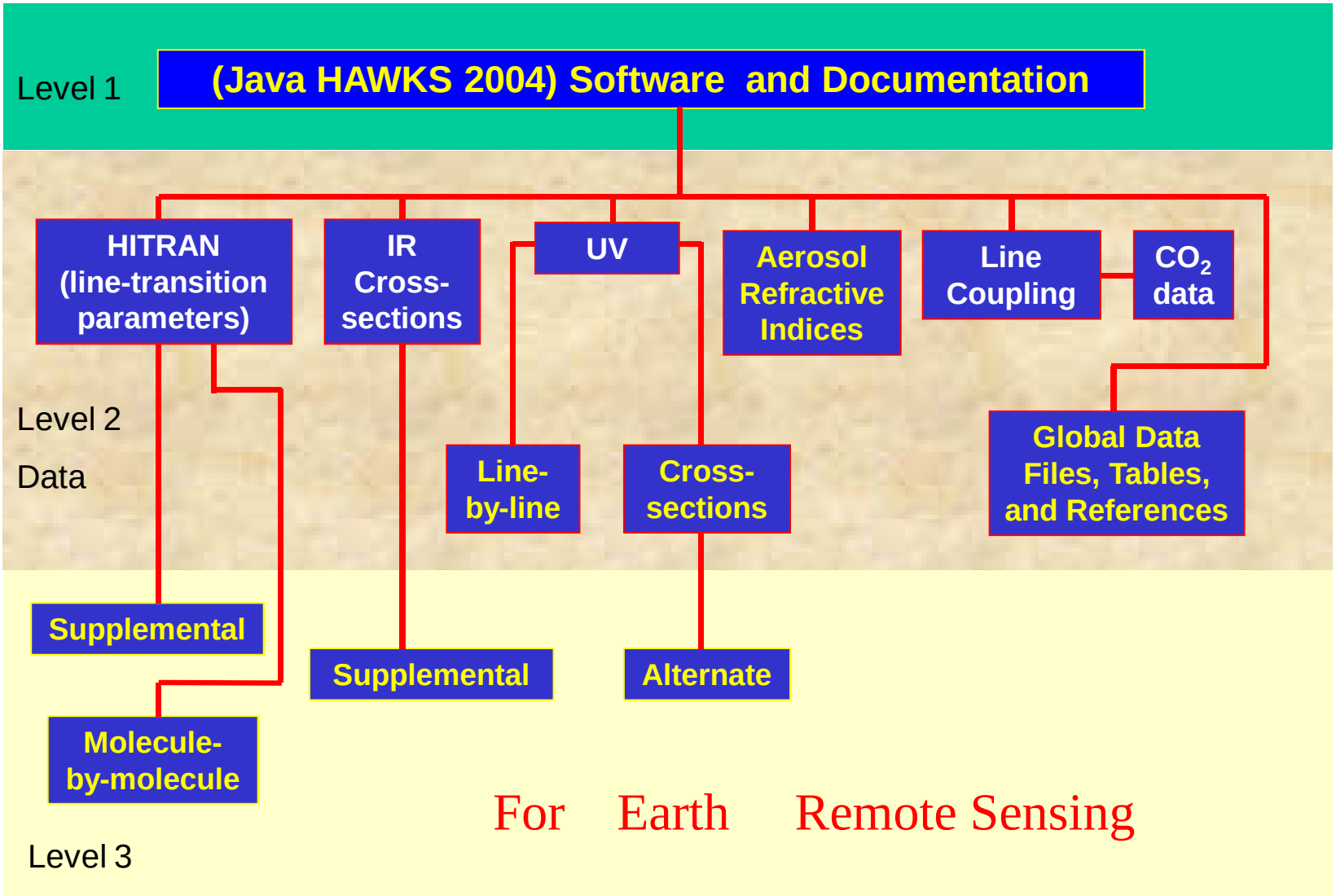
Spectroscopy presentations & advisory committee

http://www.cfa.harvard.edu/hitran

Started in 1973 for Atmospheric Remote Sensing

New editions with documentation every ~ 4 years

HITRAN Compilation



For Earth Remote Sensing

THE GEISA DATABASE 2009 EDITION: Update Description and Assessment of Spectroscopic Parameters Through Hyperspectral Remote Sensing Applications

Jacquinet-Husson N., Crépeau L., Capelle V., Scott N.A., Armante R., Boutammine C., Chédin A.

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http://ara.lmd.polytechnique.fr

- Presentation
- The Context
- Research themes
- Tools
- Geisa
- Get ARA data
- HFTP
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Last update: 18th May 2009

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The ARA Group

The Atmospheric Radiation Analysis group is specialized in the study of the variability and evolution of the climate of the Earth from space borne observations made principally by vertical sounders, in the infrared and the microwave domains.

Its main research themes relate to the collection of a long term, global, climatology of the earth-atmosphere state: temperature and moisture; cloud characteristics, including their microphysical properties; greenhouse gases, mainly CO_2, in relation with the carbon cycle; aerosols (volcanic, dust, smoke, etc.) infrared characteristics in relation with the earth radiative budget; continental surface infrared emissivities, in relation with the interaction between the surface and the atmosphere. The group is also deeply involved in statistical analysis of large spatio-temporal data bases (inverse problems, linear and non linear inference, neural networks, classification, pattern recognition, etc.).
The group has developed numerous tools in spectroscopy of the atmospheric gases, forward and inverse radiative transfer modelling, etc. In particular, the group develops and maintains the spectroscopic data base GEISA « Gestion et Etude des Informations Spectroscopiques Atmosphériques » *(Study and management of atmospheric spectroscopic information)*.

The Laboratoire de Météorologie Dynamique (LMD) is a Laboratory of the French Centre National de la Recherche Scientifique (CNRS), of the Ecole Polytechnique, of the Ecole Normale Supérieure, of the Université Pierre et Marie Curie (Paris 6), and belongs to the Institut Pierre-Simon Laplace (IPSL). It is also one of the French space laboratories working in cooperation with the Centre National d'Etudes Spatiales (CNES).

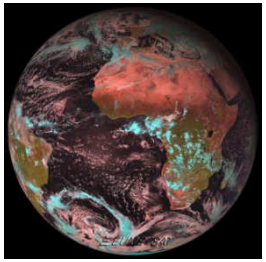
GEISA: Gestion et Etude des Informations Spectroscopiques Atmosphériques ;

Management and Study of Atmospheric Spectroscopic Information

GEISA-2009 for planets : emphasis on Earth

ThreeTypes of DATABASES

- **Line transition parameters database**
  50 molecules (111 isotopic species)
  3,807,997 transitions between 0.000001 and 35,877 cm^{-1}

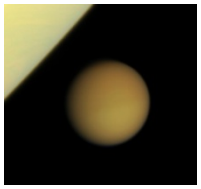


(MSG-2 25/01/06)

EARTH

- Major Permanent constituents of EARTH atmosphere : O_2,H_2O,CO_2…
- Trace molecules in the EARTH' atmosphere :
  NO, SO_2, NO_2, NH_3, HNO_3, OH,HF, HCl, HBr, HI, ClO, OCS, H_2CO, PH_3 ,.

- **Molecules in Planetary Atmospheres of**
  JUPITER, SATURN, URANUS,TITAN etc.:
  C_2H_6, CH_3D, C_2H_2, C_2H_4, GeH_4, HCN, C_3H_8, C_3H_4



(CASSINI-HUYGENS 29/01/06)

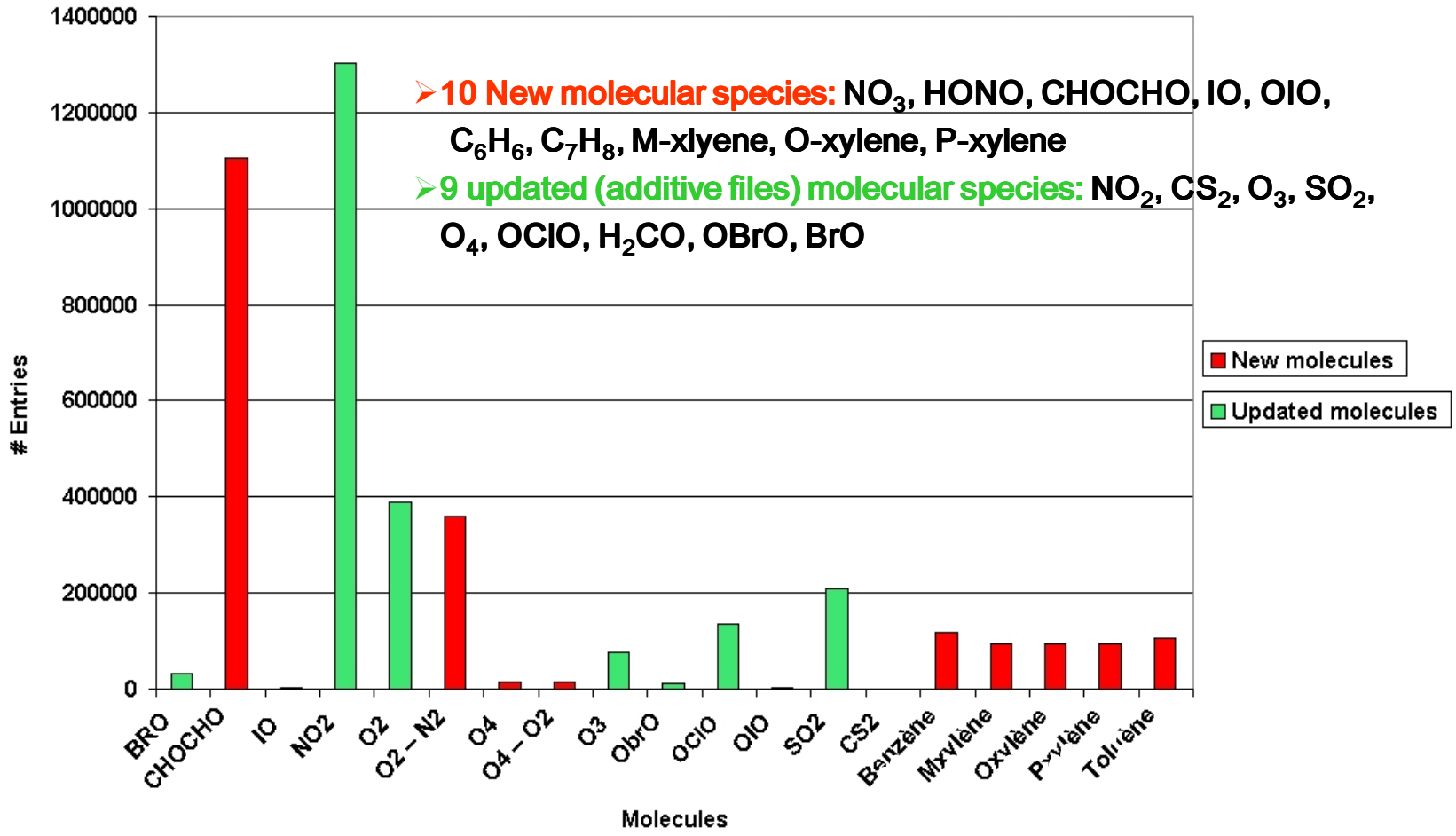
TITAN

- **Absorption cross-sections database**
  - IR: 43 molecular species (mainly CFC's)
  - UV/Visible : 19 molecular species

- **Aerosol data archive and softwares**

MANAGEMENT SOFTWARES
For each Sub-database

GEISA-09 UV/VIS CROSS-SECTIONS
(molecular species update)



- **10 New molecular species:** NO_3, HONO, CHOCHO, IO, OIO, C_6H_6, C_7H_8, M-xlyene, O-xylene, P-xylene
- **9 updated (additive files) molecular species:** NO_2, CS_2, O_3, SO_2, O_4, OClO, H_2CO, OBrO, BrO

Atmospheric Species of Solar System Objects

CLASSES OF ATMOSPHERES	SOLAR SYSTEM OBJECT	MAIN COMPONENTS (non exhaustive lists)
H_2-He atmospheres of the giant planets	JUPITER	**H2, He, CH4,** C2H2, C2H6,C2H4,H2O, C4H2, C6H6 HD, C3H4, NH3, PH3, GeH4, CO, AsH3, CO2,...
	SATURN	**H2, He, CH4,** C2H2, C2H6, C3H4,CH3, H2S, CH3, H2O, C3H8, CH3C2H, NH3, SiH4 PH3,GeH4,H2O,AsH3,C2H6,C2H4,CO,CO2...
	URANUS	**H2, He, CH4,** C3H4,C4H2, C2H6 ...
	NEPTUNE	**H2, He, CH4,** C2H4, C2H2, C3H4, C4H2, NH3 **(?), CH3, C6H6**
Terrestrial CO_2 atmospheres	VENUS	**CO2, N2, SO2, H2SO4,** CO, O, N2, O3, FeCl3(?), H2O, O2, Cl, ClO, ClO2, COCl, .. HCl, HF, Ne, H2S , OCS, H, H2, He
	MARS	**CO2, N2,** Ar, O2, H2O, CO, H2O2 ?, CH4, O3, Ne, Kr, Xe, **...**
N_2 atmospheres	TITAN	**N2, CH4,** Ar, C2H6, C3H8, H2O, CO, CO2, CH3D, CH3, C2H4, NH3, HCN, C2N2, HC3N, CH3CN, C4H2, C2HD, CH2CCH2, C6H2, C3H4, HC5N, C4N2, C6H6, CH2 ...
	EARTH	**N2, O2, Ar, H2O, CO2,** O3, N2O, CH4, C2H6, C2H2, NO, SO2, NO2,HNO3,OCS,NH3,HCN,H2CO,+ many more ...
	PLUTO	**N2,** CO, CH4**...**
	TRITON	**N2,** CO, CH4, CO2...
Volcanic	IO	**SO2 ...**
Exospheres	MOON	Na, K **...**
	MERCURY	Na, K ...
Comae	COMETS	**H2O,** CH4, C2H6, CO, CO2, H2CO, CH3OH, **.....**
Extrasolar planets	??	**H2O, CH4, CO2** ....

CDMS and JPL Catalogs for astrophysics

www.cdms.de and spec.jpl.nasa.gov

Download parameters by species

- Molecules detected or detectable in inter/circumstellar medium
- **Emphasis on Submillimeter and TeraHertz regions** for **HERSCHEL**
- Predictions based on modeling experimental frequencies via Hamiltonians
- Separate entries for rarer isotopomers or excited vibrational states (1-1)
- **Entries include species not important for Earth and planets**
  - light hydrides and deuterated species: HD_2^+, NH, ND, CH_2D^+, NH_2D, NHD_2, ND_3
  - molecules in excited vibrational states: HCN, HNC, HC_3N, HC_5N, CS, SiO
  - complex species: ethylene glycol
- ~ **580** entries as of Sept. 2010

Number of species a factor of 10 over GEISA and HITRAN

NEED *MORE*? Try specialized collections

HITEMP, the high-temperature molecular spectroscopic database

L.S. Rothman [a,*], I.E. Gordon [a], R.J. Barber [b], H. Dothe [c], R.R. Gamache [d], A. Goldman [e], V.I. Perevalov [f], S.A. Tashkun [f], J. Tennyson [b]

JQSRT 2010

Table 4
Line list comparison between HITEMP2010 and HITRAN [2].

Molecule	Spectral coverage (cm^{-1})	Number of isotopologues[a] (HITEMP2010)	Number of transitions (HITEMP2010)	Number of transitions[b] (HITRAN)	Dissociation energy (cm^{-1})
H_2O	0–30,000	6	111,377,777	69,201	41,145.94 ± 0.15 [75]
CO_2	258–9648	7	11,167,618	312,479	44,360 [76]
CO	0–8465	6	115,218	4,477	90,674 ± 15 [77]
NO	0–9274	3	105 633	105,079	52,265 [78]
OH	0–19,268	3	40,055	31,976	35,593 ± 25 [79]

Weaker lines included

[a] For H_2O, NO, and OH, only the principal isotopologue has been created for high temperature at this time. The other lesser abundant isotopologues have been transcribed from HITRAN (296 K).
[b] The number of transitions listed in this column are for the equivalent number of isotopologues and spectral range consistent with HITEMP2010.

for near-IR applications: ***(Follow 'other lists' links on HITRAN)***

UCL (Tennyson) www.tampa.phys.ucl.ac.uk/ftp/astrodata/ Ab initio

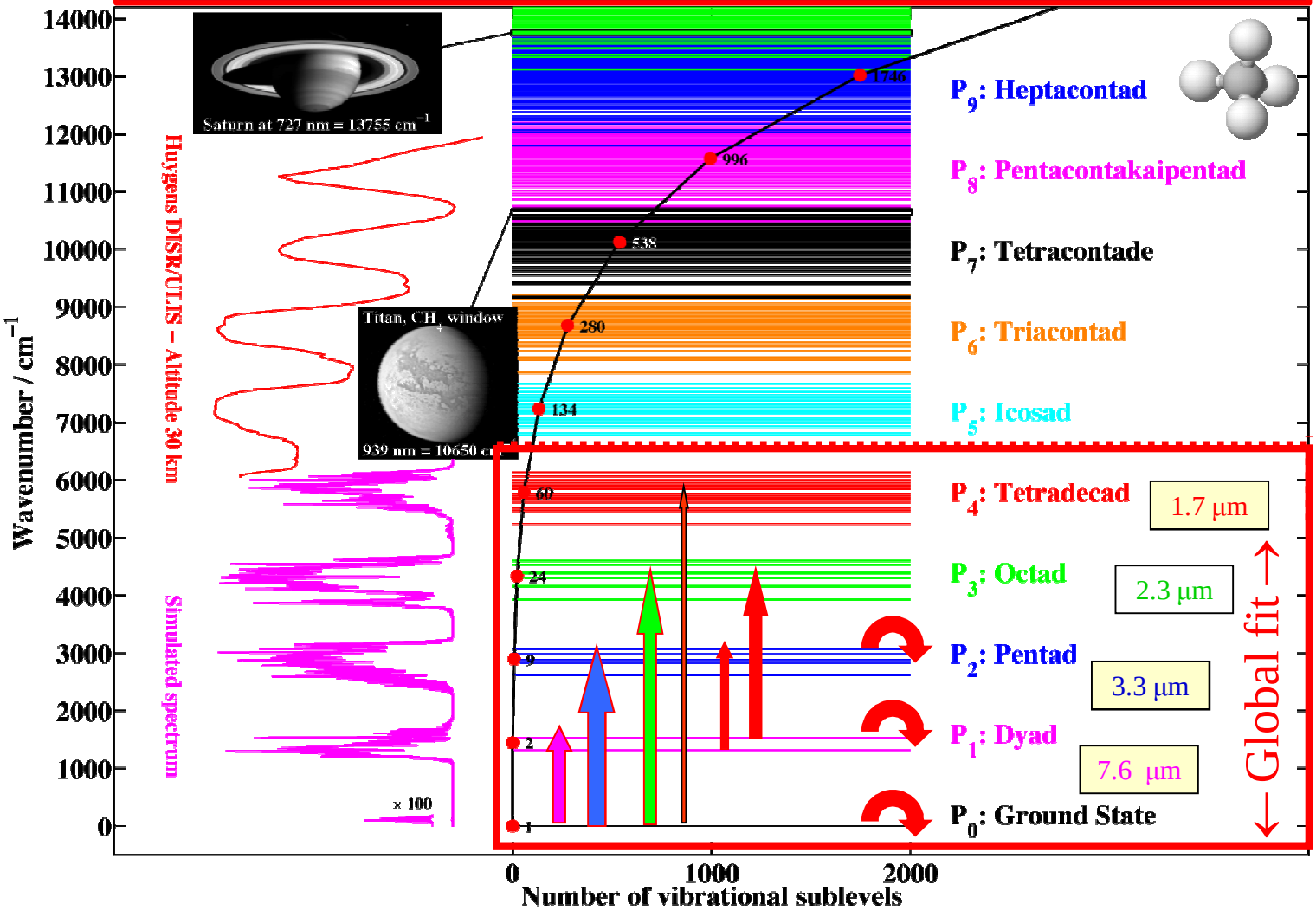
Oxford, UK (Irwin) www.atm.ox.ac.uk/user/irwin/band.html **(cross sec.** NH_3, CH_4)

PNNL nwir.pnl.gov 600-6000 cm^{-1} **336** species Cross Sections (*no funding now*)

VPL vpl.astro.washington.edu/sci/ /plots of spectra/ 0.0 –22000 cm^{-1} (PNNL+ HITRAN +)

Dijon (Boudon) icb.u-bourgogne.fr/titan **(linelists for** CH_4**)**

METHANE Polyads: 0 – 14000 cm^{-1}



From Boudon et al.

Tennyson: Ab initio Linelists

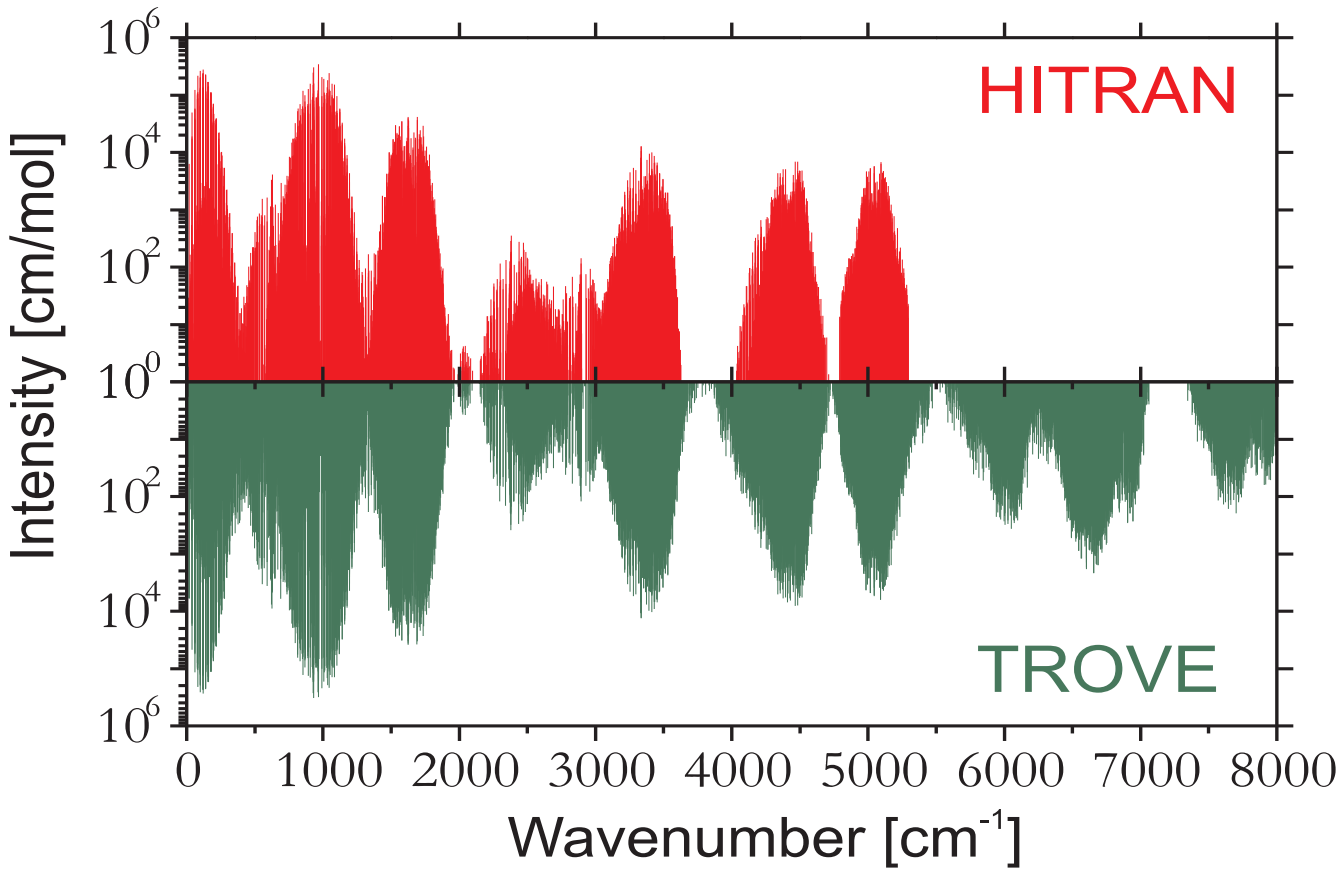
completed or under construction @ UCL

www.tampa.phys.ucl.ac.uk/ftp/astrodata/

	by
H_3^+	Neale
H_2D^+	Sochi
H_2O	Barber
HDO	Voronin
HCN/HNC ($H^{13}CN$/ $H^{13}CN$)	Harris
HeH^+	Engel
NH_3	Barber, Yurchenko (Dresden)
HCCH	Urru
C_3	La Delfa and Sochi

NH_3: Comparison of UCL predictions with HITRAN

(J. Tennyson, HITRAN 2010)



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Private collections: merging information from different sources

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ATOMIC AND MOLECULAR OPACITIES FOR BROWN DWARF AND GIANT PLANET ATMOSPHERES

C. M. Sharp[1] and A. Burrows[1]

ATOMIC AND MOLECULAR OPACITIES

TABLE 1

Summary List of Species, Section Numbers, and Band Systems

Species	Section	Comments
H	2.5 and 3.2	Lines and continuum
H^-	3.2	Continuum present when free electrons are also present
He	3.3	Important for CIA and line broadening
Li	2.6	Alkali element: lines
Na	2.6 and 3.2	Alkali element: lines and continuum
K	2.6 and 3.2	Alkali element: lines and continuum
Fe	2.5 and 3.2	Lines and continuum
Rb	2.6	Alkali element: lines
Cs	2.6	Alkali element: lines
H_2	2.5 and 3.3	CIA, and *B–X* and *C–X* UV bands
CO	2.1 and 2.5	Vib-rot bands in IR and *A–X* band system in UV
SiO	2.5	*A–X* band system in UV
H_2O	2.1 and 2.5	Rot and vib-rot bands in IR and absorption in UV
NH_3	2.1	Vib-rot bands in IR
CH_4	2.1 and 3.3	Vib-rot bands in IR
H_2S	2.4 and 2.5	Precomputed vib-rot bands in IR and absorption in UV
PH_3	2.4	Precomputed vib-rot bands in IR
TiO	2.1	α, β, γ, γ', δ, ϵ, and ϕ band systems
VO	2.1	*A–X*, *B–X*, and *C–X* band systems
TiH	2.3	*A–X* and *B–X* band systems
CrH	2.3	*A–X* band system
FeH	2.3	*F–X* band system
MgH	2.3	*X–X*, *A–X*, and *B′–X* systems
CaH	2.3	*A–X*, *B–X*, and *D–X* systems
$MgSiO_3$	3.4	Enstatite in Mie theory
H_2O	3.4	Water in Mie theory

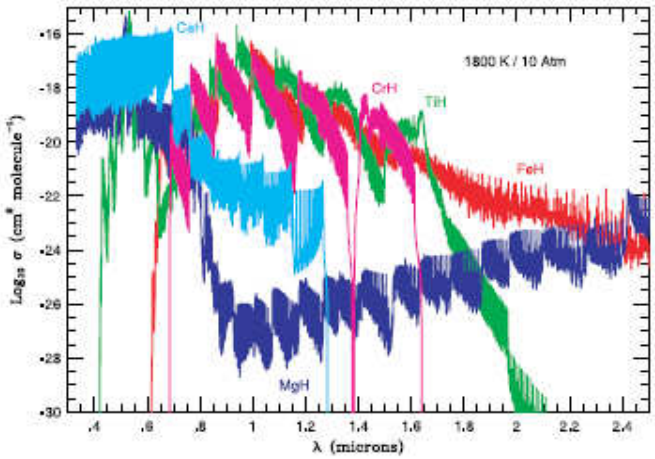
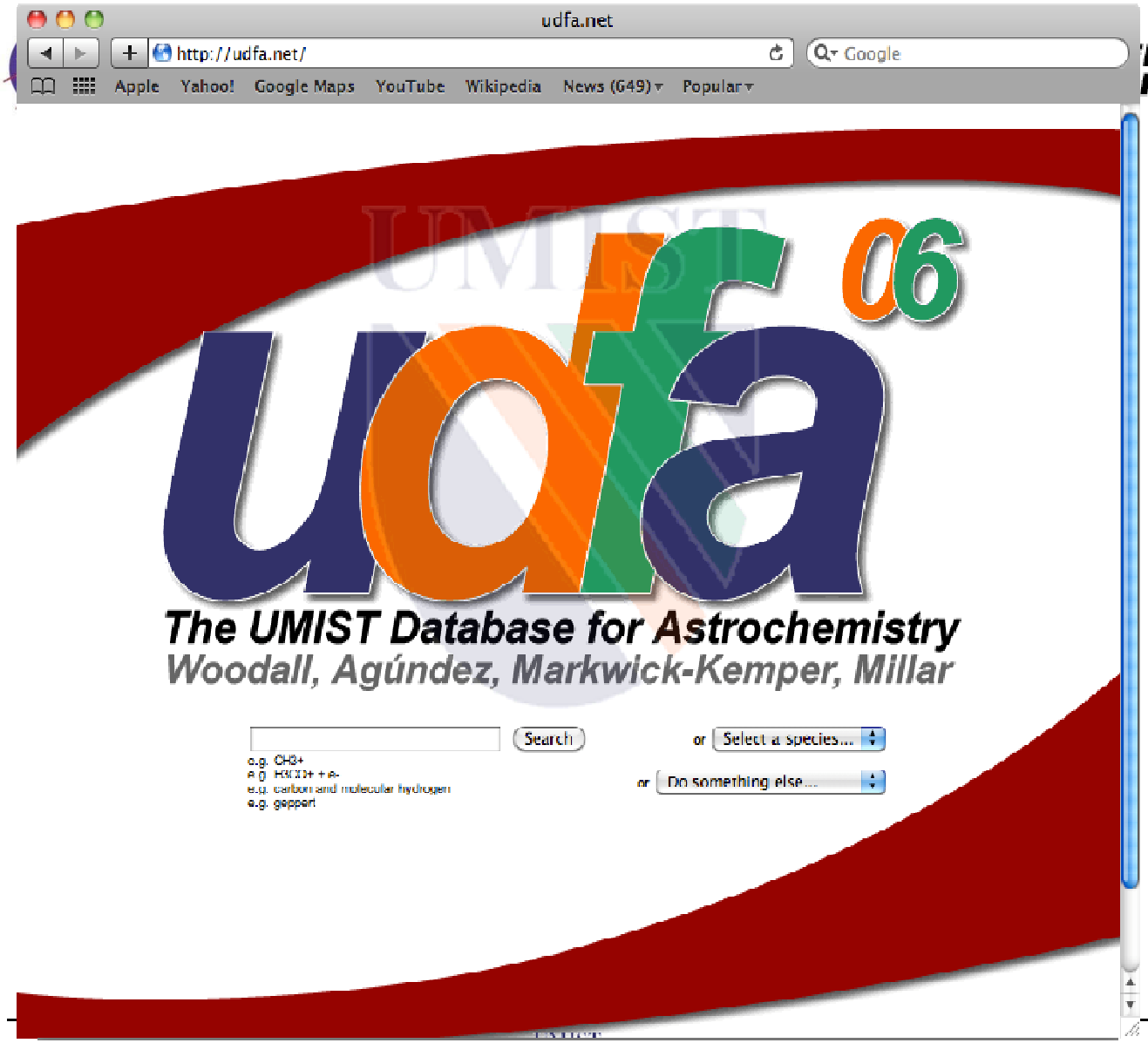


Fig. 7.—Log of the monochromatic absorption σ in cm^2 $molecule^{-1}$ as a function wavelength λ in μm in the infrared and visible at a temperature of 1800 K and a pressure of 10 atm for the five metal hydrides FeH, TiH, MgH, CrH, and CaH, represented, respectively, in red, green, blue, magenta, and cyan. All the bands are due to electronic transitions, except that for MgH, which includes vibration-rotation transitions in the ground *X* electronic state, in addition to the *A–X* and *B′–X* electronic systems.

UV-VUV info (via Web) examples?

Lists?	Websites (http://)	Data
MPI-Mainz *(Oct 2010)*	**www.atmosphere.mpg.de/enid/2295** *Easy to use*	**840** species **atlas, xsec**
CFA → *'other lists' on HITRAN*	**www.cfa.harvard.edu/amp** *VUV cross sections, energy levels and wavelengths (ASCII files)*	O_2, H_2O, O_3, C_2H_2, CO_2, CO, SO_2, N_2 NO, NO_2,N_2O
MOLAT *(2006?)*	**molat.obspm.fr/index.php?page=pages/menuSpectreMol.php**	**VUV** **H_2, D_2, CO, N_2** others
N_2 *Etc.*	**www.wellesley.edu/Physics/gstark/N2_ANU_cross_sections/**	**N_2**


udfa.net
http://udfa.net/
Google
Apple
Yahoo!
Google Maps
YouTube
Wikipedia
News (649)
Popular
udfa 06
The UMIST Database for Astrochemistry
Woodall, Agúndez, Markwick-Kemper, Millar
Search
or
Select a species...
e.g. CH3+
e.g. carbon and molecular hydrogen
e.g. geppert
or
Do something else...

STANDARD DATABASE FORMAT:

Parameter	Field size	Definition
Mol	I2	Molecule number
Iso	*I1*	*Isotope number (1 = most abundant, 2 = 2nd most abundant,..)*
ν_{if}	F12.6	Transition position in vacuum [cm^{-1}]
S_{if}	E10.3	Intensity [$cm^{-1}/(molecule \cdot cm^{-2})$ @ 296K]
A_{if}	*E10.3*	*Einstein A-coefficient [s^{-1}]*
γ_{air}	F5.4	Air-broadened half-width (HWHM) [cm^{-1}/atm @ 296K]
γ_{self}	*F5.4*	*Self-broadened half-width (HWHM) [cm^{-1}/atm @ 296K]*
E''	F10.4	Lower-state energy [cm^{-1}]
n_{air}	*F4.2*	*Temperature-dependence coefficient of air width*
δ_{air}	F8.6	Air pressure-induced shift [cm^{-1}/atm @ 296K]
v', v''	*2A15*	*Upper and Lower "global" quantum numbers*
q', q''	*2A15*	*Upper and Lower "local" quantum numbers*
ierr	6I1	Uncertainty indices for ν_{if}, S_{if}, γ_{air}, γ_{self}, n_{air}, δ_{air}
iref	6I2	*Reference pointers for* ν_{if}, S_{if}, γ_{air}, γ_{self}, n_{air}, δ_{air}
*	A1	Flag for line-coupling algorithm (line mixing)
g', g''	2F7.1	Upper and Lower statistical weights

CONCLUSIONS

- **No public database tailored for astrophysics at shorter wavelengths**
- **Astronomers often must use their own private (undocumented) collections.**
- **Basic molecular parameters (positions, intensities) available for dozens, but needed for hundreds (*thousands?*) of astrophysics species.**
- **Join efforts with others: http://www.vamdc.org/**

VAMDC

Virtual Atomic and Molecular Data Centre

Marie-Lise Dubernet, LPMAA Université Pierre et Marie Curie, Paris

- *e-Infrastructure Project (to collect spectroscopic lists)*
- **15 legal partners - 21 institutes or departments in 7 EU countries, Russian Federation (4 institutes) and Venezuela (2 institutes)**
- **Started July 2009 – (funded for) 42 months**
- **Possible outcome: legal entity or *laboratory without walls***

www.vamdc.org