



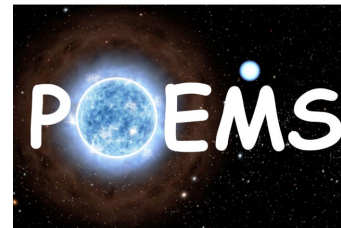
# *Modeling diatomic molecules in circumstellar disk*

*Rodolfo Vallverdú*

*Ondrejov, June 29, 2023*



Facultad de Ciencias  
**Astronómicas  
y Geofísicas**  
UNIVERSIDAD NACIONAL DE LA PLATA





## **Molecules in circumstellar disk.**

The temperature is low enough to allow the formation of molecules.

Molecules are evidenced by the presence of molecular emission bands in the star's spectrum.

The shape of the lines in the molecular bands indicates that they are formed in a rotating disk.

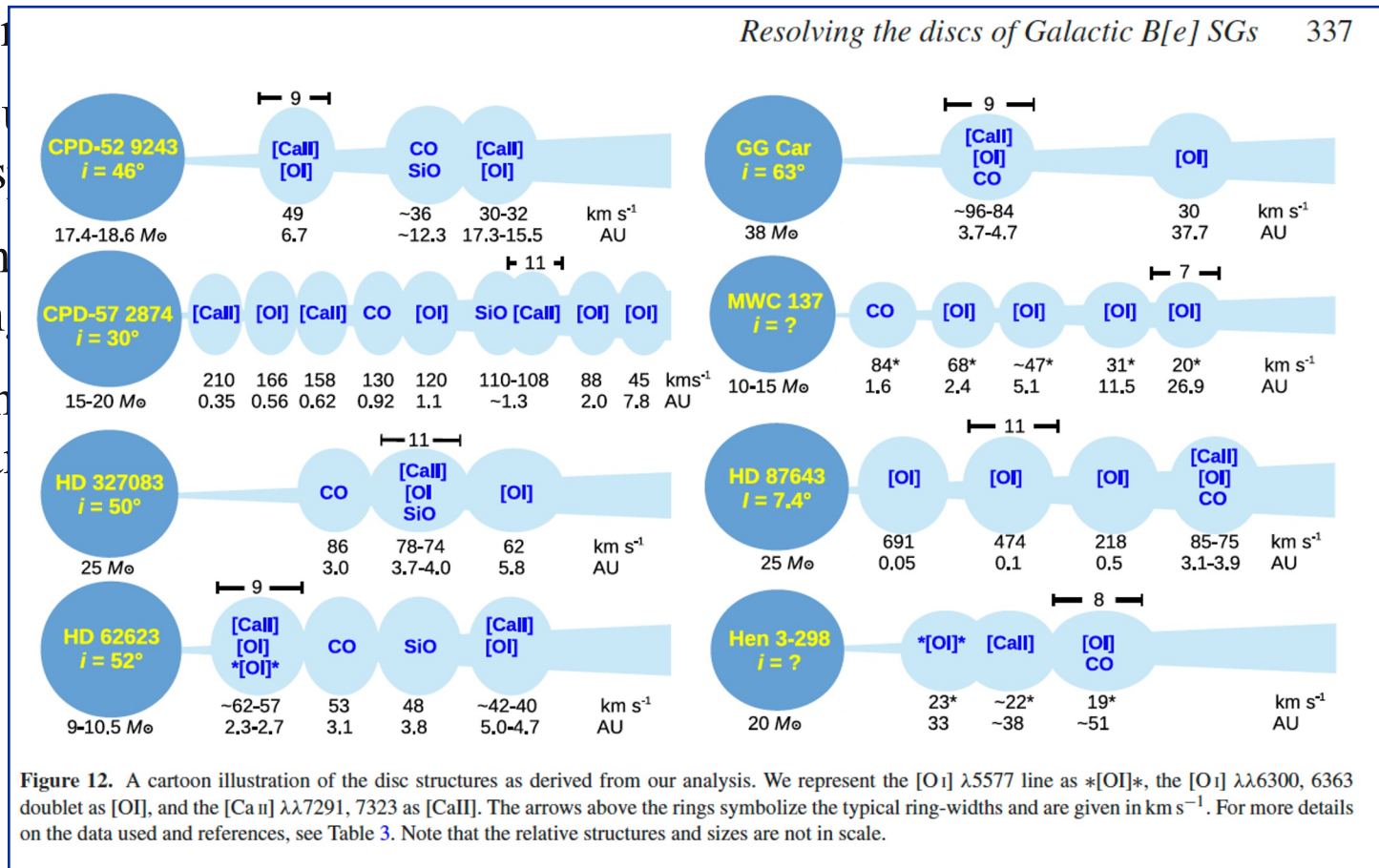
Each molecule is located in specific regions of the disk at a given distance from the star (Maravelias et al., 2018).



# Molecules in circumstellar disk.

The temperature  
Molecular  
star's surface  
The shock  
rotating  
Each molecule  
the star

in the  
ed in a  
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## **Molecules in circumstellar disk.**

The temperature is low enough to allow the formation of molecules.

Molecules are evidenced by the presence of molecular emission bands in the star's spectrum.

The shape of the lines in the molecular bands indicates that they are formed in a rotating disk.

Each molecule is located in specific regions of the disk at a given distance from the star (Maravelias et al., 2018).

It is necessary to have synthetic spectra in order to identify the molecules present in circumstellar disks and determine the disk parameters in the regions where these molecules are found.



## **The Code.**

Programmed in FORTRAN 95.

The code does not have a name, for now it is temporarily called DisMol.

It allows calculating the spectrum of a single molecule or the combined spectrum of multiple molecules with overlapping molecular bands.

The code considers each isotopic variant as a separate molecule.

The code requires multiple input files. Some files need to be manipulated by the user to input the spectrum characteristics, while others contain specific data for each molecule that should not be altered.

Depending on the number of rovibrational levels and their respective transitions of the considered molecule, the computational requirements can be demanding.



```
emacs@electra
File Edit Options Buffers Tools Help
=====
# File with the data of the molecules and the disk. English version.
#-----
# --- Lenguaje. -----|-----
ES                               Selected language.
# --- Spectrum data. -----|-----
Disco-C0-2000.sal                 File name with the spectrum.
C0                               Molecule (if there are several, write them).
30000                            Number of grid points.
2.29                             Minimum wavelength [Microns].
2.80                             Maximum wavelength [Microns].
16.0                             V Res [km/s], spectral resolution.
2.0                              Grid spacing delta V [km/s].
# --- Molecule data. -----|-----
2                               Number of molecules.
Entrada-C12-016.dat              File name of molecule 01.
Entrada-C13-016.dat              File name of molecule 02.
# --- Disk data. -----|-----
40.0                             Disk inclination [deg].
2                               Number of rings.
# ... Ring 01 .....|.....
72                               Number of points on ring 01.
3000.0                           Temperature of ring 01 [K].
86.0                             Rotation velocity of ring 01 [km/s].
# ... Ring 02 .....|.....
10                               Number of points on ring 01.
1000.0                           Temperature of ring 02 [K].
20.0                             Rotation velocity of ring 02 [km/s].
#=== End of file. =====
# This file should be named "Dismol.dat".
#
# It is important that when modifying this file, the descriptive text is not to
# the left of the "|" symbol, as it could be read and cause errors.
#
# The number of listed files must match the number of molecules, otherwise rea-
# ding errors may occur.
#
# In the case of ring data, the structure must be preserved, and the number of
# data sets must match the number of rings. If there are more data sets, there
# wouldn't be any reading issues.
#
# Currently, the code only calculates for one ring.
#
# The language options are: ES for Spanish (castellano o español), EN for En-
# glish, FR for French (Français), DE for German (Deutsch), BR or PO for Brazi-
# lian or Portuguese (Brasileiro o Português), IT for Italian (Italiano), and
# CZ for Czech (Český).
#-----
U:--- Dismol.dat All L1 (Fundamental)
For information about GNU Emacs and the GNU system, type C-h C-a.
```

## Dismol.dat

Input file containing the general information of the model.

Data of the spectrum.

Number of molecules and associated files.

Data of the disk.

Information about this file.



```
=====
# File with the data of the molecules and the disk. English version.
#=====
#--- Languaje. -----|-----
ES                          Selected language.

#--- Spectrum data. -----|-----
Disco-C0-2000.sal           File name with the spectrum.
C0                           Molecule (if there are several, write them).
30000                        Number of grid points.
2.29                         Minimum wavelength [Microns].
2.80                         Maximum wavelength [Microns].
16.0                         V Res [km/s], spectral resolution.
2.0                          Grid spacing delta V [km/s].

#--- Molecule data. -----|-----
2                             Number of molecules.
Entrada-C12-016.dat          File name of molecule 01.
Entrada-C13-016.dat          File name of molecule 02.

#--- Disk data. -----|-----
40.0                         Disk inclination [deg].
2                             Number of rings.

#... Ring 01 .....|.....
72                            Number of points on ring 01.
3000.0                        Temperature of ring 01 [K].
86.0                          Rotation velocity of ring 01 [km/s].

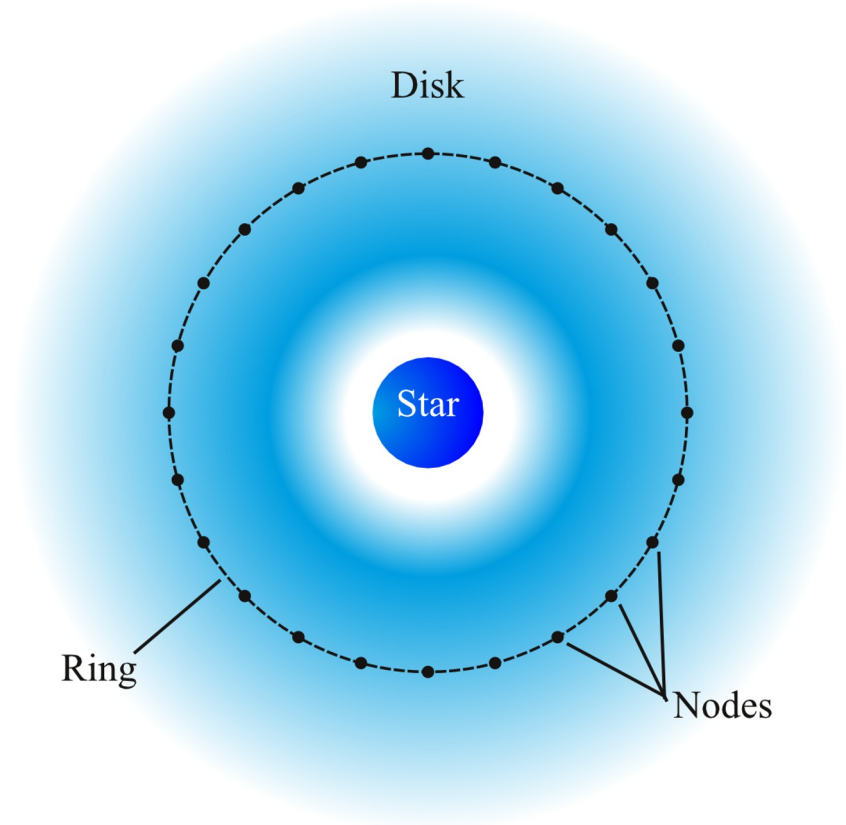
#... Ring 02 .....|.....
10                             Number of points on ring 01.
1000.0                        Temperature of ring 02 [K].
20.0                          Rotation velocity of ring 02 [km/s].

#=== End of file =====
```



## Disk representation

- Ring with equidistant nodes with the same physical and geometric parameters (temperature, density, chemical composition, rotation speed, inclination, etc.).
- Consequently, each node has a different radial velocity.





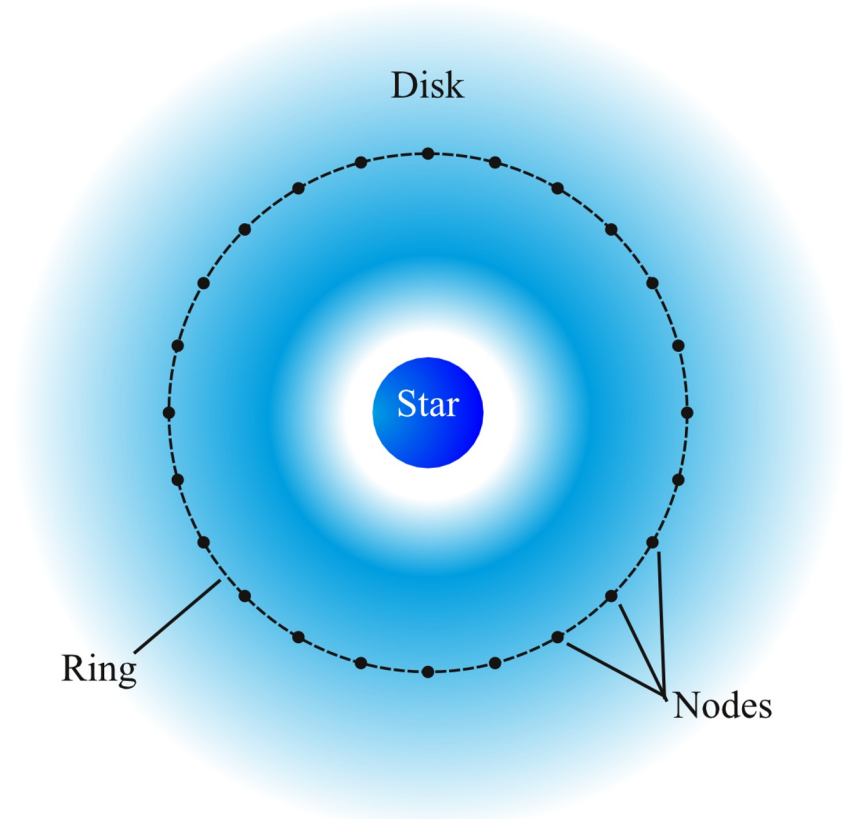


## Disk representation

- Ring with equidistant nodes with the same physical and geometric parameters (temperature, density, chemical composition, rotation speed, inclination, etc.).
- Consequently, each node has a different radial velocity.

### In the future:

- Incorporation of additional rings with different conditions.
- Consider the possibility of partial rings.





```
emacs@electra
File Edit Options Buffers Tools Help
[Icons: Save, Undo, Cut, Copy, Paste, Find]
#=====
# File with the data of the molecule 12C-16O. English version.
#=====
#--- Molecule. -----|-----
12C-16O                Molecule identification.
 6 12                  Atomic and mass numbers of the first atom.
 8 16                  Atomic and mass numbers of the second atom.

#--- Associated files. -----|-----
Datos-CO/Einstein-12C-16O.dat  File with the Einstein coefficients.
10920                          Total number of transitions.
Datos-CO/Energias-12C-16O.dat  File with the energy levels.
2961                            Total number of levels.
20                              Highest vibrational level.
140                             Highest rotational level.
1                               Option for the partition function (1 or 2).
Datos-CO/FP-12C-16O.dat        File with the partition function.
C12-016-Espectro-2000          File name with the spectrum.

#--- Physical parameters. -----|-----
2000.0                       Kinetic temperature [K].
1.0D19                        Column density of CO [1/cm^2].
0.95                          Abundance ratio (12C-16O/CO).
5.0                            Turbulence velocity [km/s].

#=== End of file. =====
# The options for the partition function are:
# 1   Z is obtained by interpolation of the data from the corresponding file.
# 2   Z is obtained by direct calculation (the file is ignored).
#
# It is important that when modifying this file, the descriptive text is not to
# the left of the "|" symbol, as it could be read and cause errors.
#
# For now, the total number of transitions and the total number of levels are
# read from here. Later on, if they are read from the respective files, they
# can be removed.
#=====
-:--- Entrada-C12-016.dat  All L37  (Fundamental)
Beginning of buffer
```

## Entrada-C12-O16.dat

Input file containing the data for each isotopic variant. One file per variant.

Data of the isotopic variant.

Information about the files containing the data of the variant.

Physical parameters of the variant.

Information about this file.



```
#=====
# File with the data of the molecule 12C-16O. English version.
#=====
#--- Molecule. -----|-----
12C-16O                Molecule identification.
 6 12                  Atomic and mass numbers of the first atom.
 8 16                  Atomic and mass numbers of the second atom.

#--- Associated files. -----|-----
Datos-C0/Einstein-12C-16O.dat  File with the Einstein coefficients.
10920                          Total number of transitions.
Datos-C0/Energias-12C-16O.dat  File with the energy levels.
2961                            Total number of levels.
20                               Highest vibrational level.
140                              Highest rotational level.
1                                Option for the partition function (1 or 2).
Datos-C0/FP-12C-16O.dat        File with the partition function.
C12-016-Espectro-2000          File name with the spectrum.

#--- Physical parameters. -----|-----
2000.0                         Kinetic temperature [K].
1.0D19                          Column density of CO [1/cm^2].
0.95                             Abundance ratio (12C-16O/CO).
5.0                               Turbulence velocity [km/s].

#=== End of file. =====
# The options for the partition function are:
# 1      Z is obtained by interpolation of the data from the corresponding file.
# 2      Z is obtained by direct interpolation of the data from the corresponding file.
```



ExoMol High temperature molecular line lists for modelling exoplanet atmospheres

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## Molecules

Search molecules:

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MgH	NH	VO	CO
NaH	CH	AlO	NO
NIH	OH	YO	PO
AlH	HCl	MgO	O <sub>2</sub>
CrH	SiH	TiO	
CaH	SH	SiO	
BeH	HF	CaO	
TiH	PH	NaO	
FeH		LaO	

triatomic molecules

H <sub>2</sub> O
CO <sub>2</sub>



ExoMol High temperature molecular line lists for modelling exoplanet atmospheres

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- By Molecule**
- By Data Type
- Bibliography
- Licence

## Isotopologues of CO

$^{12}\text{C}^{16}\text{O}$
$^{13}\text{C}^{16}\text{O}$
$^{12}\text{C}^{18}\text{O}$
$^{12}\text{C}^{17}\text{O}$
$^{13}\text{C}^{18}\text{O}$
$^{13}\text{C}^{17}\text{O}$
$^{14}\text{C}^{16}\text{O}$
$^{14}\text{C}^{17}\text{O}$
$^{14}\text{C}^{18}\text{O}$

Broadening coefficients for CO



The screenshot shows a web browser window with the ExoMol website. The URL is [exomol.com/data/molecules/CO/12C-16O/](https://exomol.com/data/molecules/CO/12C-16O/). The page title is "Data sets for  $^{12}\text{C}^{16}\text{O}$ ". On the left, there is a navigation menu with options: Search, By Molecule (selected), By Data Type, Bibliography, and Licence. The main content area lists five data sets:

- Li2015** (recommended): Hot line list for  $^{12}\text{C}^{16}\text{O}$  by Li et al, ApJSS, 216, 15 (2015)
- HITEMP**: The HITEMP high temperature molecular line list
- Li**: Ro-vibrational line lists for nine isotopologues of CO
- xsec-Li2015**: Online absorption cross section service: this CO cross section has been generated from data in the empirical line list Li2015 using the procedure described in [Hill et al. (2013)].
- xsec-VUV-DTU**: Experimental temperature-dependent far-UV absorption cross sections ( $\text{cm}^2/\text{molecule}$ ) measured/obtained by Dr Alexander Fateev (DTU) vs wavelength (nm). Please contact Alexander Fateev [alfa@kt.dtu.dk](mailto:alfa@kt.dtu.dk) for more details and more data.



ExoMol | exomol.com/data/molecules/CO/12C-16O/Li2015/

### Li2015: line list (external)

Hot line list for 12C16O by Li et al, ApJSS, 216, 15 (2015)

- [12C-16O\\_Li2015.trans.bz2 \[796.3 KB\]](#)  
Li2015 transitions for (12C)(16O) by Li et al 2015
- [12C-16O\\_Li2015.states.bz2 \[49.8 KB\]](#)  
Li2015 states for (12C)(16O) by Li et al 2015
- [12C-16O\\_Li2015\\_E2.trans.bz2 \[62.0 KB\]](#)  
Li2015 quadrupole transitions for (12C)(16O) by Li et al 2015

### References

- Li, G., Gordon, I. E., Rothman, L. S., Tan, Y., Hu, S.-M., Kass, S., Campargue, A., Medvedev, E. S., "Rovibrational line lists for nine isotopologues of the CO molecule in the X  $^1\Sigma^+$  ground electronic state", *Astrophysical Journal Supplement Series* **216**, 15 (2015). [[link to article](#)][15LiGoRo.CO]
- Somogyi, W., Yurchenko, S. N., Yachmenev, A., "Calculation of electric quadrupole linestrengths for diatomic molecules: Application to the H<sub>2</sub>, CO, HF, and O<sub>2</sub> molecules", *The Journal of Chemical Physics* **155** (2021). [[link to article](#)]

### Li2015: partition function (external)

Hot line list for 12C16O by Li et al, ApJSS, 216, 15 (2015)

- [12C-16O\\_Li2015.pf \[237.3 KB\]](#)  
Calculated partition function for (12C)(16O) to 9000 K from Li et al 2015

### References

- Li, G., Gordon, I. E., Rothman, L. S., Tan, Y., Hu, S.-M., Kass, S., Campargue, A., Medvedev, E. S., "Rovibrational line lists for nine isotopologues of the CO molecule in the X  $^1\Sigma^+$  ground electronic state", *Astrophysical Journal Supplement Series* **216**, 15 (2015). [[link to article](#)]



## Einstein-12C-16O.dat

Input file containing the transitions.

Data of the isotopic variant.

Reference.

Information of the header.

Number of transitions.

Data.

```
emacs@electra
File Edit Options Buffers Tools Help
[Icons: Save, Undo, Cut, Copy, Paste, Find]
=====
# Coeficientes A de Einstein, Energía del nivel inferior y frecuencia de la
# la transición para moléculas (12)C(16)O, (CO).
#-----
# Rovibrational line lists for nine isotopologues of the CO molecule in the
# X1 Σ+ ground electronic state.
# G. Li, I. Gordon, L. Rothman, Y. Tan, S. Hu, S. Kassı, et al.
# APJSS 216, 15 (2015).
#-----
# Vi = Número cuántico vibracional del nivel inferior.
# Ji = Número cuántico rotacional del nivel inferior.
# Vs = Número cuántico vibracional del nivel superior.
# Js = Número cuántico rotacional del nivel superior.
# A = Coeficiente A de Einstein [1/seg].
# Einf = Energía del nivel inferior [1/cm].
# Frec = Frecuencia de la transición [1/cm].
# ID = Identificador de la transición.
# IDNI = Identificador del nivel inferior.
# IDNS = Identificador del nivel superior.
#-----
# 10920 Número de transiciones.
#-----
# Vi Ji Vs Js A Einf Frec ID IDNI IDNS
#-----
19 140 20 139 0.324D+02 65262.8879 930.6251 1 5900 5859
19 139 20 138 0.330D+02 64885.0924 937.3934 2 5858 5817
19 138 20 137 0.336D+02 64509.0340 944.1420 3 5816 5775
19 137 20 136 0.343D+02 64134.7340 950.8709 4 5774 5733
18 140 19 139 0.332D+02 63934.1228 950.9696 5 5899 5858
19 136 20 135 0.349D+02 63762.2133 957.5803 6 5732 5691
18 139 19 138 0.338D+02 63551.2684 957.7656 7 5857 5816
19 135 20 134 0.356D+02 63391.4930 964.2698 8 5690 5649
18 138 19 137 0.344D+02 63170.1917 964.5423 9 5815 5774
19 134 20 133 0.363D+02 63022.5935 970.9397 10 5648 5607
U:--- Einstein-12C-16O.dat Top L1 (Fundamental)
For information about GNU Emacs and the GNU system, type C-h C-a.
```





## Einstein-40Ca-16O.dat

Input file containing the transitions.

Data of the isotopic variant.

Reference.

Information of the header.

Number of transitions.

Data.

```
emacs@electra
File Edit Options Buffers Tools Help
[Icons: Save, Undo, Cut, Copy, Paste, Find]
=====
# Coeficientes A de Einstein, Energía del nivel inferior y frecuencia de
# la transición para moléculas de (40)Ca(16)O, (CaO).
#-----
# ExoMol molecular line lists - XIII: The spectrum of CaO.
# S. Yurchenko, A. Blissett, U. Asari, M. Vasilios, C. Hill & J. Tennyson.
# MNRAS 456, 4524-4532 (2016).
#
#-----
# Vi = Número cuántico vibracional del nivel inferior.
# Ji = Número cuántico rotacional del nivel inferior.
# Vs = Número cuántico vibracional del nivel superior.
# Js = Número cuántico rotacional del nivel superior.
# A = Coeficiente A de Einstein [1/seg].
# Einf = Energía del nivel inferior [1/cm].
# Frec = Frecuencia de la transición [1/cm].
# ID = Identificador de la transición.
# IDNI = Identificador del nivel inferior.
# IDNS = Identificador del nivel superior.
#-----
# 453331 Número de transiciones.
#-----
# Vi Ji Vs Js A Einf Frec ID IDNI IDNS
#-----
15 31 14 32 0.157D-16 16035.8151 0.0075 1 20039 20386
5 51 3 50 0.488D-15 12134.1136 0.0172 2 32585 32288
10 59 11 58 0.124D-15 14902.2498 0.0175 3 38070 37133
3 31 5 30 0.107D-12 11570.1296 0.0824 4 19664 19365
14 38 13 39 0.884D-13 15720.5134 0.1165 5 24597 24896
20 11 19 10 0.626D-13 18038.2531 0.1354 6 7086 6137
17 15 16 16 0.255D-13 16726.6319 0.1378 7 9347 10346
13 45 12 46 0.170D-12 15432.1311 0.1504 8 29087 29431
17 15 16 16 0.361D-13 16726.6298 0.1508 9 9669 10018
U:--- Einstein-40Ca-16O.dat Top L1 (Fundamental)
File Einstein-40Ca-16O.dat is large (33.7 MiB), really open? (y)es or (n)o or (l)iterally y
```



## Einstein-12C-1H.dat

Input file containing the transitions.

Data of the isotopic variant.

Reference.

Information of the header.

Number of transitions.

Data.

```
emacs@electra
File Edit Options Buffers Tools Help
[Icons: Save, Undo, Cut, Copy, Paste, Find]
=====
# Coeficientes A de Einstein, Energía del nivel inferior y frecuencia de
# la transición para moléculas de (12)C(1)H, (CH).
#-----
# MoLLIST: Molecular Line Lists, Intensities and Spectra.
# P. Bernath.
# J. Quant. Spectrosc. Radiat. Transf. 240, 106687 (2020).
#
#-----
# Vi = Número cuántico vibracional del nivel inferior.
# Ji = Número cuántico rotacional del nivel inferior.
# Vs = Número cuántico vibracional del nivel superior.
# Js = Número cuántico rotacional del nivel superior.
# A = Coeficiente A de Einstein [1/seg].
# Einf = Energía del nivel inferior [1/cm].
# Frec = Frecuencia de la transición [1/cm].
# ID = Identificador de la transición.
# IDNI = Identificador del nivel inferior.
# IDNS = Identificador del nivel superior.
#-----
# 20080 Número de transiciones.
#-----
# Vi Ji Vs Js A Einf Frec ID IDNI IDNS
#-----
20 20.5 19 19.5 0.158D-03 15488.5998 1127.5182 1 1253 1357
20 20.5 19 19.5 0.172D-03 15475.6976 1150.4346 2 1247 1359
19 19.5 18 18.5 0.212D-03 15029.1683 1184.0623 3 1205 1309
19 19.5 18 18.5 0.228D-03 15017.2258 1205.1511 4 1199 1312
20 20.5 19 19.5 0.186D-03 13367.5976 1209.2884 5 1023 1148
20 20.5 19 19.5 0.209D-03 13354.1174 1233.2505 6 1013 1150
18 18.5 17 17.5 0.286D-03 14587.4158 1240.7089 7 1152 1281
18 18.5 17 17.5 0.305D-03 14576.4230 1259.9974 8 1145 1285
19 19.5 18 18.5 0.246D-03 12886.7399 1267.6289 9 963 1092
19 19.5 18 18.5 0.274D-03 12874.2663 1289.6714 10 957 1096
U:--- Einstein-12C-1H.dat Top L23 (Fundamental)
Wrote /home/vallverdu/Pictures/Einstein-12C-1H.dat
```



```
emacs@electra
File Edit Options Buffers Tools Help
[Icons: Save, Undo, Cut, Copy, Paste, Search]
=====
# Niveles de energía de la molécula (12)C(16)O, (C0).
#-----
# Rovibrational line lists for nine isotopologues of the CO molecule in
# the X1 Σ+ ground electronic state.
# G. Li, I. Gordon, L. Rothman, Y. Tan, S. Hu, S. Kassı, et al.
# APJSS 216, 15 (2015).
#-----
# V = Número cuántico vibracional.
# J = Número cuántico rotacional, puro o total.
# Ener = Energía del nivel [1/cm].
# ID = Identificador del nivel.
#-----
# 2961 Número de niveles.
#-----
# ID V J Ener
#-----
  1  0  0  0.0000
  2  1  0 2143.2711
  3  2  0 4260.0622
  4  3  0 6350.4391
  5  4  0 8414.4693
  6  5  0 10452.2222
  7  6  0 12463.7686
  8  7  0 14449.1813
  9  8  0 16408.5346
 10  9  0 18341.9044
 11 10  0 20249.3682
 12 11  0 22131.0050
 13 12  0 23986.8951
 14 13  0 25817.1200
 15 14  0 27621.7622
 16 15  0 29400.9053
 17 16  0 31154.6335
U:**- Energias-12C-16O.dat Top L4 (Fundamental)
```

## Energías-12C-16O.dat

Input file containing the energy levels.

Data of the isotopic variant.

Reference.

Information of the header.

Number of levels.

Data.



```
emacs@electra
File Edit Options Buffers Tools Help
[Icons: Save, Undo, Cut, Copy, Paste, Search]
=====
# Función de partición del (12)C(16)O, (C0).
#-----
# Rovibrational line lists for nine isotopologues of the C0 molecule in
# the X1Σ+ ground electronic state.
# G. Li, I. Gordon, L. Rothman, Y. Tan, S. Hu, S. Kassı, et al.
# ApJSS, 216, 15-33 (2015).
#-----
# T = Temperatura [K].
# Z = Función de partición.
#-----
# 1.0 Temperatura mínima.
# 9000.0 Temperatura máxima.
#-----
# T      Z
#-----
1.0      1.011900
2.0      1.190000
3.0      1.494400
4.0      1.833100
5.0      2.182400
6.0      2.536300
7.0      2.892600
8.0      3.250300
9.0      3.608900
10.0     3.968100
11.0     4.327800
12.0     4.687800
13.0     5.048000
14.0     5.408500
15.0     5.769100
16.0     6.129800
17.0     6.490600
18.0     6.851500
U: --- FP-12C-160.dat Top L1 (Fundamental)
For information about GNU Emacs and the GNU system, type C-h C-a.
```

## FP-12C-160.dat

Input file containing the partition function.

Data of the isotopic variant.

Reference.

Information of the header.

Range of temperatura.

Data.



```
emacs@electra
File Edit Options Buffers Tools Help
[Icons: Save, Undo, Cut, Copy, Paste, Find]
=====
# Molécula: CO
=====
# Temperatura cinética [K]: 3000.00
# Densidad de columna [1/cm^2]: 0.1000D+20
# Cociente de abundancias: 0.95
# Velocidad térmica [km/s]: 1.3293
# Velocidad de turbulencia [km/s]: 5.0000
# Resolución instrumental [km/s]: 16.0000
# Velocidad interna [km/s]: 16.8157
# Rango de longitudes de onda [A]: 22900.00 28000.00
=====
#
# Longitud de onda      Flujo      Flujo
# [Micrones]          [erg / s cm^2 A] [erg / s cm^2 Hz]
#=====
█ 2.29259828      0.25305959E-01 0.44366791E-11
  2.29262150      0.79464765E-01 0.13932165E-10
  2.29264473      0.23397783E+00 0.41023011E-10
  2.29266796      0.64621556E+00 0.11330238E-09
  2.29269118      0.16747996E+01 0.29365220E-09
  2.29271441      0.40751253E+01 0.71452953E-09
  2.29273764      0.93144309E+01 0.16332187E-08
  2.29276087      0.20012146E+02 0.35090575E-08
  2.29278409      0.40446841E+02 0.70923510E-08
  2.29280732      0.76968943E+02 0.13496773E-07
  2.29283055      0.13805015E+03 0.24208066E-07
  2.29285378      0.23365451E+03 0.40973795E-07
  2.29287701      0.37371498E+03 0.65536211E-07
  2.29290025      0.56578438E+03 0.99220308E-07
  2.29292348      0.81234085E+03 0.14246124E-06
  2.29294671      0.11085868E+04 0.19441821E-06
  2.29296994      0.14416623E+04 0.25283637E-06
  2.29299318      0.17918612E+04 0.31426005E-06
U:**- Disco-CO-3000.sal Top L17 (Fundamental)
Auto-saving...done
```

## Disco-12C-16O-2000.sal

Output file containing the data for the spectrum.

Information of the model.

Spectrum.



## **Models**

In the first models, it is calculated for a range of temperatures.

In the latest models, only for 2000 K.

Column density =  $10^{19} \text{ cm}^{-2}$ .

Rotation velocity = 86 km/s.

Inclination =  $40^\circ$ .

Resolution = 16.0 km/s



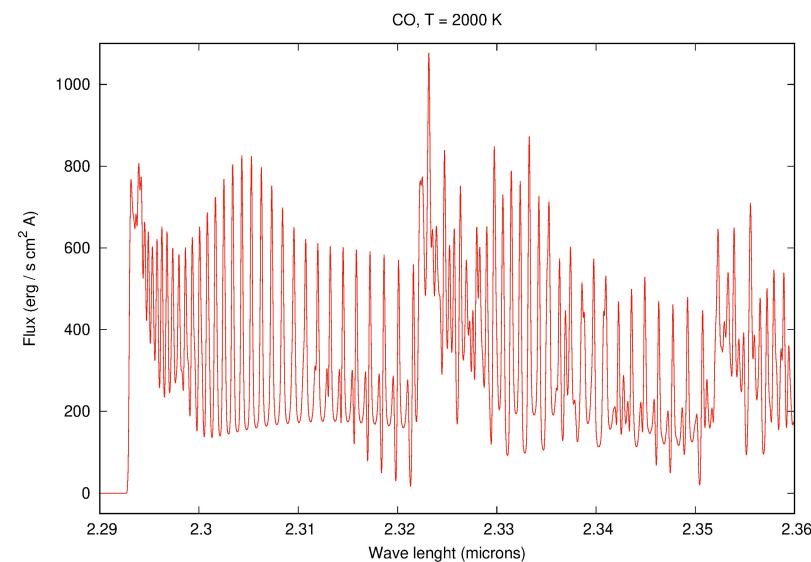
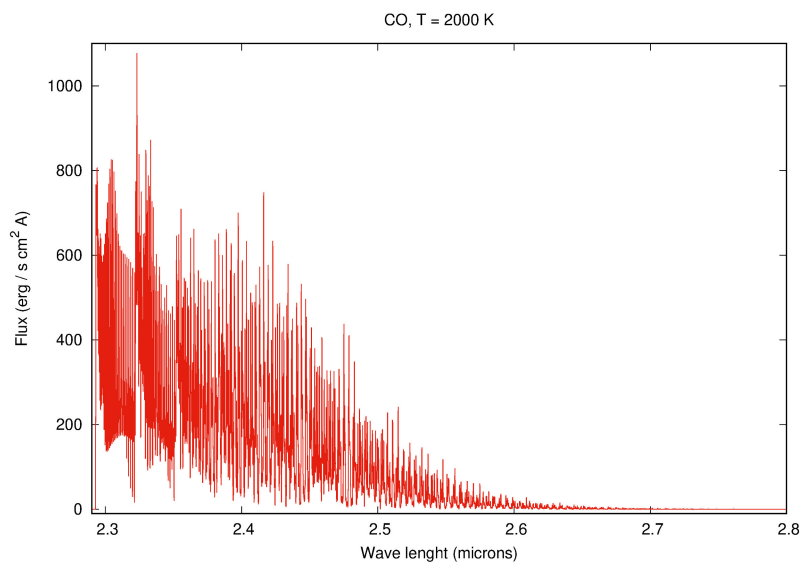
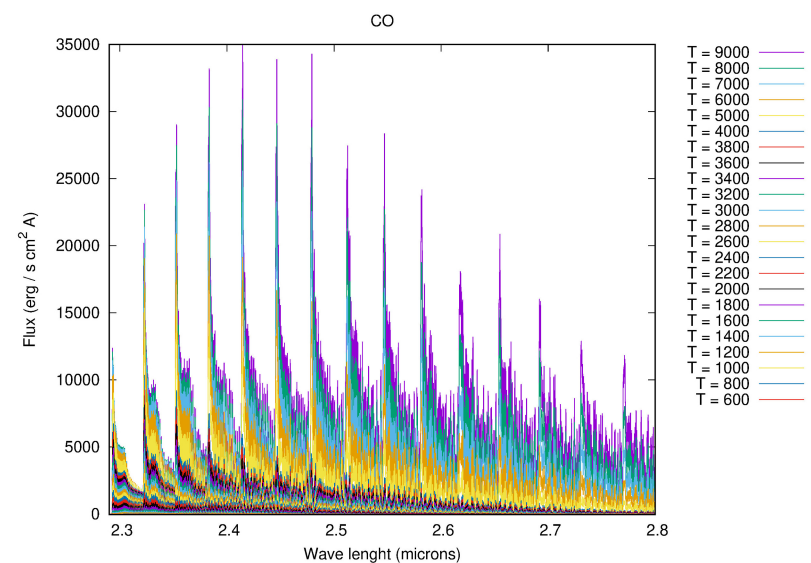
# Carbon monoxide (CO).

10920 transitions, (2.29 - 2.80  $\mu$ ).

2961 energy levels.

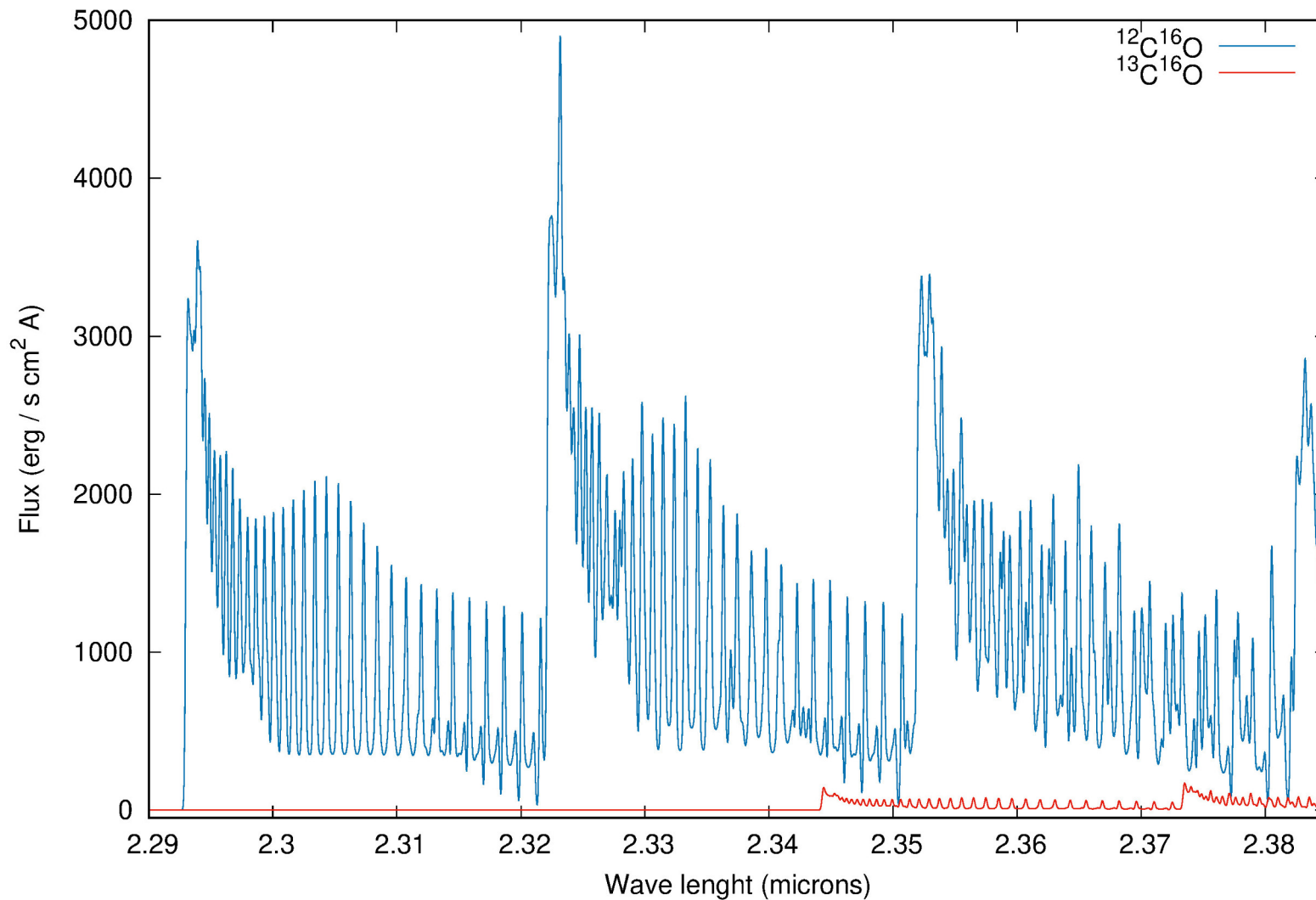
$v_{\max} = 20$ ,  $J_{\max} = 140$ .

$^{12}\text{C}^{16}\text{O}$ ,  $^{13}\text{C}^{16}\text{O}$ ,  $^{12}\text{C}^{17}\text{O}$ ,  $^{13}\text{C}^{17}\text{O}$ ,  $^{12}\text{C}^{18}\text{O}$ ,  
 $^{13}\text{C}^{18}\text{O}$ .





$^{12}\text{C}^{16}\text{O}$  and  $^{13}\text{C}^{16}\text{O}$







## CPD-52 9243

$$T_{\text{CO}} = 2400 \text{ K}$$

$$N_{\text{CO}} = 4.0 \times 10^{22} \text{ cm}^{-2}$$

$$[^{12}\text{C}^{16}\text{O}] = 0.95$$

$$[^{13}\text{C}^{16}\text{O}] = 0.05$$

$$\text{Resolution} = 6 \text{ km/s}$$

$$2.29 \mu \text{ a } 2.51 \mu$$

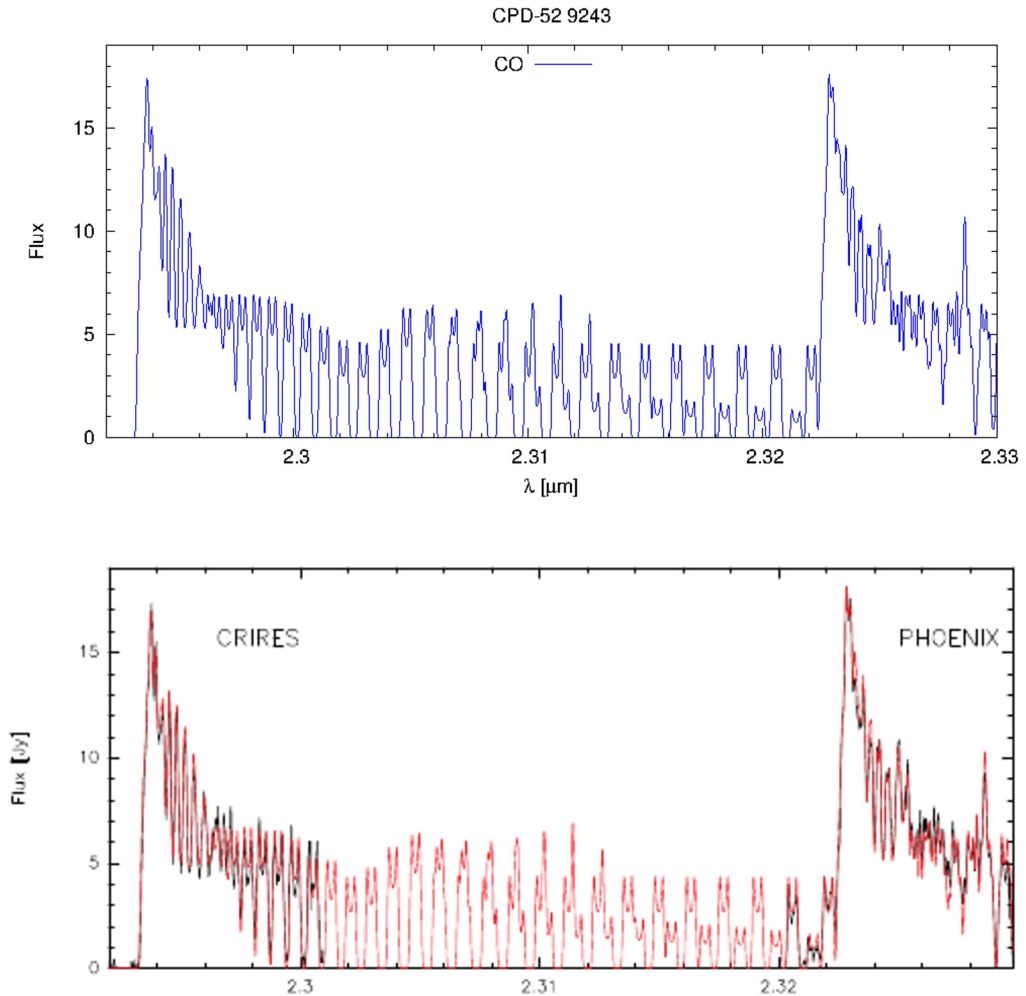
$$16000 \text{ points}$$

$$i = 40^\circ$$

$$V_{\text{rot}} = 33 \text{ km/s}$$

$$72 \text{ nodes}$$

*Cidale et al, 2012*





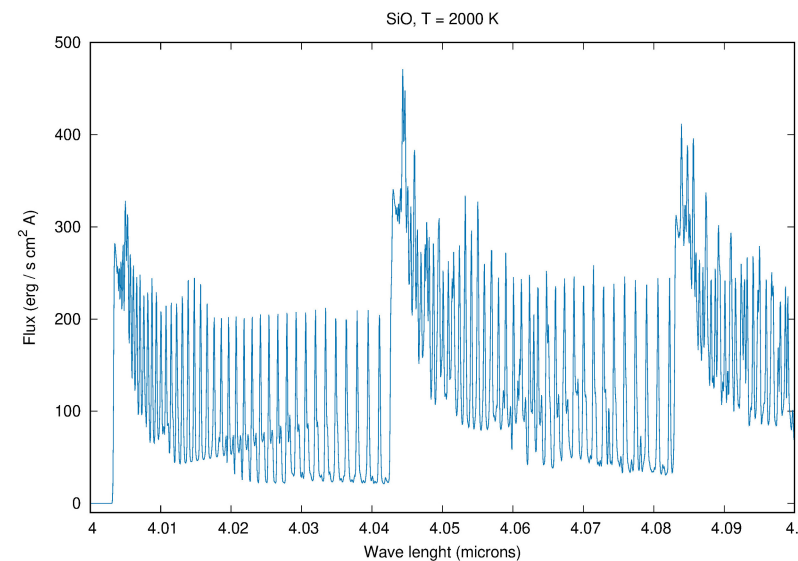
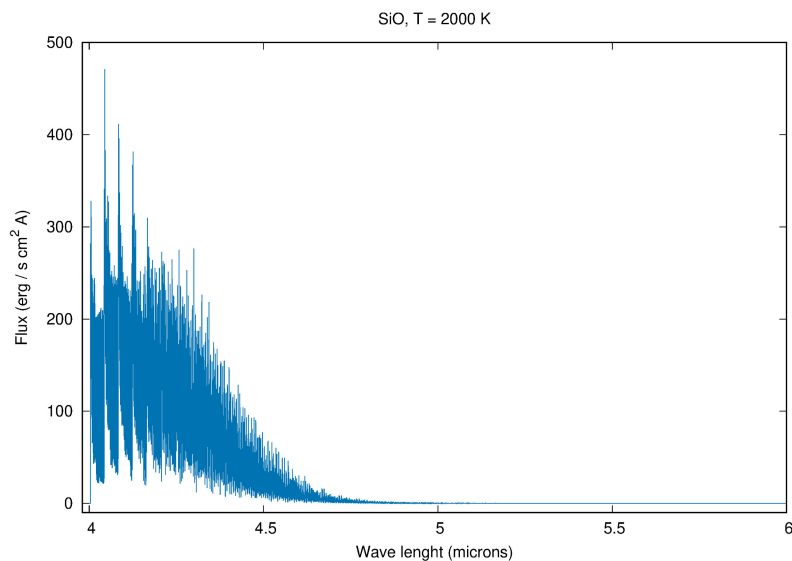
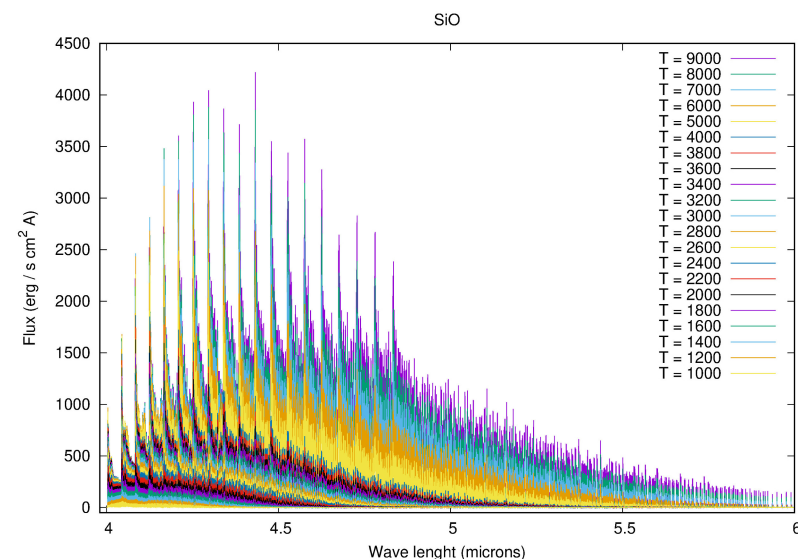
# Silicon monoxide (SiO).

10920 transitions, (4.00 - 6.00  $\mu$ ).

2961 energy levels.

$v_{\max} = 20, J_{\max} = 140.$

$^{28}\text{Si}^{16}\text{O}, ^{29}\text{Si}^{16}\text{O}, ^{30}\text{Si}^{16}\text{O}, ^{28}\text{Si}^{17}\text{O}, ^{28}\text{Si}^{18}\text{O}.$





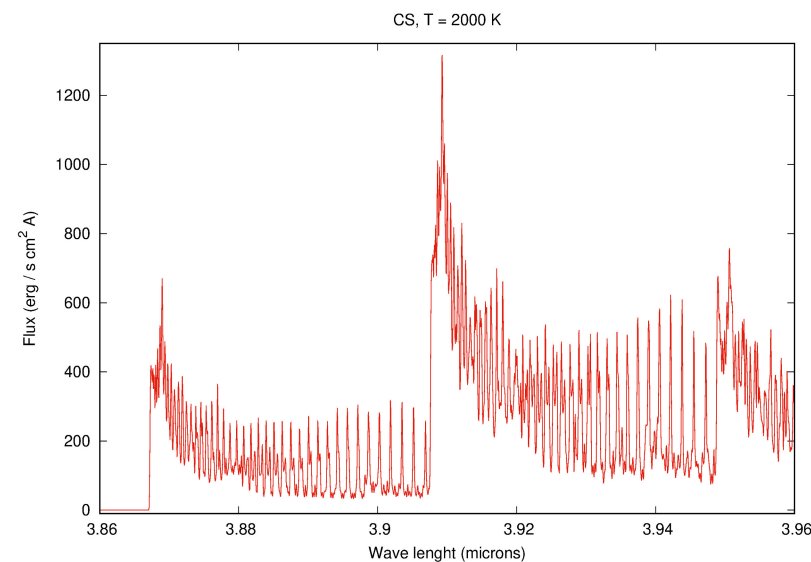
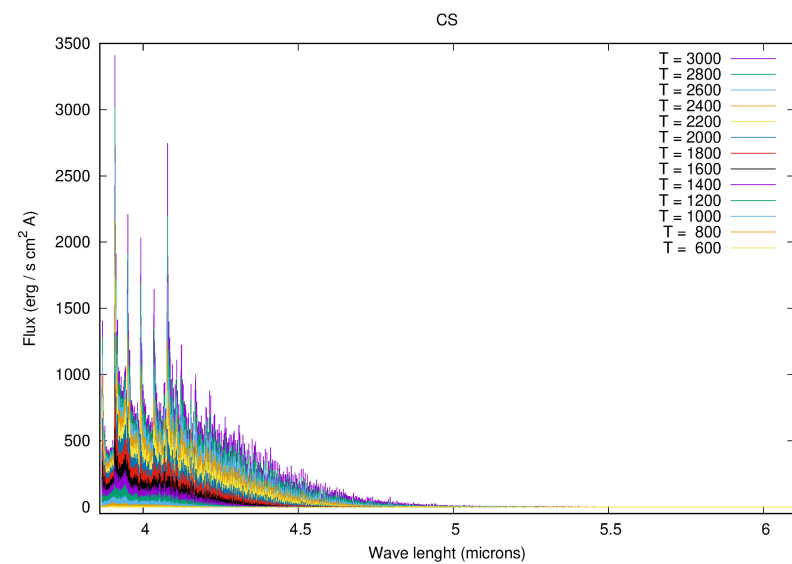
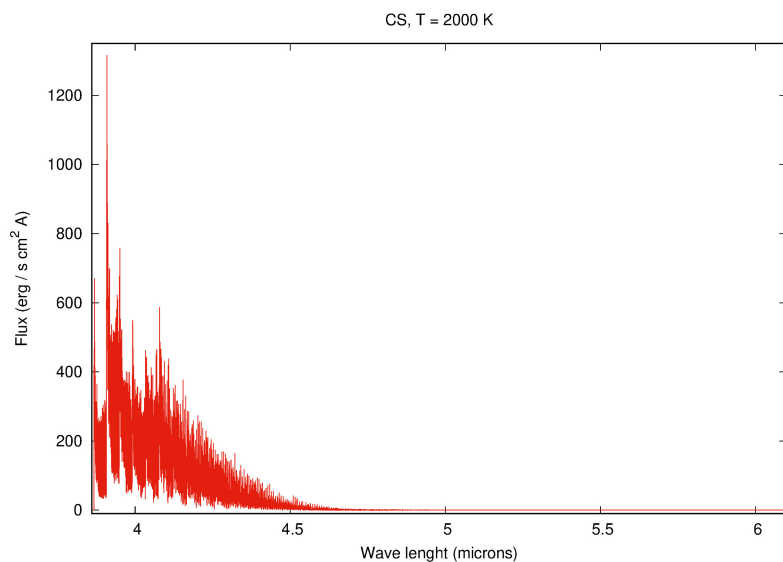
# Carbon sulfide (CS).

11480 transitions, (3.86 - 6.10  $\mu$ ).

2961 energy levels.

$v_{\max} = 20$ ,  $J_{\max} = 140$ .

$^{12}\text{C}^{32}\text{S}$ ,  $^{12}\text{C}^{34}\text{S}$ ,  $^{13}\text{C}^{32}\text{S}$ ,  $^{12}\text{C}^{35}\text{S}$ ,  $^{12}\text{C}^{36}\text{S}$ ,  
 $^{13}\text{C}^{33}\text{S}$ ,  $^{13}\text{C}^{34}\text{S}$ ,  $^{13}\text{C}^{36}\text{S}$ .





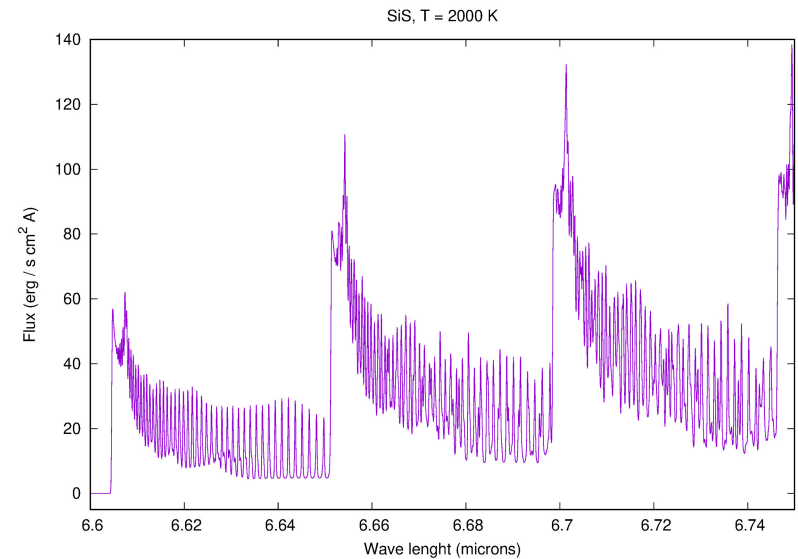
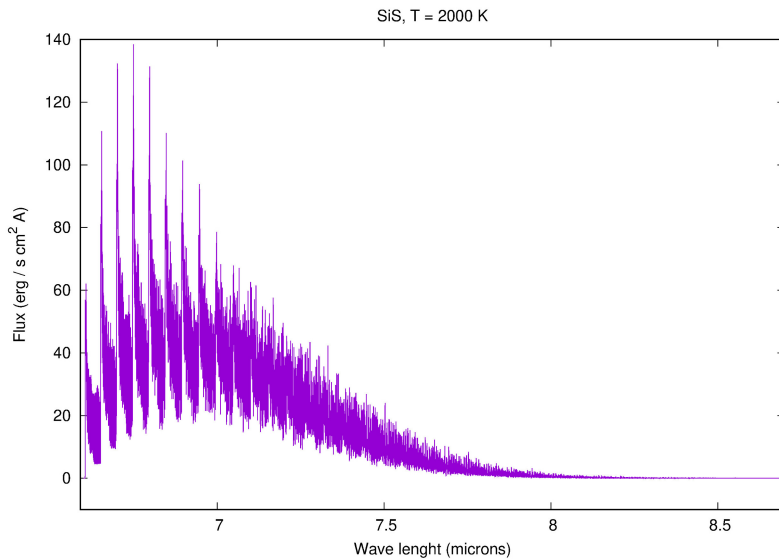
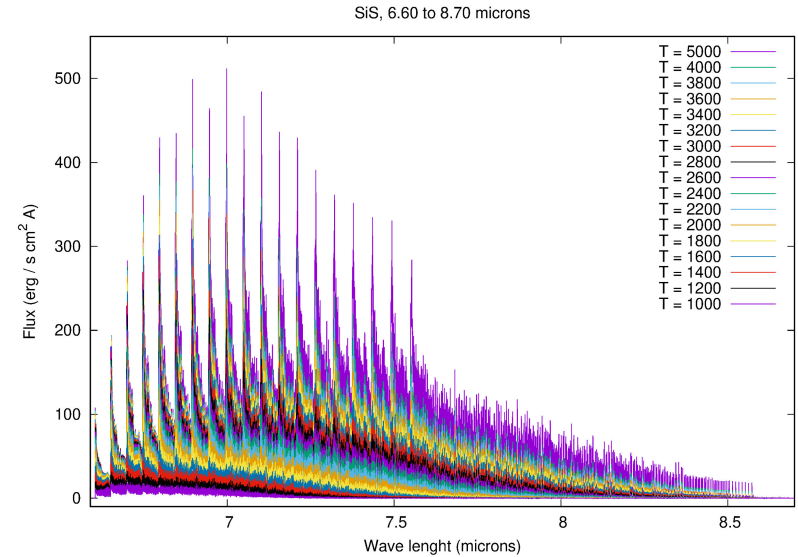
# Silicon sulfide (SiS).

10920 transitions, (6.60 - 8.70  $\mu$ ).

2961 energy levels.

$v_{\max} = 20$ ,  $J_{\max} = 140$ .

$^{28}\text{Si}^{32}\text{S}$ ,  $^{28}\text{Si}^{34}\text{S}$ ,  $^{29}\text{Si}^{32}\text{S}$ ,  $^{30}\text{Si}^{32}\text{S}$ ,  $^{28}\text{Si}^{33}\text{S}$ ,  
 $^{28}\text{Si}^{36}\text{S}$ ,  $^{29}\text{Si}^{33}\text{S}$ ,  $^{29}\text{Si}^{34}\text{S}$ ,  $^{29}\text{Si}^{36}\text{S}$ ,  $^{30}\text{Si}^{33}\text{S}$ ,  
 $^{30}\text{Si}^{34}\text{S}$ ,  $^{30}\text{Si}^{36}\text{S}$ .





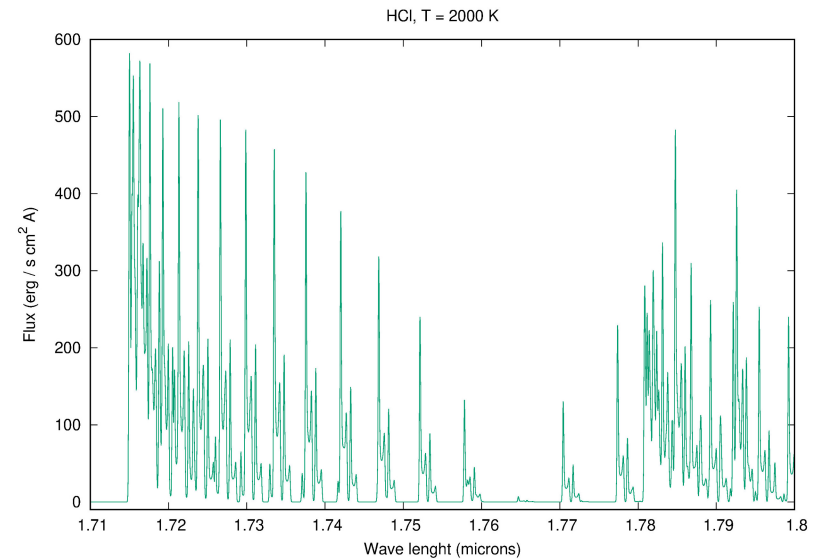
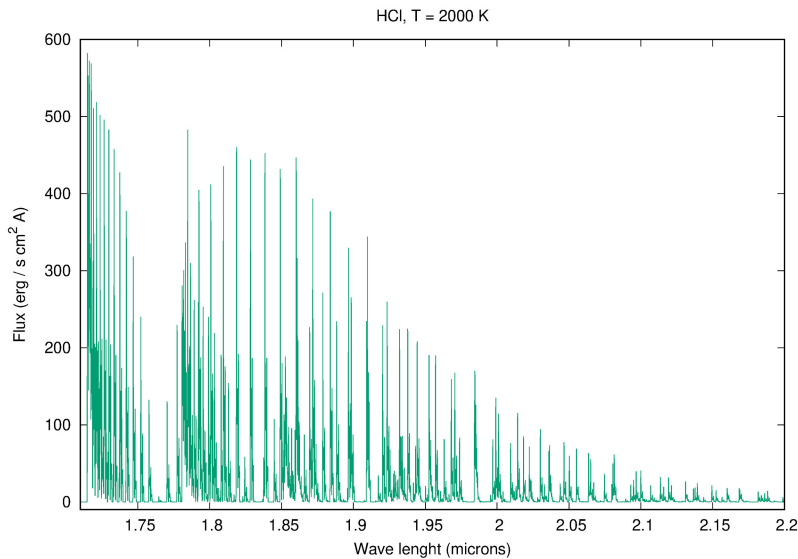
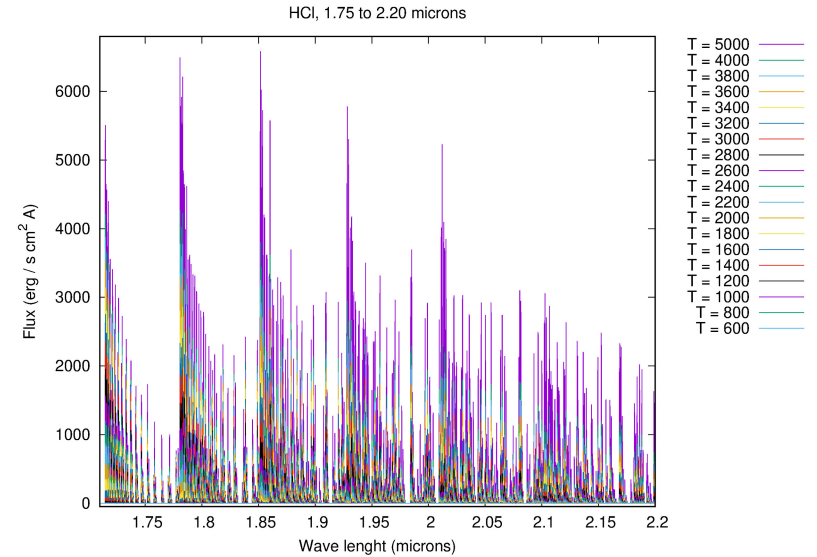
# Chlorine hydride (HCl).

2509 transitions, (1.71 - 2.20  $\mu$ ).

710 energy levels.

$v_{\max} = 17, J_{\max} = 41.$

$^{35}\text{Cl}^1\text{H}, ^{37}\text{Cl}^1\text{H}, ^{35}\text{Cl}^2\text{H}, ^{37}\text{Cl}^2\text{H}.$





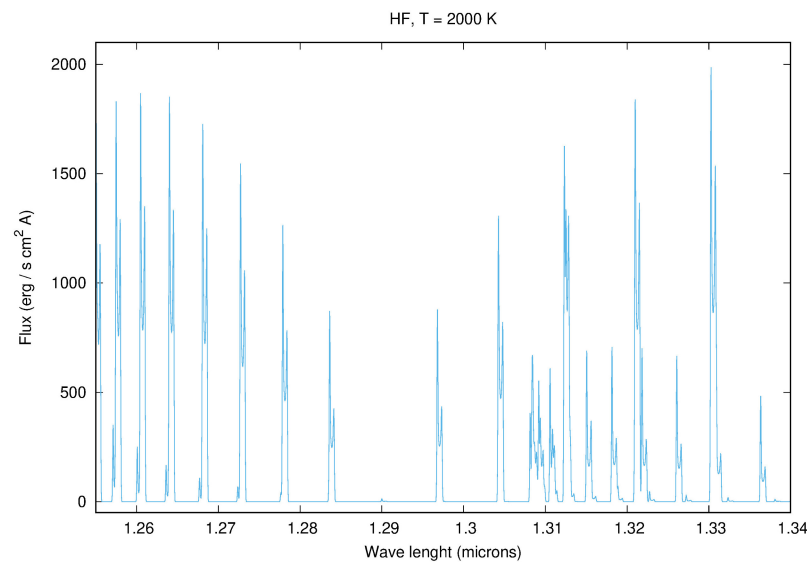
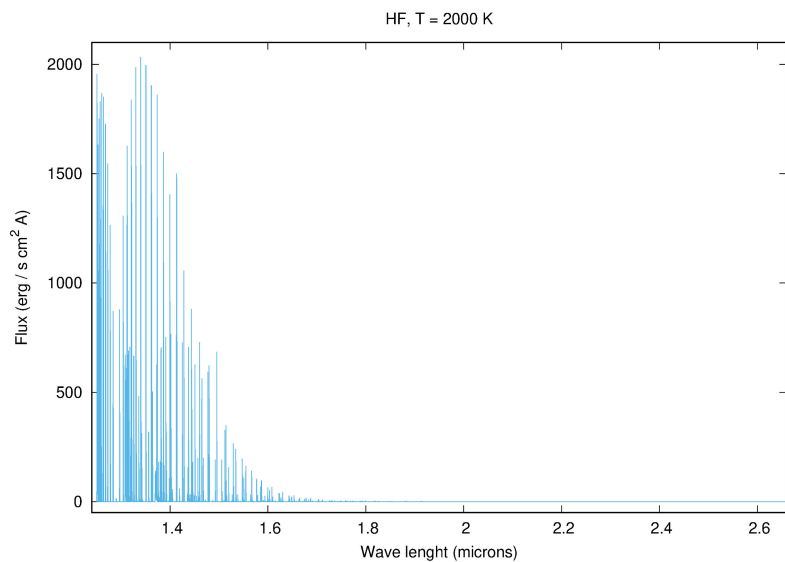
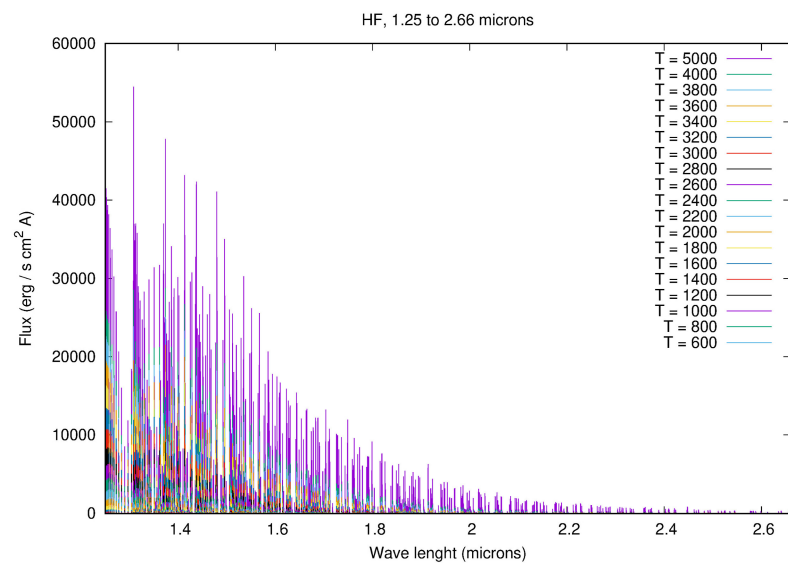
# Fluorine hydride (HF).

1457 transitions, (1.25 - 2.66  $\mu$ ).

468 energy levels.

$v_{\max} = 11, J_{\max} = 38.$

**$^1\text{H}^{19}\text{F}$ .**





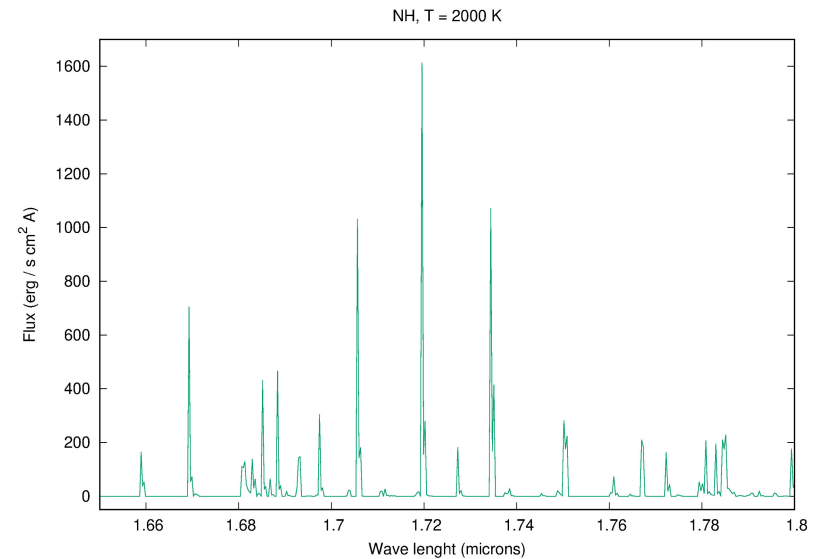
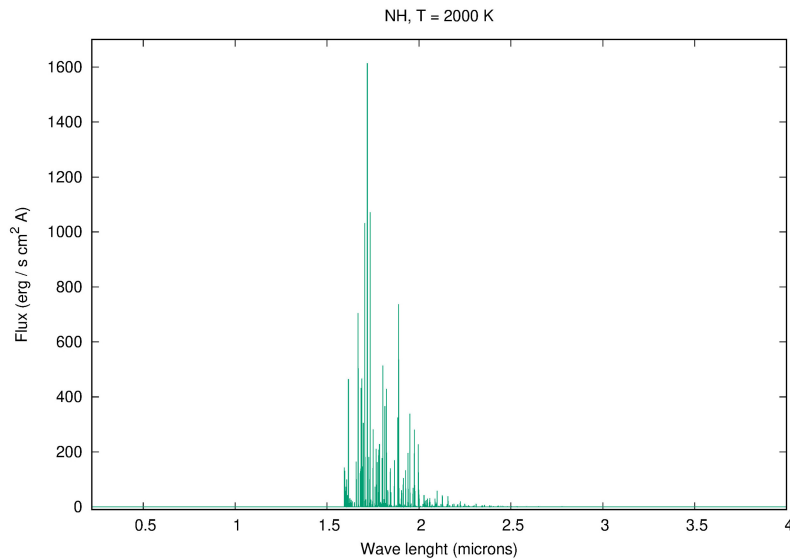
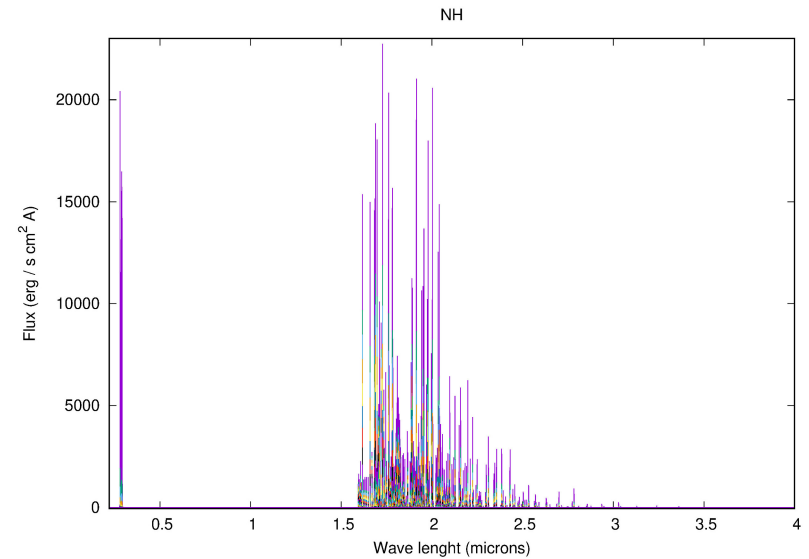
# Nitrogen hydride (NH).

7561 transitions, (1.57 - 2.90  $\mu$ ).

1285 energy levels.

$v_{\max} = 6, J_{\max} = 44.$

$^{14}\text{N}^1\text{H}.$





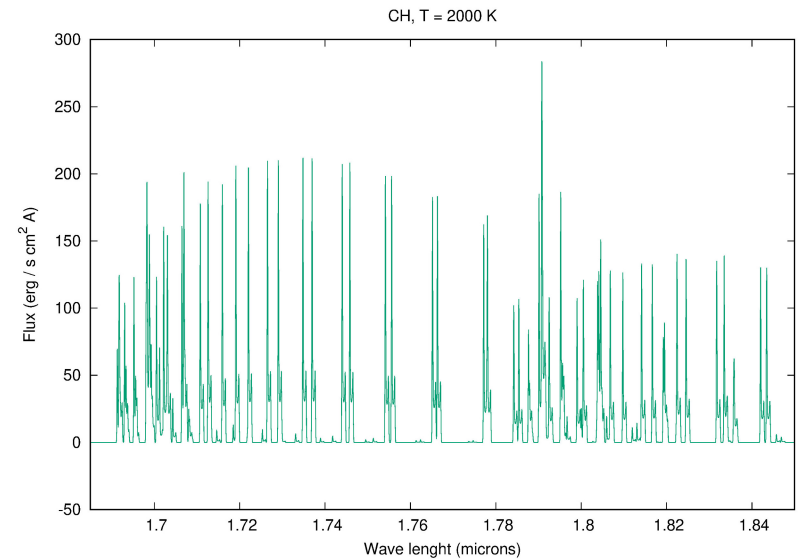
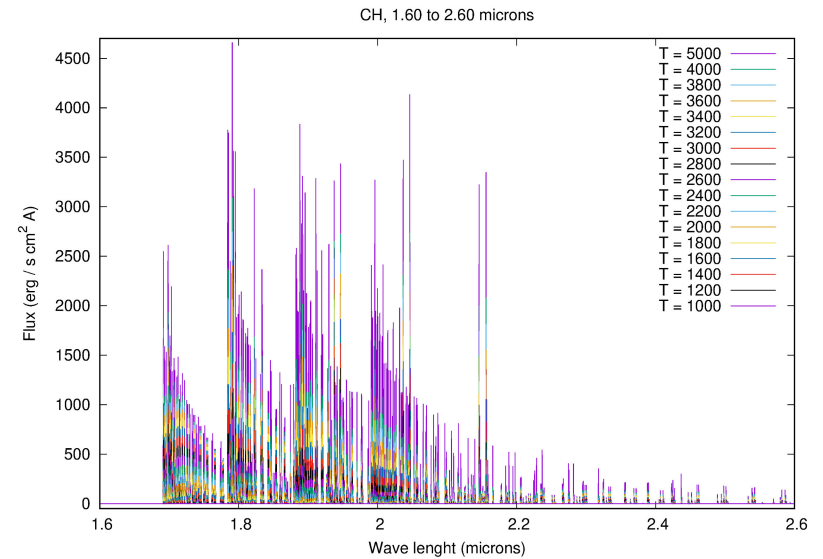
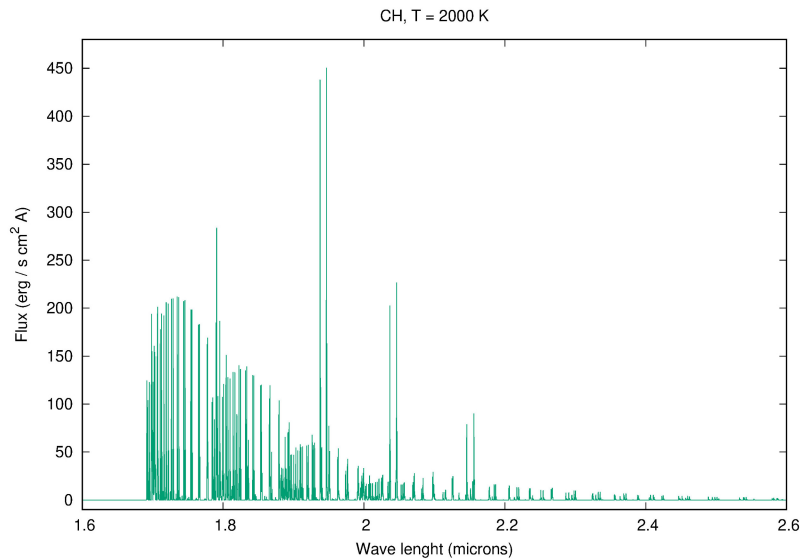
# Carbon hydride (CH).

20080 transitions, (1.60 - 2.60  $\mu$ ).

1596 energy levels.

$v_{\max} = 20, J_{\max} = 21.$

$^{12}\text{C}^1\text{H}, ^{13}\text{C}^1\text{H}.$







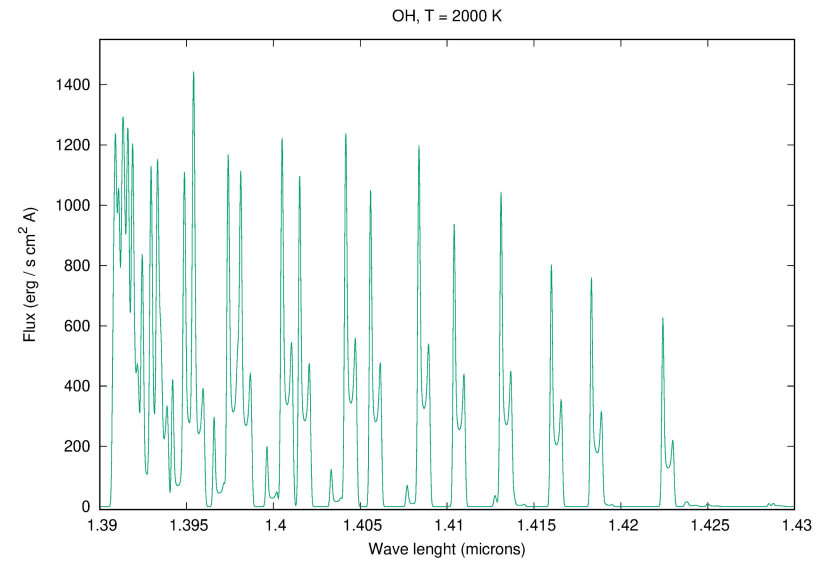
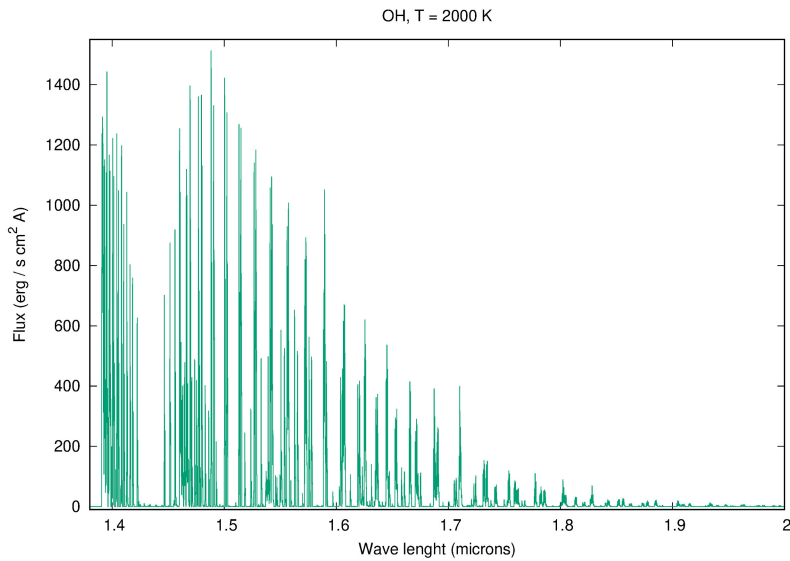
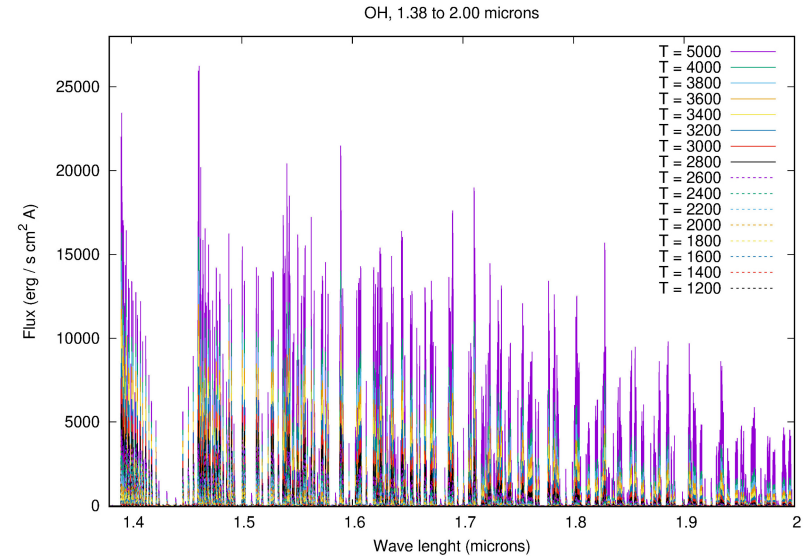
# Hydroxyl (OH).

12306 transitions, (1.38 - 2.00  $\mu$ ).

1878 energy levels.

$v_{\max} = 4, J_{\max} = 44.$

$^{16}\text{O}^1\text{H}.$





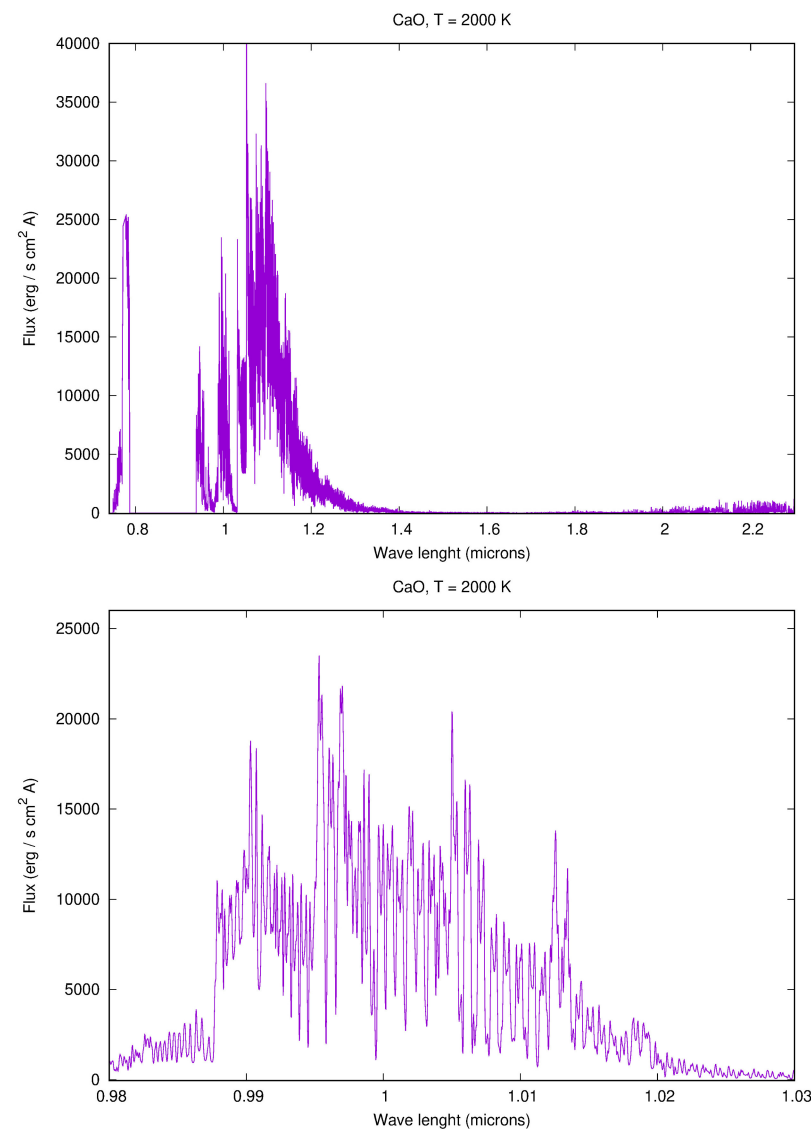
## Calcium monoxide (CaO).

453331 transitions, (0.74 - 2.30  $\mu$ ).

19113 energy levels.

$v_{\max} = 20$ ,  $J_{\max} = 70$ .

$^{40}\text{Ca}^{16}\text{O}$ .





## Iron hydride (FeH).

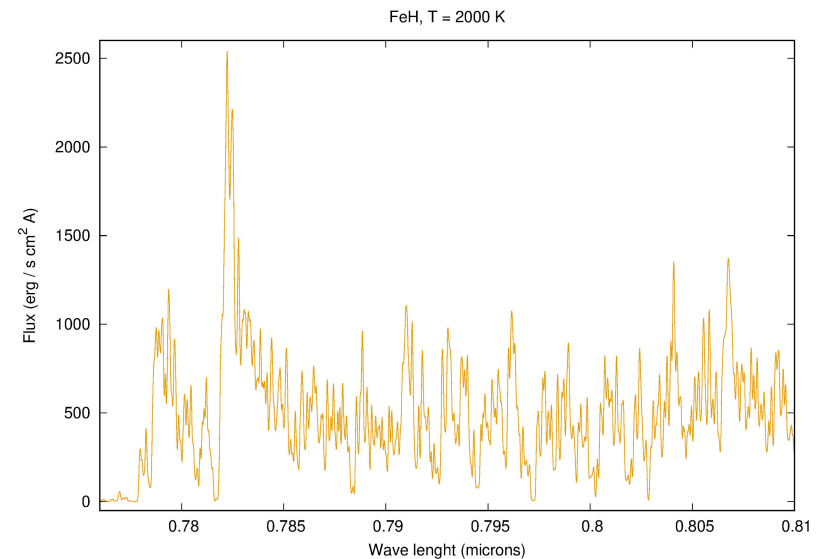
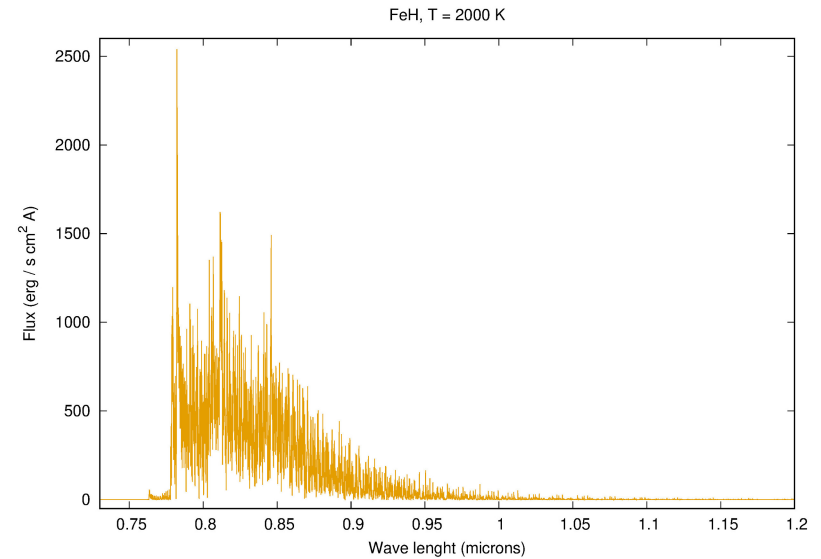
45232 transitions, (0.73 - 1.20  $\mu$ ).

3960 energy levels.

$v_{\max} = 4$ ,  $J_{\max} = 51$ .

**$^{56}\text{Fe}^1\text{H}$** .  $^{54}\text{Fe}^1\text{H}$  and  $^{57}\text{Fe}^1\text{H}$  they are relevant but there is no data available.

Column density =  $10^{17} \text{ cm}^{-2}$





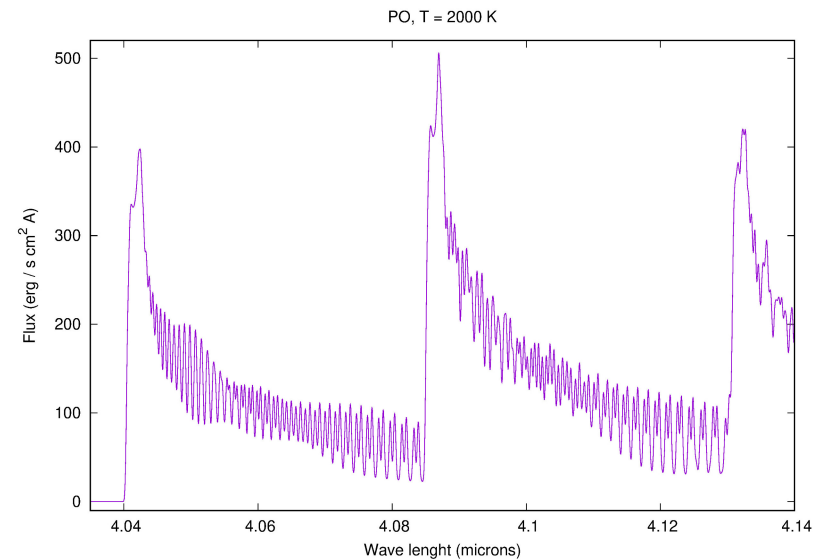
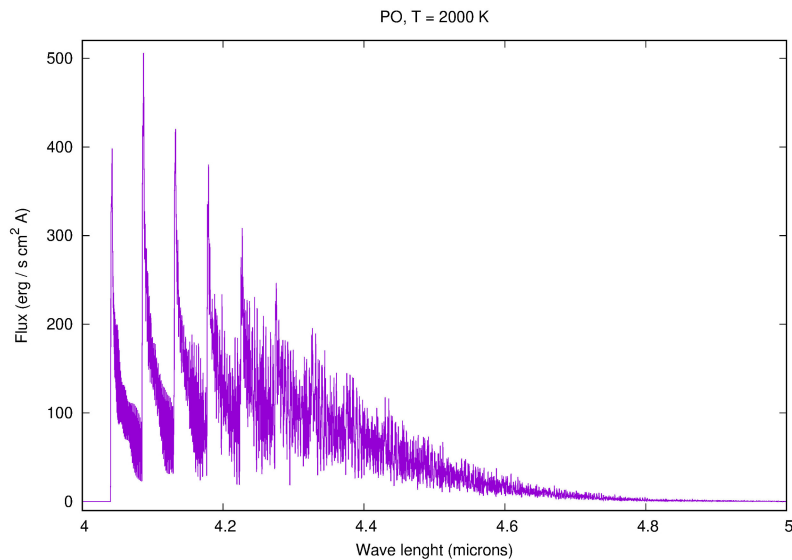
# Phosphorus monoxide (PO).

79353 transitions, (4.00 - 5.00  $\mu$ ), (7.60 - 8.60  $\mu$ ).

11278 energy levels.

$v_{\max} = 20$ ,  $J_{\max} = 140.5$ .

**$^{31}\text{P}^{16}\text{O}$ .**





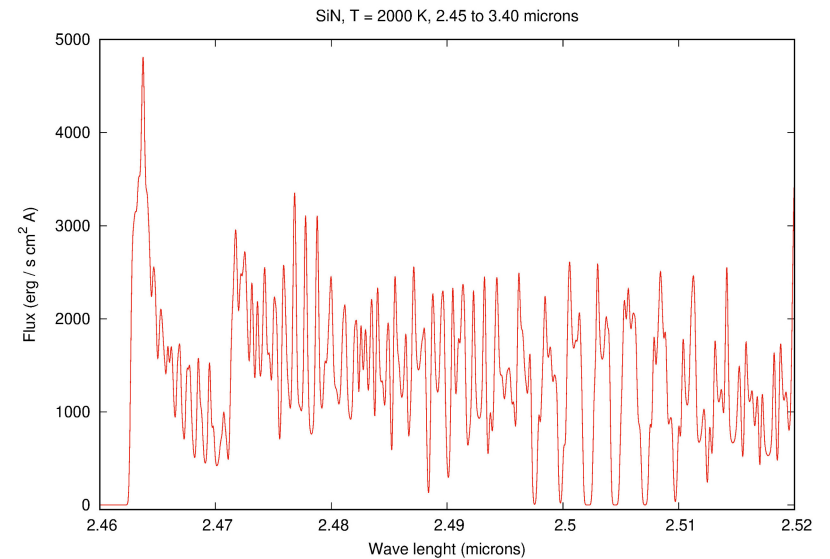
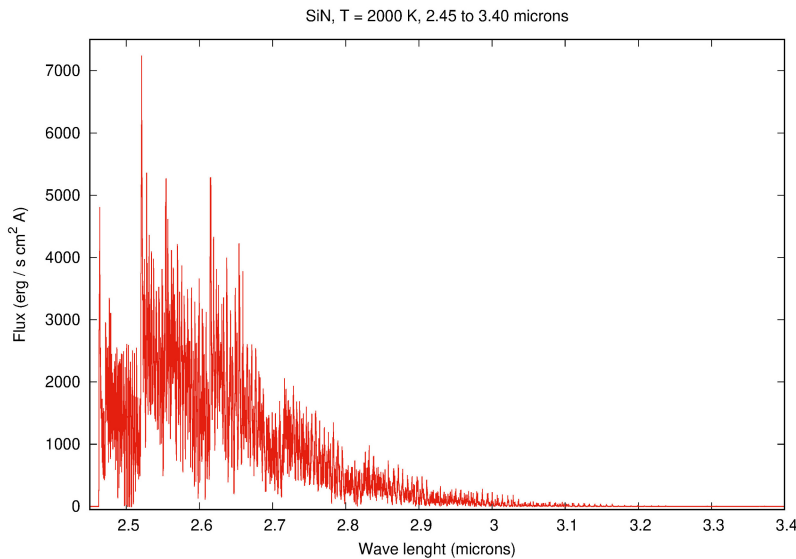
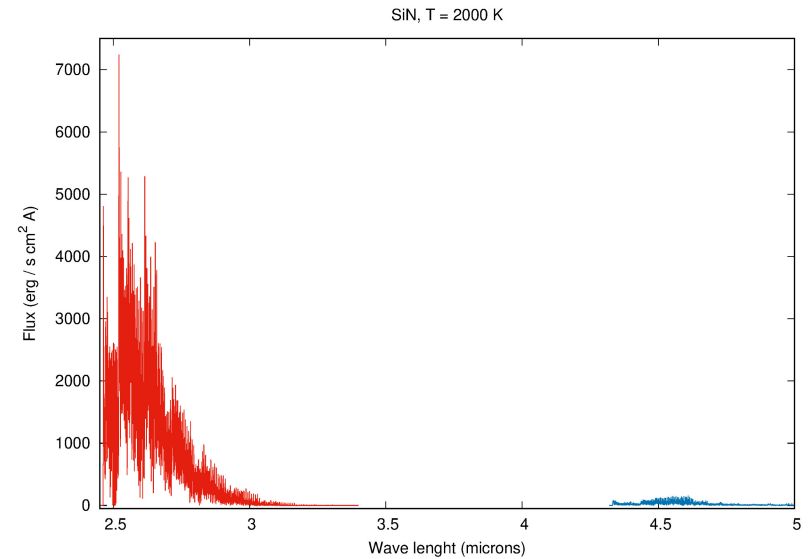
# Silicon nitride (SiN).

1051315 transitions, (2.45 - 3.40  $\mu$ ),  
(4.32 - 5.00  $\mu$ ).

24764 energy levels.

$v_{\max} = 20$ ,  $J_{\max} = 50.5$ .

$^{28}\text{Si}^{14}\text{N}$ ,  $^{29}\text{Si}^{14}\text{N}$ ,  $^{30}\text{Si}^{14}\text{N}$ ,  $^{28}\text{Si}^{15}\text{N}$ .





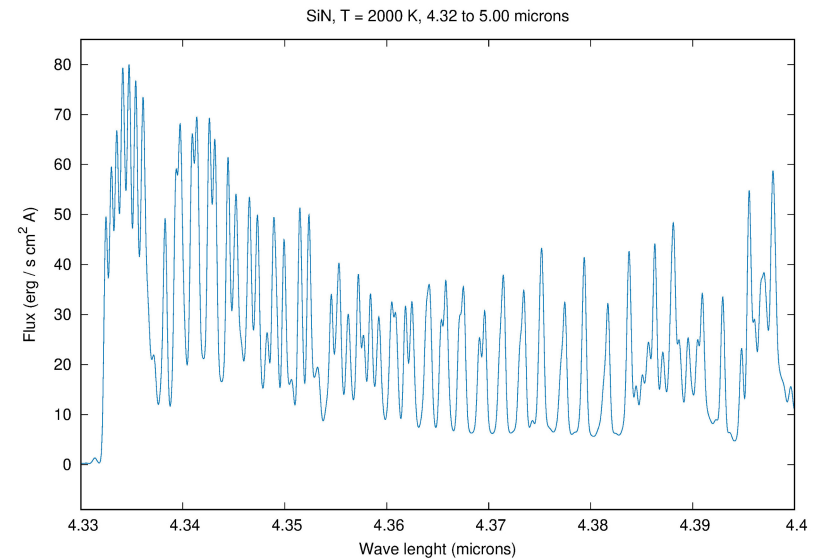
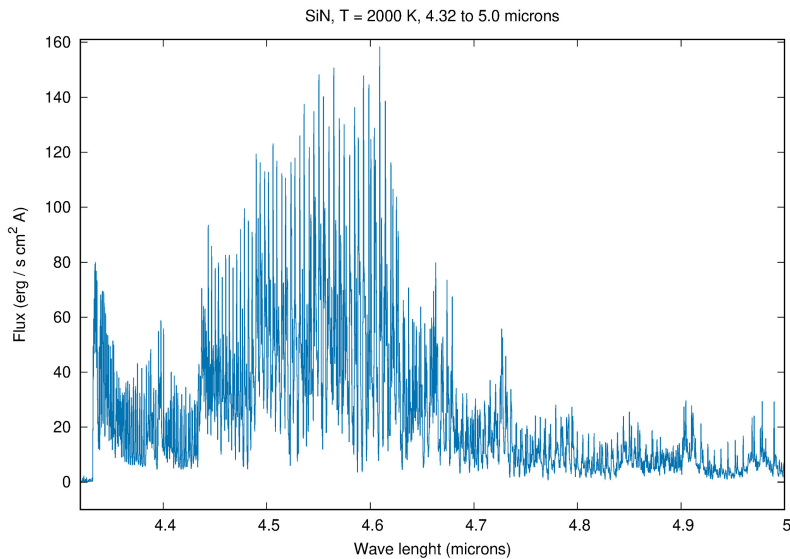
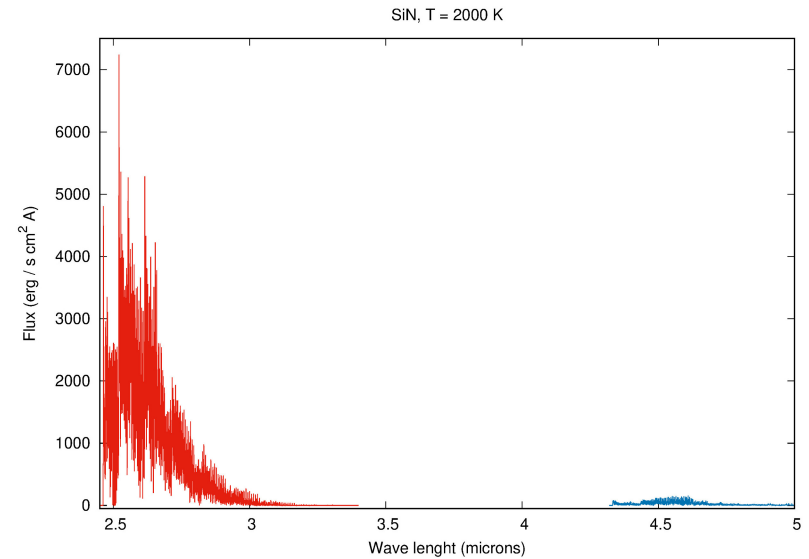
# Silicon nitride (SiN).

1051315 transitions, (2.45 - 3.40  $\mu$ ),  
(4.32 - 5.00  $\mu$ ).

24764 energy levels.

$v_{\max} = 20$ ,  $J_{\max} = 50.5$ .

$^{28}\text{Si}^{14}\text{N}$ ,  $^{29}\text{Si}^{14}\text{N}$ ,  $^{30}\text{Si}^{14}\text{N}$ ,  $^{28}\text{Si}^{15}\text{N}$ .





# Molecular carbon ( $C_2$ ).

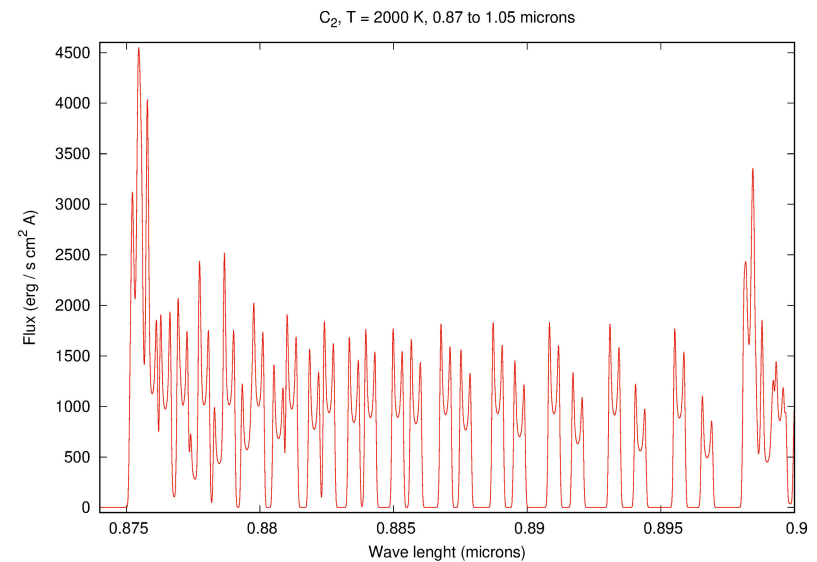
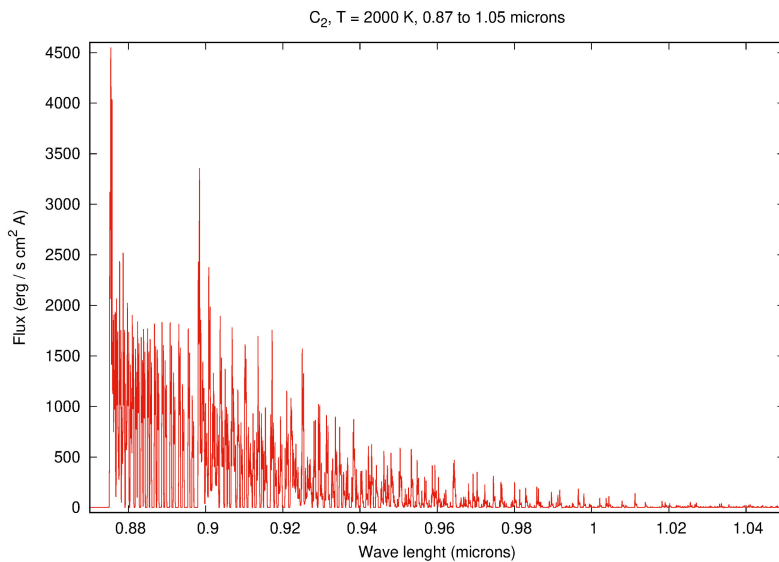
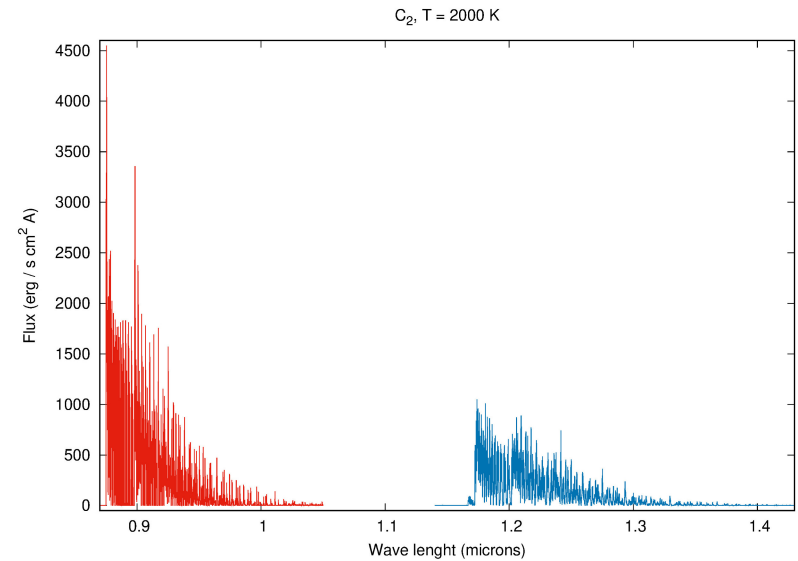
429843 transitions, (0.87 - 1.05  $\mu$ ),  
(1.14 - 1.43  $\mu$ ).

31353 energy levels.

$v_{\max} = 20, J_{\max} = 140.$

$^{12}C^{12}C, ^{12}C^{13}C, ^{13}C^{13}C.$

Column density =  $10^{17} \text{ cm}^{-2}$





# Molecular carbon ( $C_2$ ).

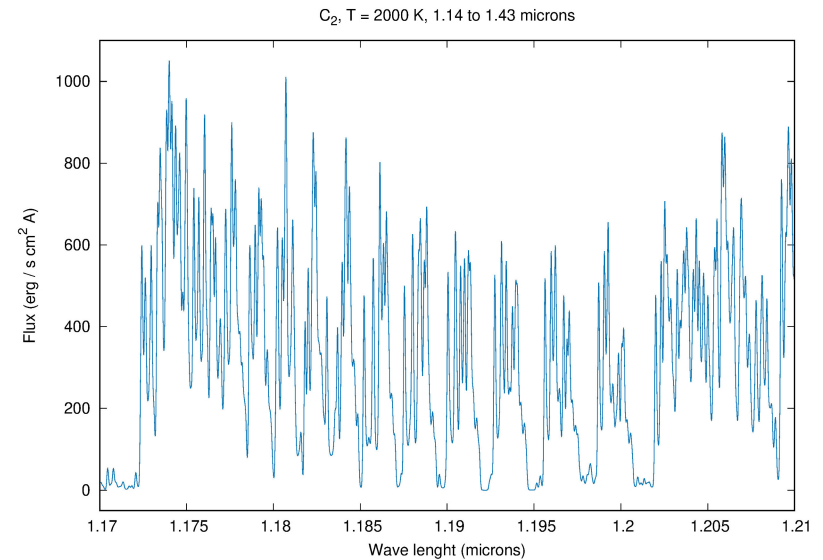
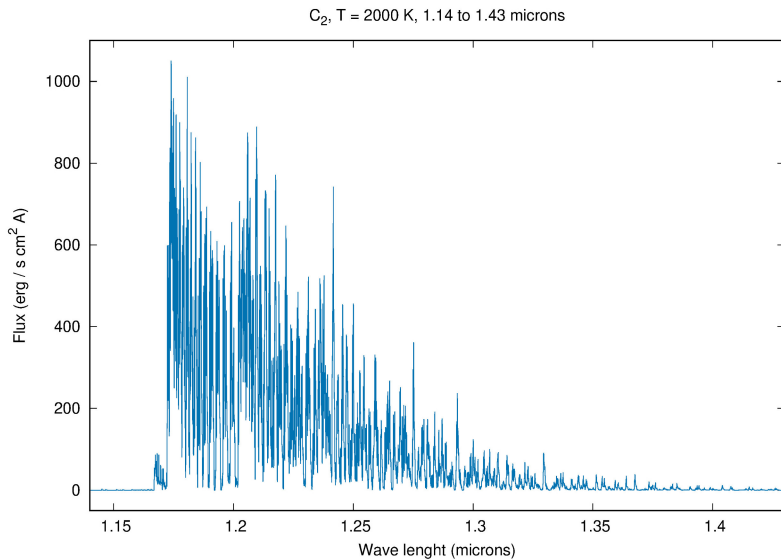
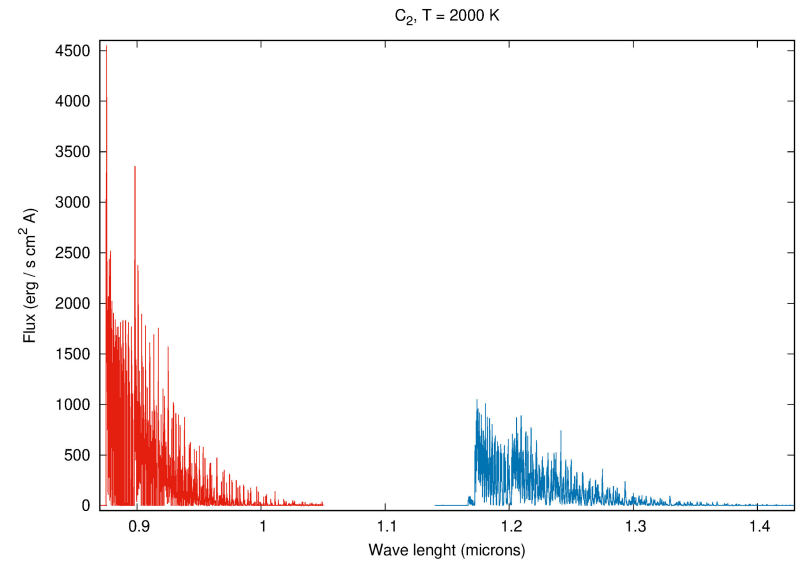
429843 transitions, (0.87 - 1.05  $\mu$ ),  
(1.14 - 1.43  $\mu$ ).

31353 energy levels.

$v_{\max} = 20, J_{\max} = 140.$

$^{12}C^{12}C, ^{12}C^{13}C, ^{13}C^{13}C.$

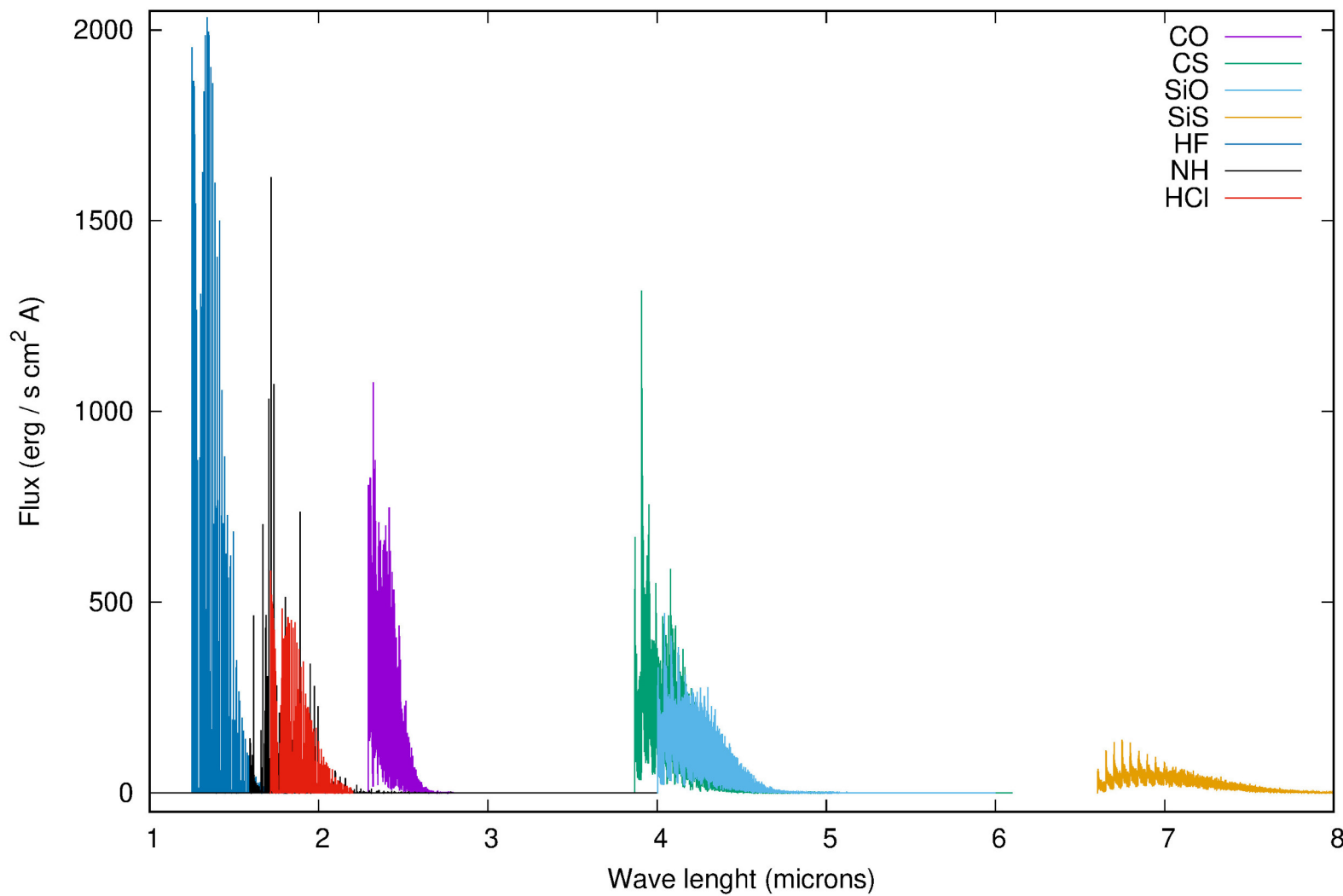
Column density =  $10^{17} \text{ cm}^{-2}$

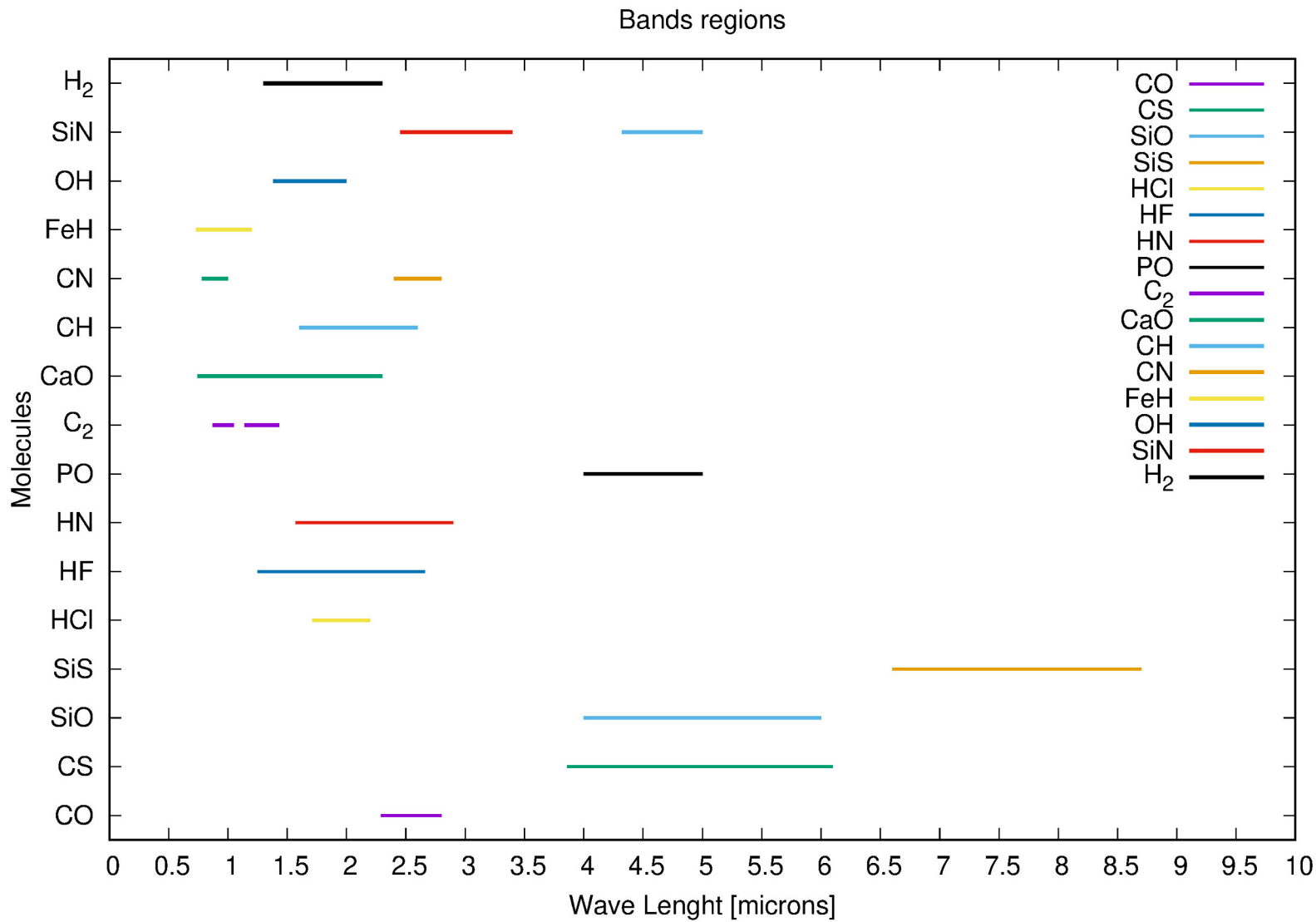






Comparison, T = 2000 K







## Future work:

SiH	LiH	PN	AlF
SH	ScH	KCl	KF
PH	VO	NaCl	LiF
MgH	AlO	LiCl	CaF
NaH	YO	CN	MgF
NiH	MgO	H <sub>2</sub>	N <sub>2</sub>
AlH	TiO	CP	SiN
CrH	NaO	PS	LiH <sup>+</sup>
CaH	LaO	NS	H <sub>2</sub> <sup>+</sup>
BeH	ZrO	NaF	HeH <sup>+</sup>
TiH	O <sub>2</sub>	AlCl	OH <sup>+</sup>



## **Conclusions:**

I think it is a good tool for identifying specific molecules and fitting the spectra to determine certain parameters of circumstellar disks.

The application of the code will depend on the available observations.

When considering molecules with a large number of transitions, we need to be careful and determine the optimal number of wavelength grid points.

.



*Muchas gracias*

*Thank you very much*

*Děkuji moc*