A dynamic database of molecular model spectra

http://www.spectrafactory.net
Outline

• Motivation / introduction
• The model calculations
• The web interface
• Current status
• Some examples
• Future prospects & needs
Motivation

• We live in a *molecular universe*! Molecules detected in/around young stars, old stars, interstellar medium, planetary atmospheres, comets, entire galaxies, ...

• Molecules are observed from UV to sub-mm wavelengths

• Important diagnostic *tools* & probes !!
Sensitive to temperature

 normalized flux + offset

 - $T = 800 \text{ K}$
 - $T = 400 \text{ K}$
 - $T = 100 \text{ K}$

 Wavelength ($\mu$m)
Sensitive to density

Log $N = 17$

Log $N = 18$

Log $N = 19$

Normalized flux + offset

Wavelength ($\mu$m)
Sensitive to exact species

Normalized flux + offset

Wavelength (μm)
Extracting physical parameters

Identification of species
- Where to find frequencies & line strengths?
- Which one of those millions of molecules?
- What band profile?

Spectral dependence on physical parameters
- Some knowledge of molecular spectroscopy
- Some knowledge of radiative transfer

Model fit
- All of the above, plus some statistics
In an ideal world...

Observed Spectrum

Black box

Perfect Fit

Physical/chemical parameters
Our aim

Observed Spectrum

Grey box

Best Fit given limitations

Estimate of Physical/chemical parameters
<table>
<thead>
<tr>
<th>Black box</th>
<th>Grey box</th>
</tr>
</thead>
<tbody>
<tr>
<td>All possible molecular species</td>
<td>What’s available</td>
</tr>
<tr>
<td>All possible transitions</td>
<td>What’s available</td>
</tr>
<tr>
<td>Full non-LTE radiative transfer</td>
<td>Isotherm, LTE</td>
</tr>
<tr>
<td>Various geometries</td>
<td>Slab</td>
</tr>
<tr>
<td>All possible instruments</td>
<td>On request</td>
</tr>
<tr>
<td>Robust statistics, fast</td>
<td>Future</td>
</tr>
</tbody>
</table>
Molecular species

143 molecules detected in space
212 including isotopologues
most in sub-mm

42 molecules studied in earth atmosphere
line lists available at 296 K (HITRAN)
often infrared

5 molecules with good line lists
\( \text{H}_2\text{O}, \text{TiO}, \text{SiO}, \text{CO}, \text{CO}_2 \)
Large frequency range
Many levels (electronic, vibrational, rotational)
High temperatures
Model calculations I

Line list: Frequencies of transition

Intrinsic line strength at $T_{ref}$

→ Calculate line strength at desired $T$
Model calculations II

- Multiply line strength by column density
- Convolve with intrinsic line profile

→ Calculate optical depth
Model calculations III

Assume LTE & slab

How does this absorb radiation?

Radiative transfer
Model calculations IV

Convolve with instrument spectral response

Instrument simulation

![Graph showing normalized flux over wavelength (μm) with CDSD at 100 K and 1000 K, and Spitzer-IRS HiRes simulation.](image-url)
Current contents of database

- 42 molecules (95 isotopologues)
- 25 different temperatures (100 K – 2500 K)
- 9 column densities ($10^{16} - 10^{24}$ cm$^{-2}$)
- 5 Instrument presets

291,213 model spectra (as of today)

Model spectra added by user requests!
The web interface - architecture

MySQL
 php

XML
 DHTML

Javascript
 Flash

Server

Client

http://www.spectrafactory.net/
<table>
<thead>
<tr>
<th>Molecule</th>
<th>Isotopologue</th>
<th>Line List</th>
<th>Temperature (K)</th>
<th>log Column Density (cm(^{-2}))</th>
<th>Resolution</th>
<th>Oversample</th>
<th>Instrument</th>
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<tbody>
<tr>
<td>H(_2)O</td>
<td>H(_2)(^{16})O</td>
<td>Schwenke</td>
<td>500</td>
<td>18</td>
<td>2000</td>
<td>2</td>
<td>IRTF SpeX</td>
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Found 15 spectra, showing 1 - 15.
Needs & prospects

More / better line lists
- Inaccurate line lists better than no line list
- Theoretical calculations and/or laboratory work
- Availability is only limit to our database!

Funding
- This project is 0% funded

Observatories
- Spitzer (now), soon SOFIA, Herschel, ALMA, ...

143 molecules detected in space; many more will be detected in the next years