Modeling diatomic molecules in circumstellar disk

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Ondrejov, June 29, 2023

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y Geofísicas
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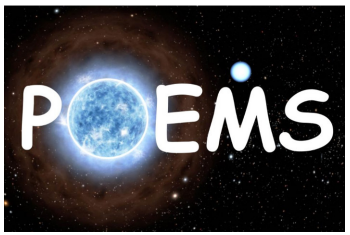

Molecules in circumstellar disk.

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).

Molecules in circumstellar disk.

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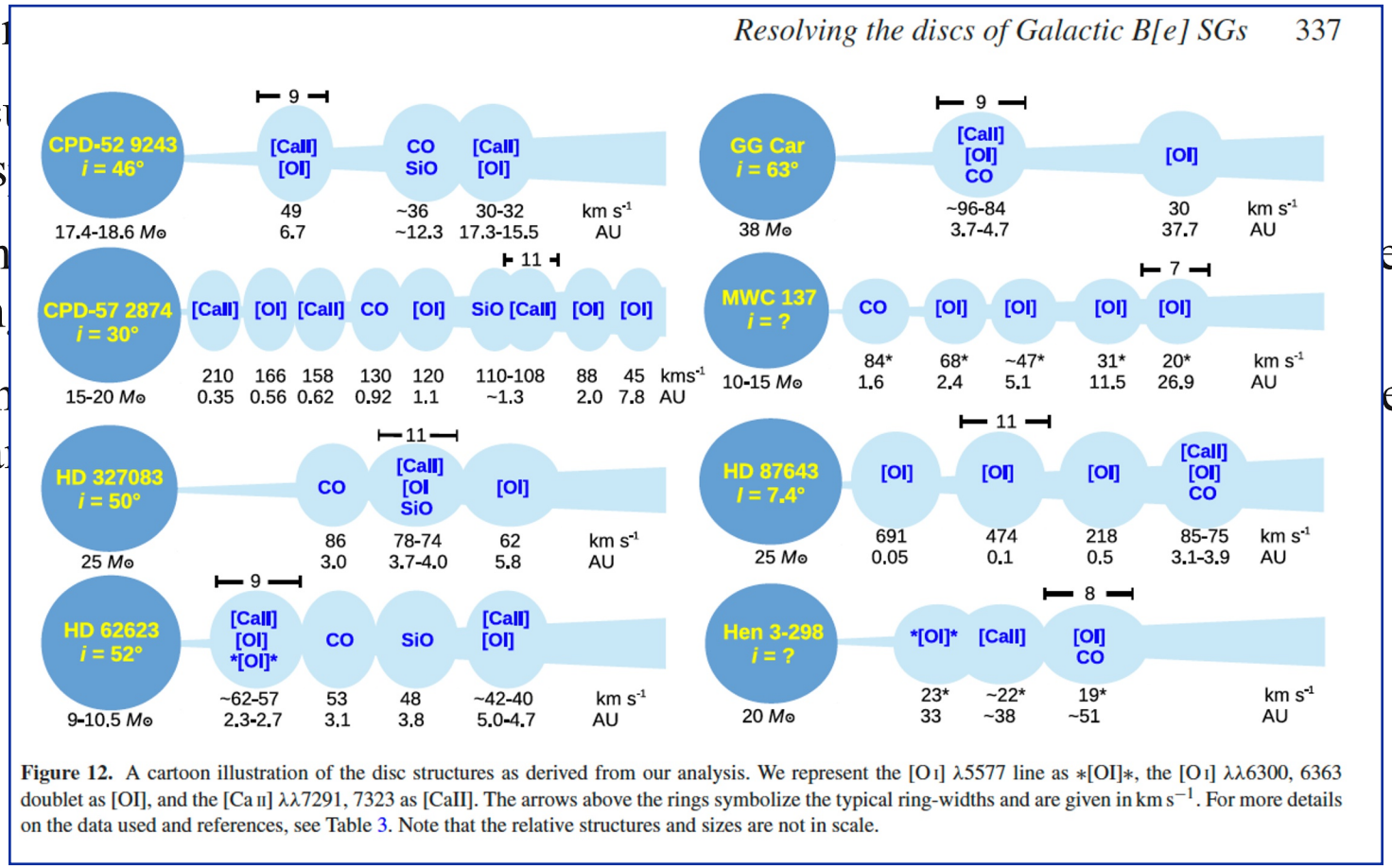

Figure 12. A cartoon illustration of the disc structures as derived from our analysis. We represent the [O I] λ5577 line as ∗[OI]∗, the [O I] λλ6300, 6363 doublet as [OI], and the [Ca II] λλ7291, 7323 as [CaII]. The arrows above the rings symbolize the typical ring-widths and are given in km s^{-1}. For more details on the data used and references, see Table 3. Note that the relative structures and sizes are not in scale.

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.

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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.

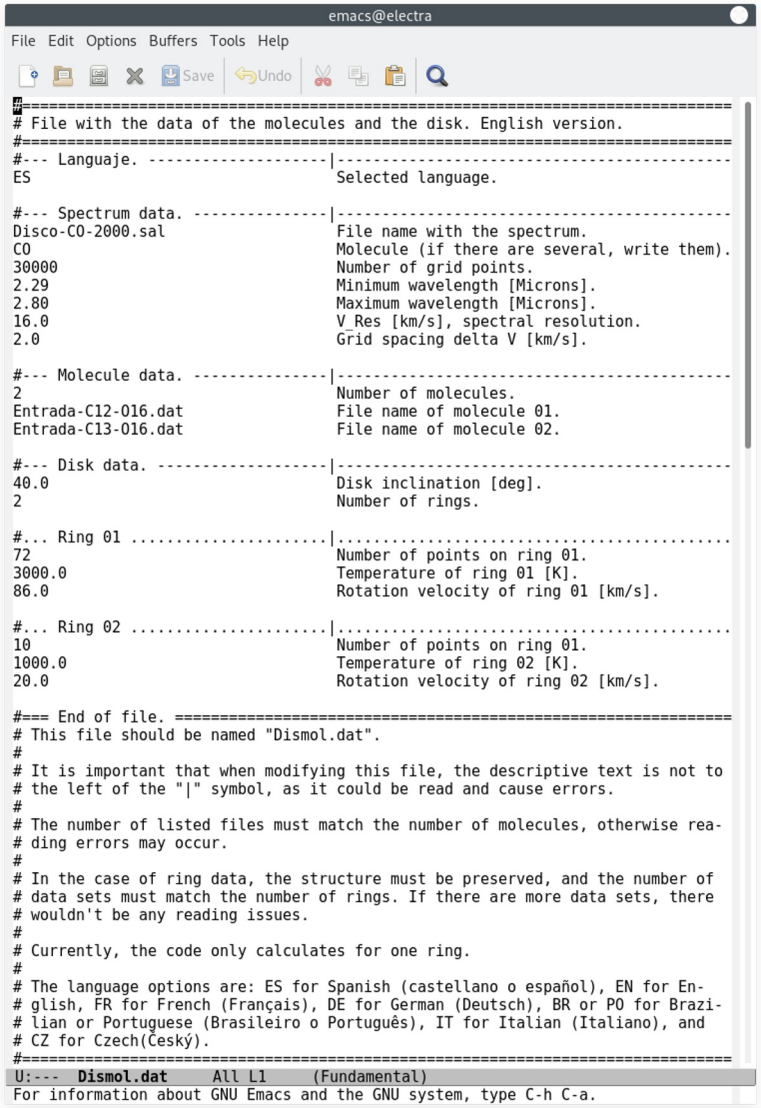
The code does not have a name, for now it is temporarily called DisMol.

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.



Dismol.dat

Input file containing the general information of the model.

Data of the spectrum.

Number of molecules and associated files.

Data of de disk.

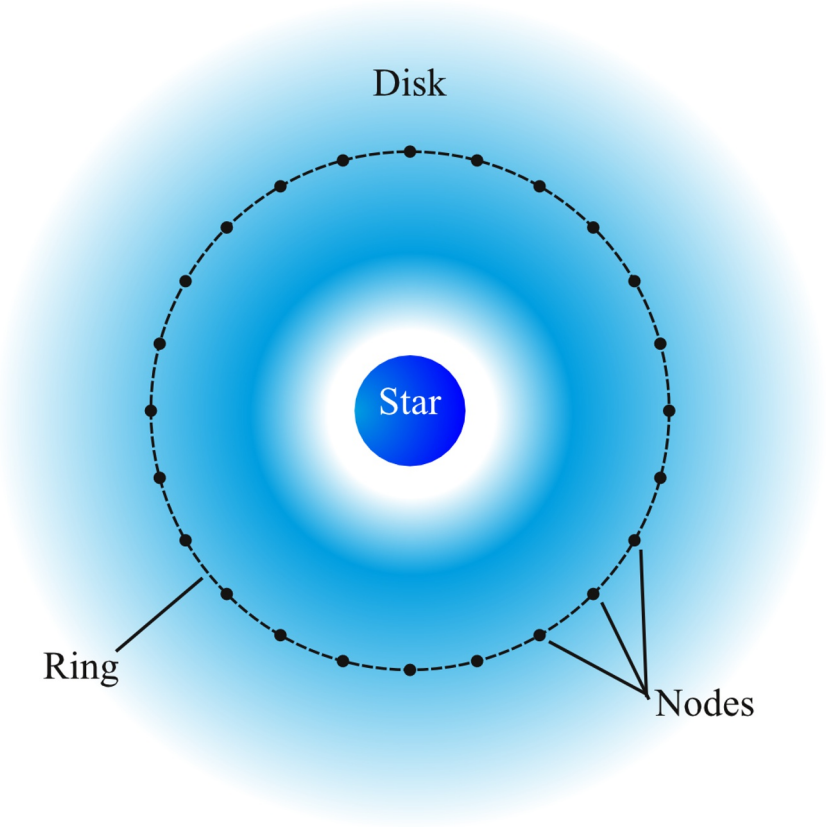
Information about this file.

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

#--- Spectrum data. --------------|-------------------------------------------
Disco-CO-2000.sal                  File name with the spectrum.
CO                                 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-O16.dat                File name of molecule 01.
Entrada-C13-O16.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

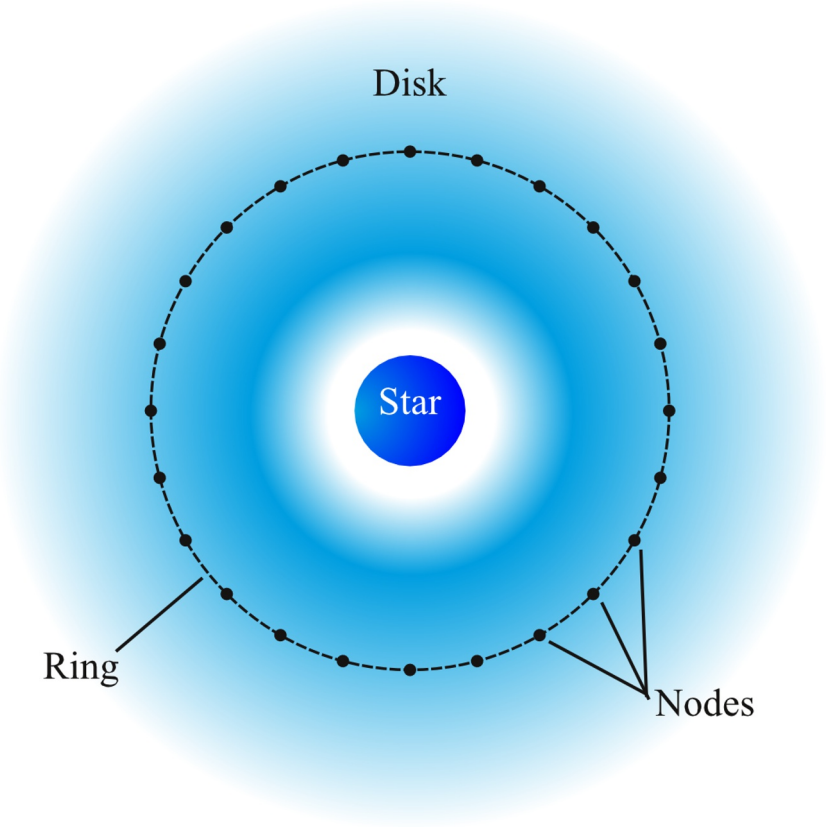
- Ring with equidistant nodes with the same physical and geometric parameters (temperature, density, chemical composition, rotation speed, inclination, etc.).

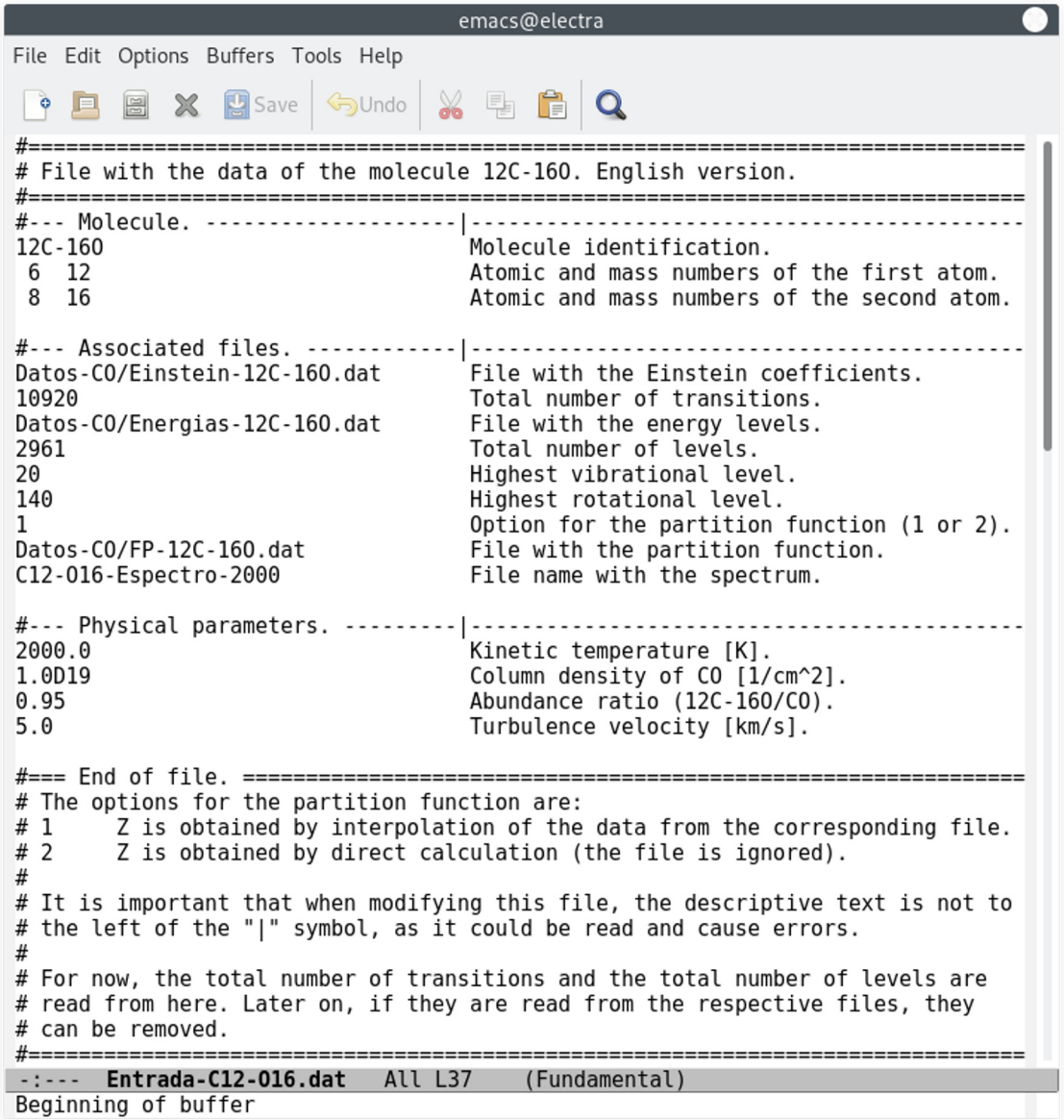
- Consequently, each node has a different radial velocity.

In the future:

- Incorporation of additional rings with different conditions.

- Consider the possibility of partial rings.





Entrada-C12-O16.dat

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

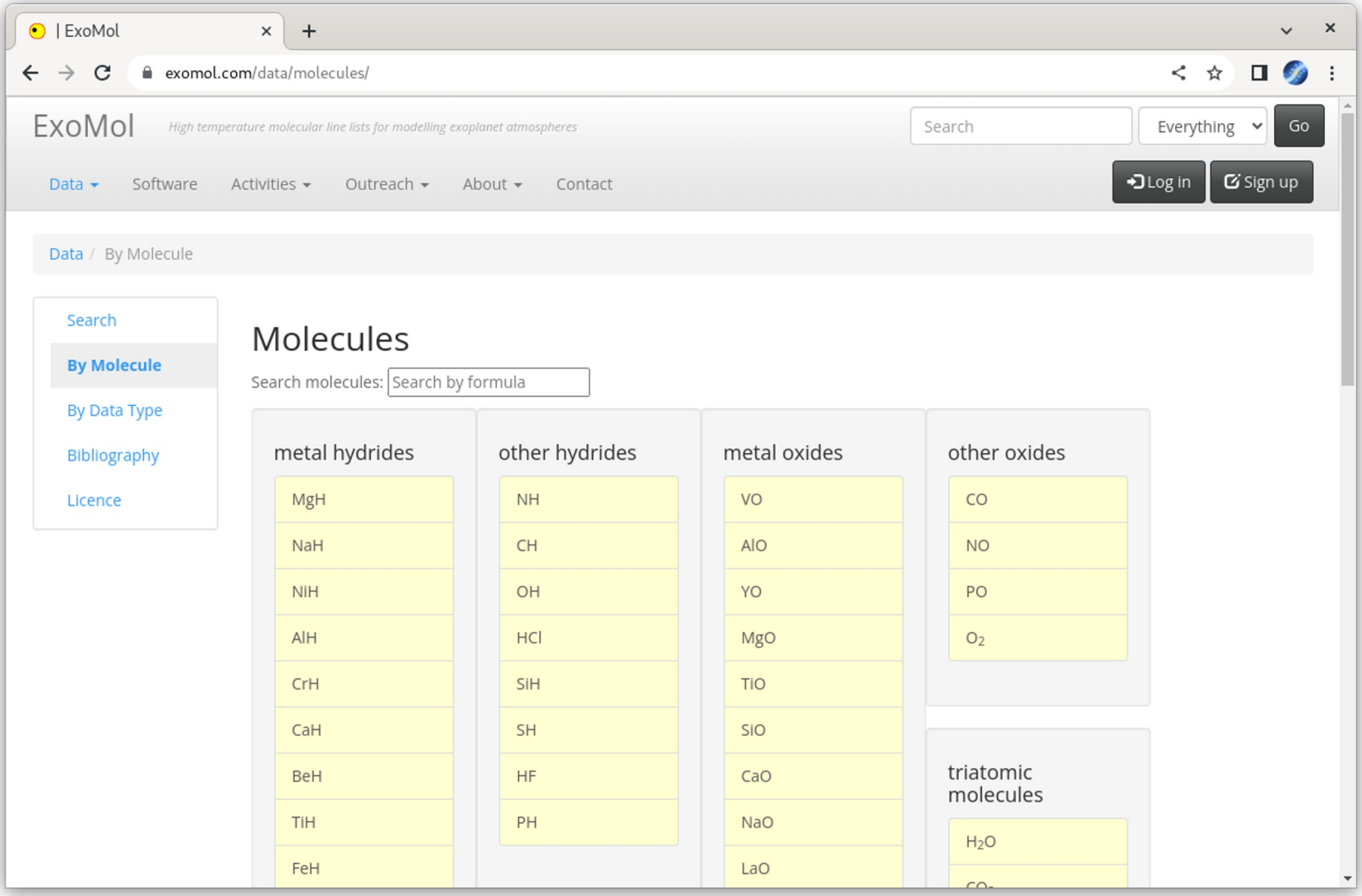
Data of the isotopic variant.

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-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-O16-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.
```


| ExoMol
exomol.com/data/molecules/
ExoMol
High temperature molecular line lists for modelling exoplanet atmospheres
Search
Everything
Go
Data
Software
Activities
Outreach
About
Contact
Log in
Sign up
Data / By Molecule
Search
By Molecule
By Data Type
Bibliography
Licence
Molecules
Search molecules: Search by formula
metal hydrides
MgH
NaH
NiH
AlH
CrH
CaH
BeH
TiH
FeH
other hydrides
NH
CH
OH
HCl
SiH
SH
HF
PH
metal oxides
VO
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YO
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CaO
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LaO
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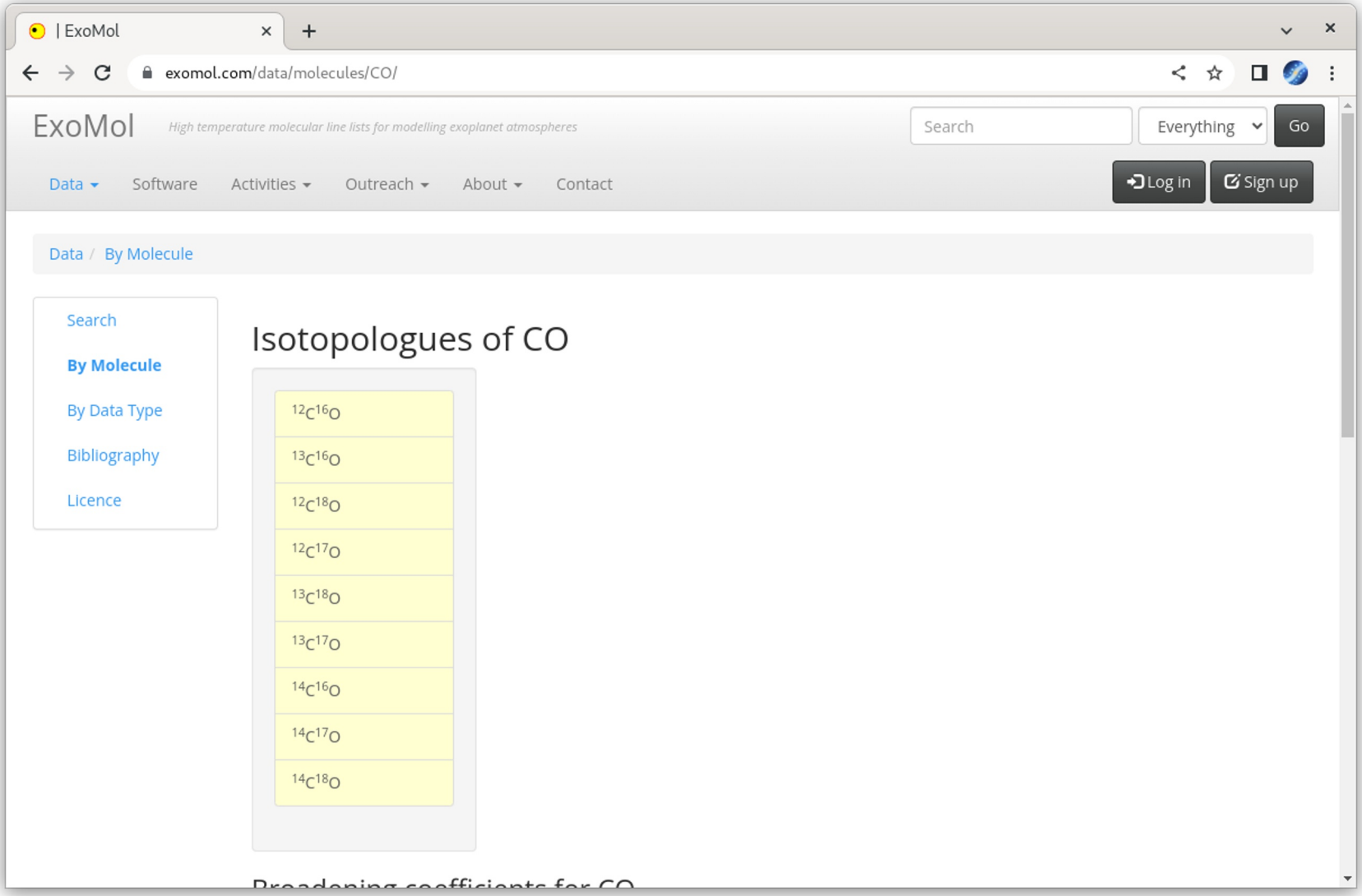
CO
NO
PO
O2
triatomic molecules
H2O


| ExoMol
exomol.com/data/molecules/CO/
ExoMol
High temperature molecular line lists for modelling exoplanet atmospheres
Search
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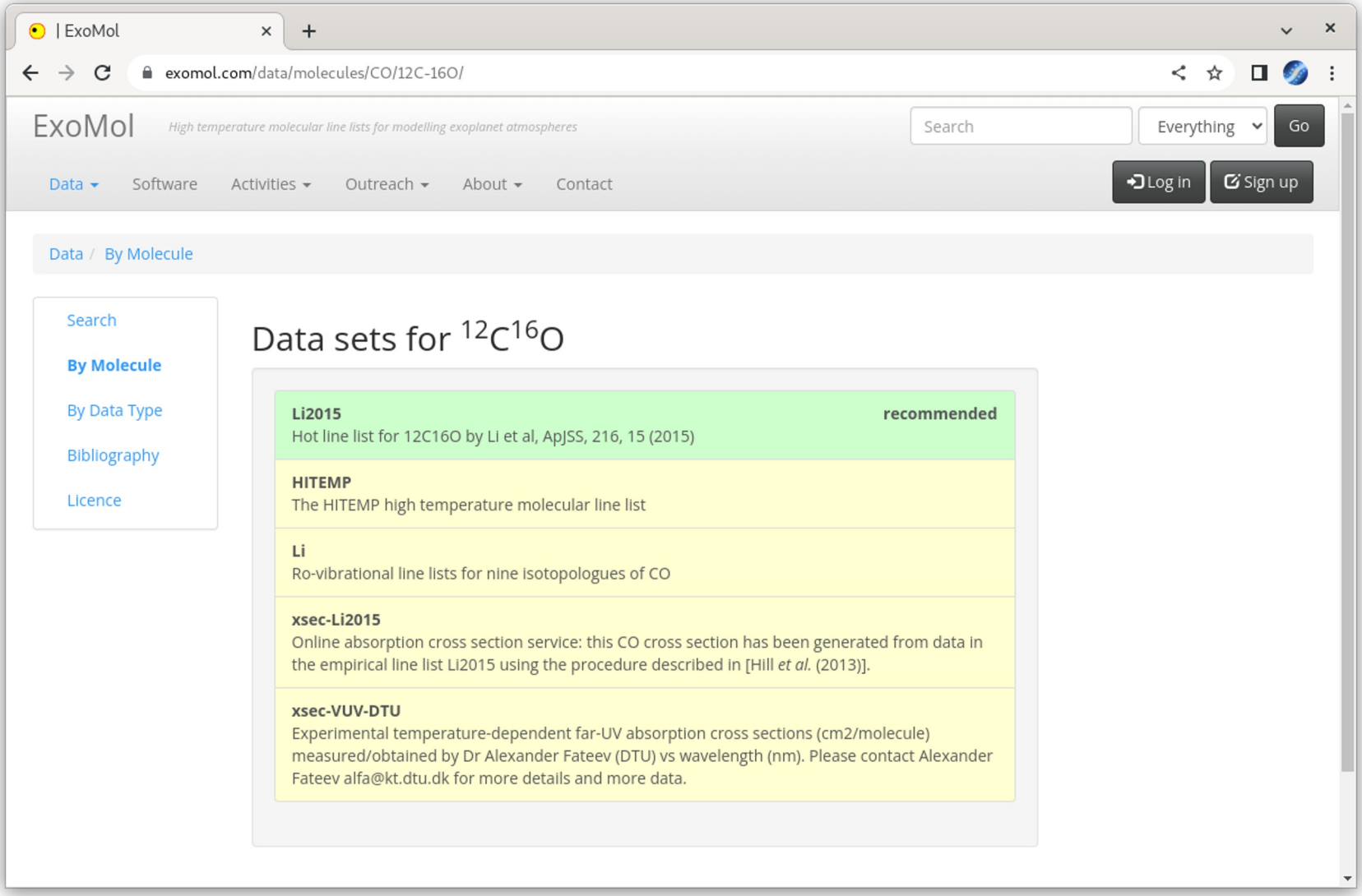
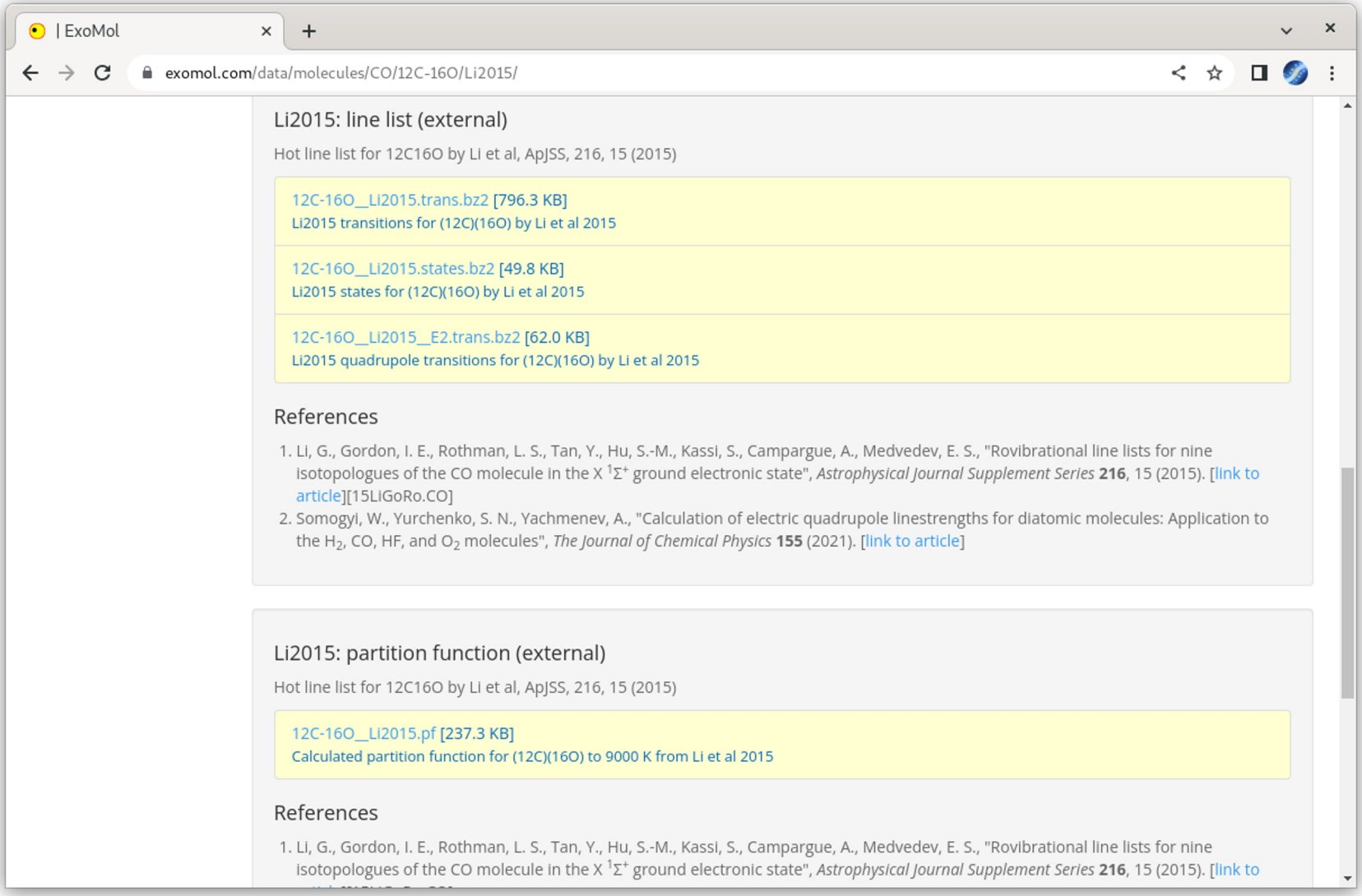
Activities
Outreach
About
Contact
Log in
Sign up
Data / By Molecule
Search
By Molecule
By Data Type
Bibliography
Licence
Isotopologues of CO
12C16O
13C16O
12C18O
12C17O
13C18O
13C17O
14C16O
14C17O
14C18O


| ExoMol
exomol.com/data/molecules/CO/12C-16O/
ExoMol
High temperature molecular line lists for modelling exoplanet atmospheres
Search
Everything
Go
Data
Software
Activities
Outreach
About
Contact
Log in
Sign up
Data / By Molecule
Search
By Molecule
By Data Type
Bibliography
Licence
Data sets for 12C16O
Li2015
recommended
Hot line list for 12C16O 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 (cm2/molecule) measured/obtained by Dr Alexander Fateev (DTU) vs wavelength (nm). Please contact Alexander Fateev 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
1. Li, G., Gordon, I. E., Rothman, L. S., Tan, Y., Hu, S.-M., Kassi, 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]
2. Somogyi, W., Yurchenko, S. N., Yachmenev, A., "Calculation of electric quadrupole linestrengths for diatomic molecules: Application to the H_2, CO, HF, and O_2 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
1. Li, G., Gordon, I. E., Rothman, L. S., Tan, Y., Hu, S.-M., Kassi, 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

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#================================================================================
# 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. Kassi, 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-12C-16O.dat

Input file containing the transitions.

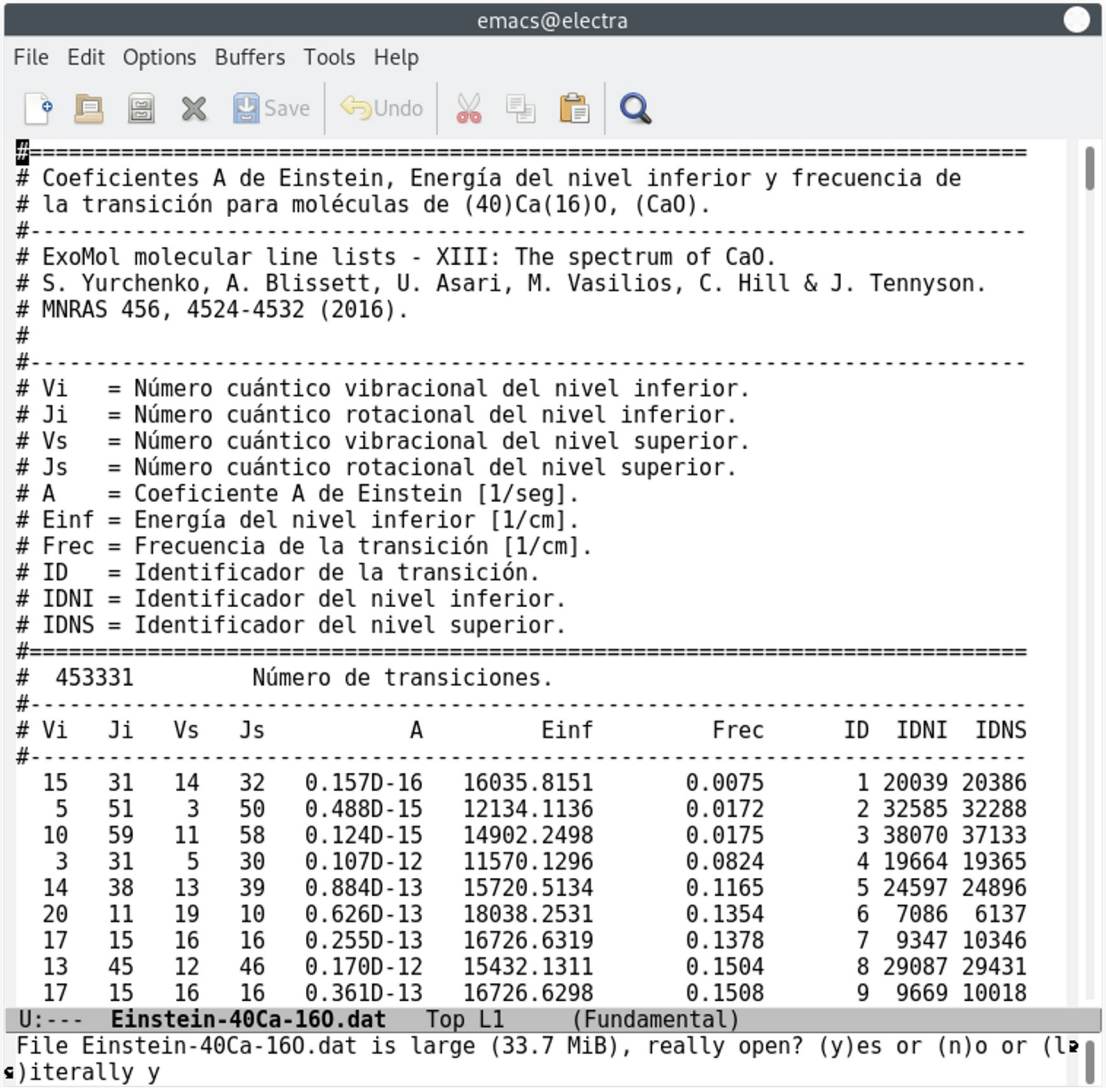
Data of the isotopic variant.

Reference.

Information of the header.

Number of transitions.

Data.



Einstein-40Ca-16O.dat

Input file containing the transitions.

Data of the isotopic variant.

Reference.

Information of the header.

Number of transitions.

Data.

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File Edit Options Buffers Tools Help

Save Undo

```
#================================================================================
# 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
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Einstein-12C-1H.dat

Input file containing the transitions.

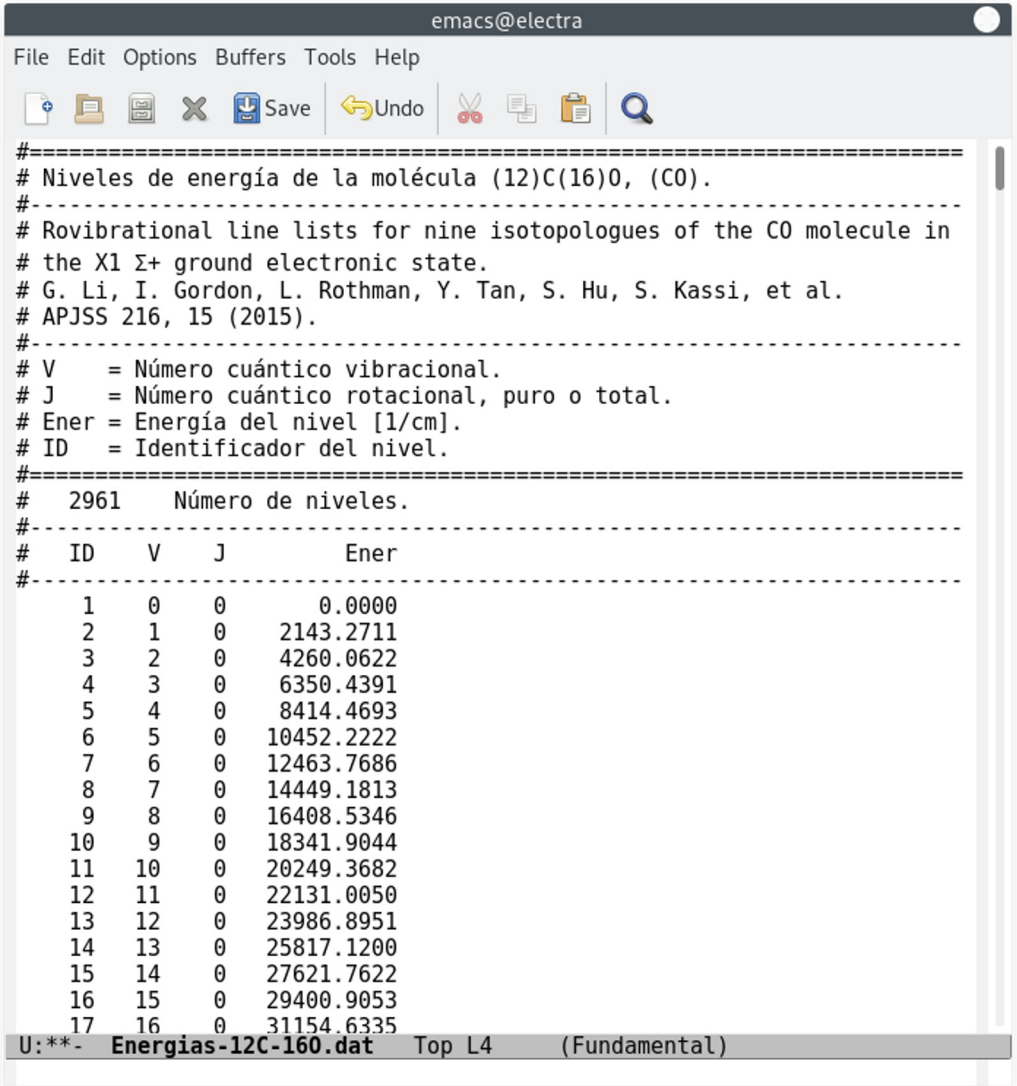
Data of the isotopic variant.

Reference.

Information of the header.

Number of transitions.

Data.



Energías-12C-16O.dat

Input file containing the energy levels.

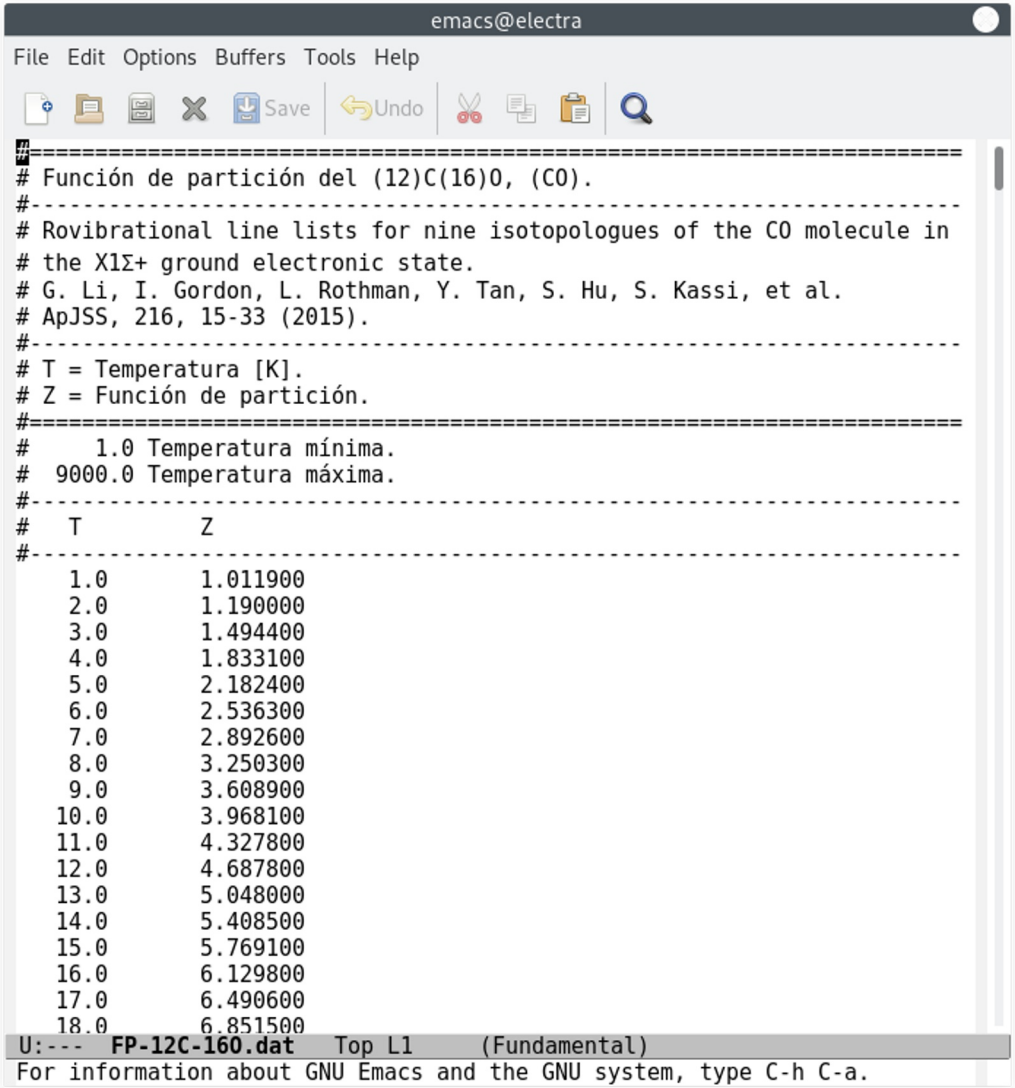
Data of the isotopic variant.

Reference.

Information of the header.

Number of levels.

Data.



FP-12C-16O.dat

Input file containing the partition function.

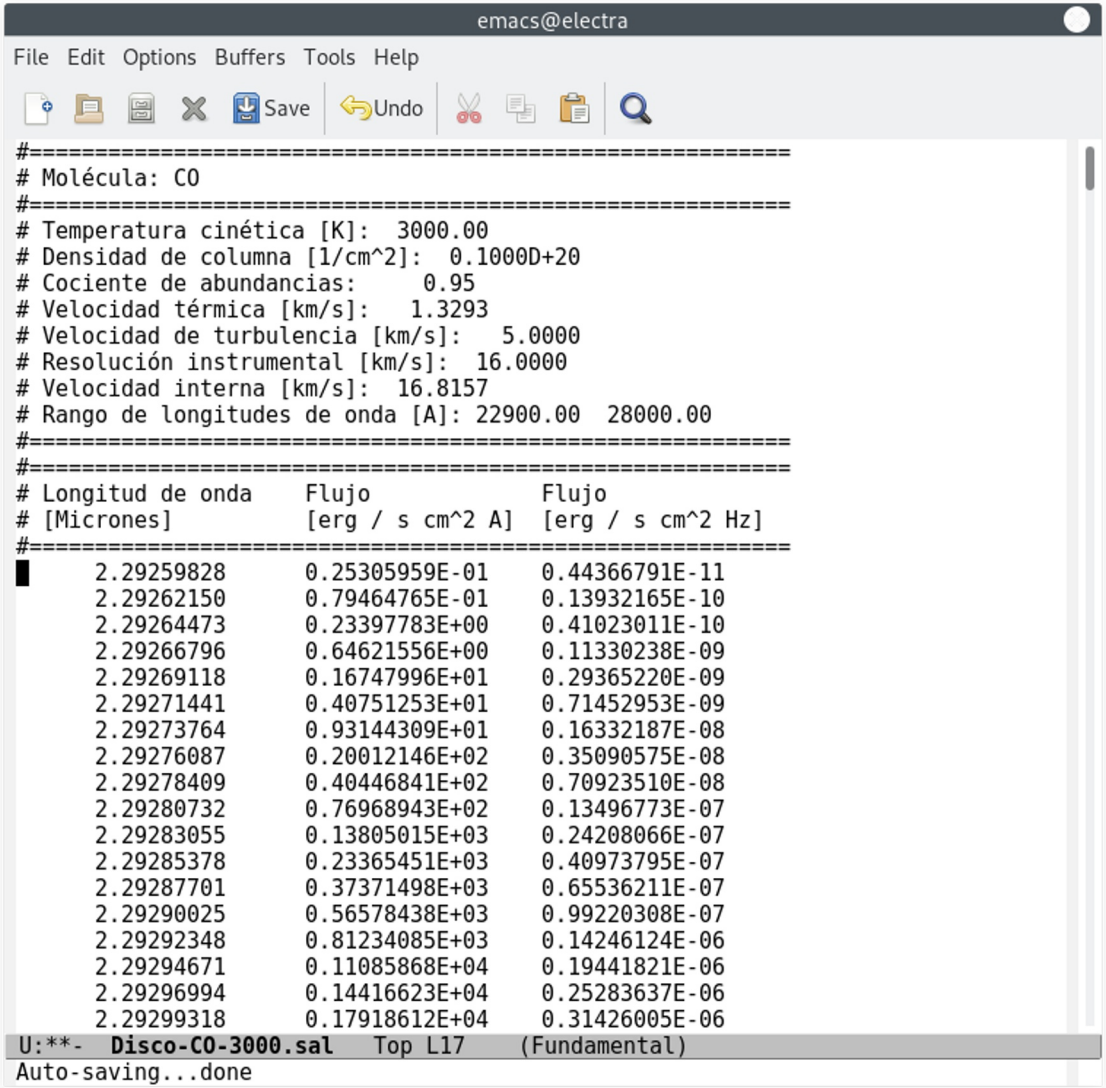
Data of the isotopic variant.

Reference.

Information of the header.

Range of temperatura.

Data.



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} cm^{-2}.

Rotation velocity = 86 km/s.

Inclination = 40˚.

Resolution = 16.0 km/s

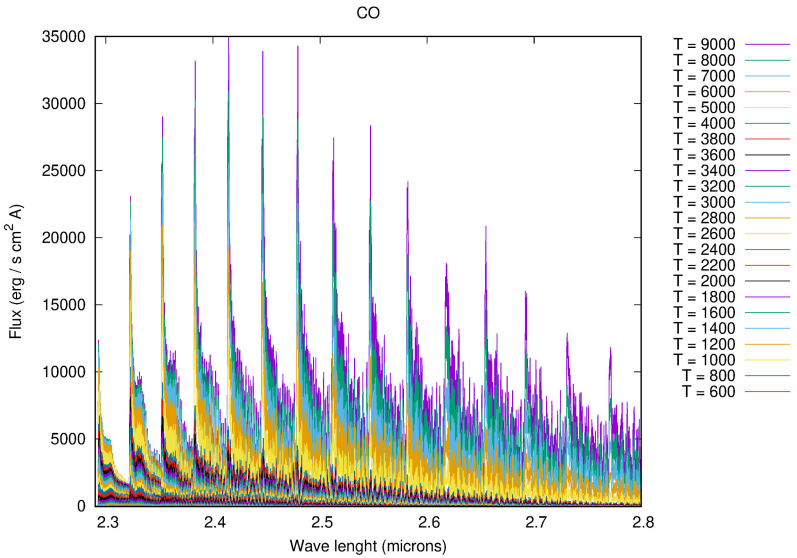
Carbon monoxide (CO).

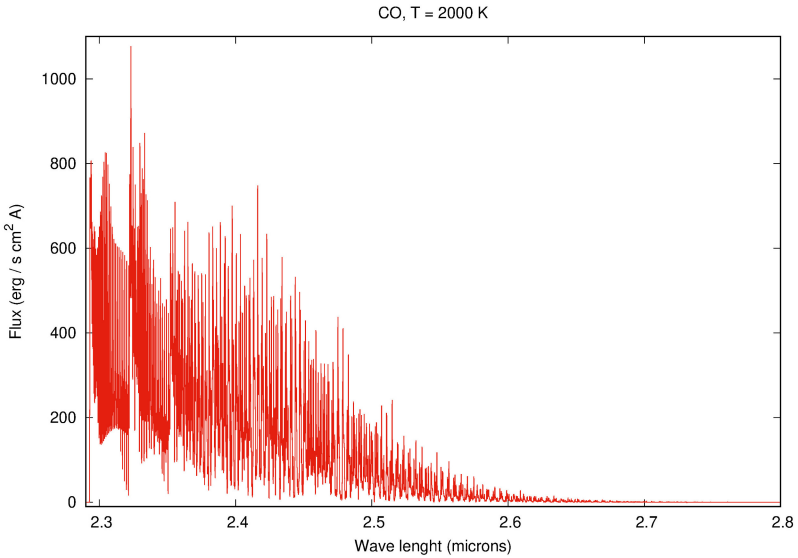
10920 transitions, (2.29 - 2.80 μ).

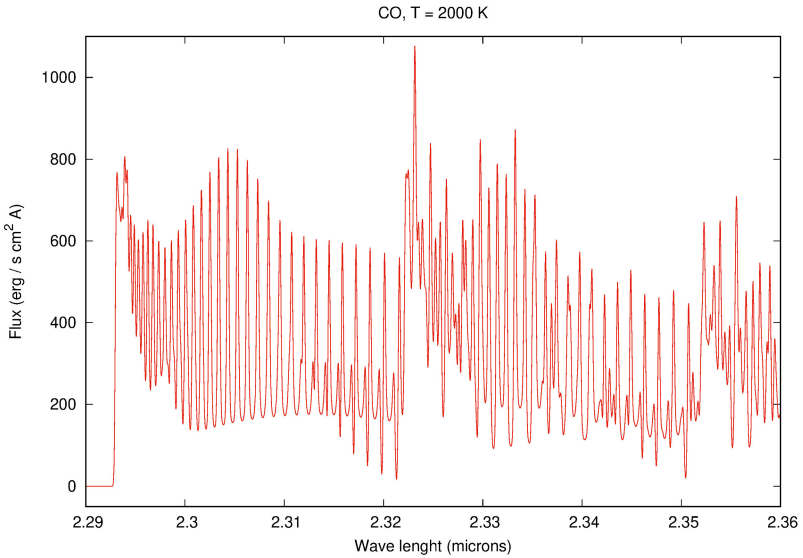
2961 energy levels.

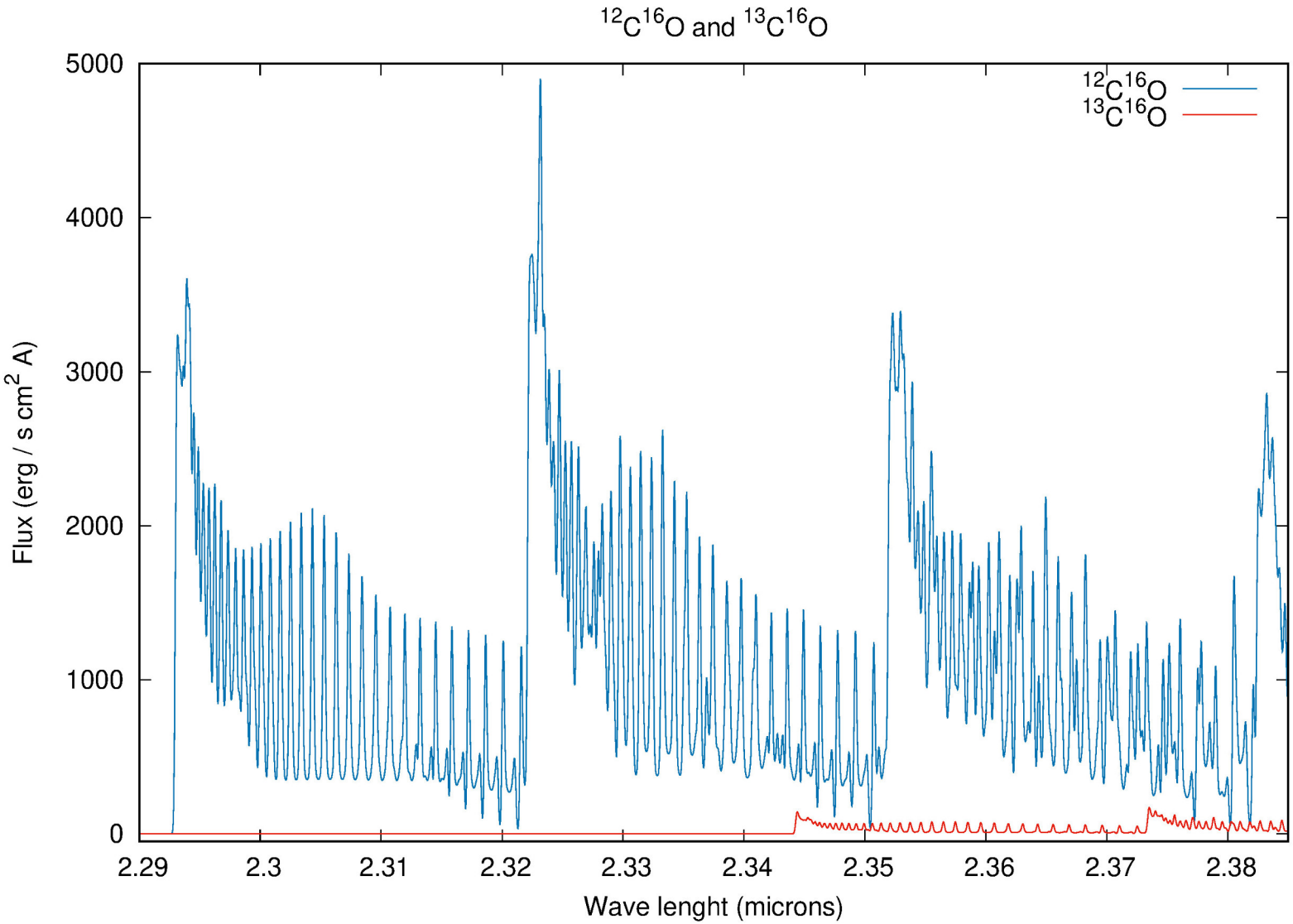
$v_{max} = 20$, $J_{max} = 140$.

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








$^{12}C^{16}O$ and $^{13}C^{16}O$
$^{12}C^{16}O$
$^{13}C^{16}O$
Flux (erg / s cm^2 A)
5000
4000
3000
2000
1000
0
2.29
2.3
2.31
2.32
2.33
2.34
2.35
2.36
2.37
2.38
Wave lenght (microns)

CPD-52 9243

T_{CO} = 2400 K

N_{CO} = 4.0x10^{22} cm^{-2}

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

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

Resolution = 6 km/s

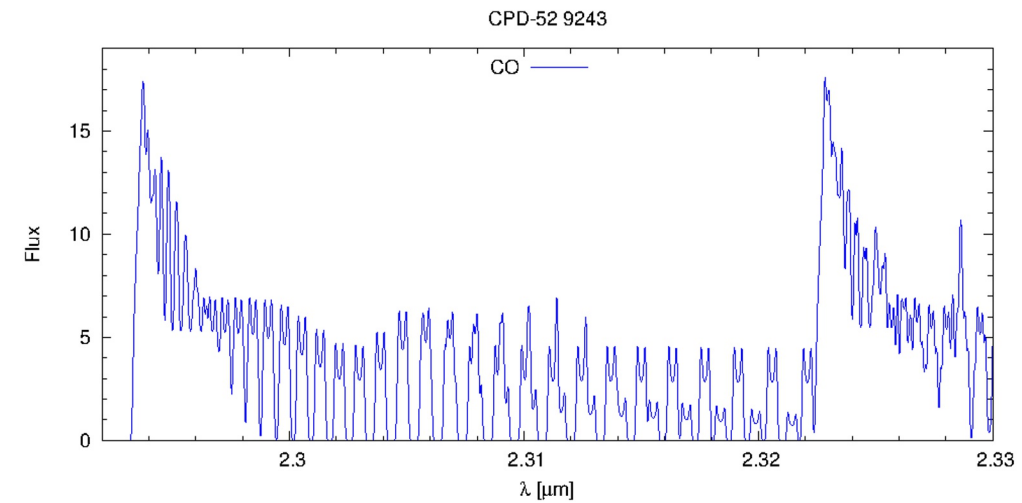
2.29 μ a 2.51μ

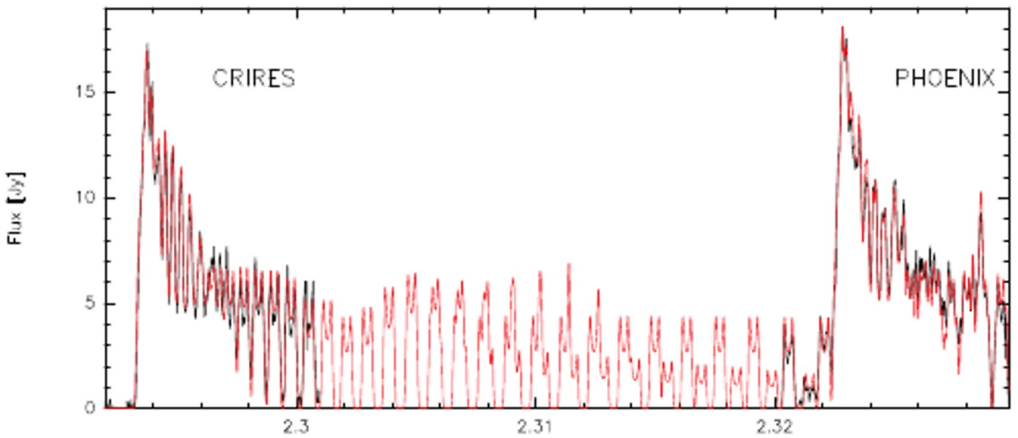
16000 points

i = 40º

V_{rot} = 33 km/s

72 nodes





Cidale et al, 2012

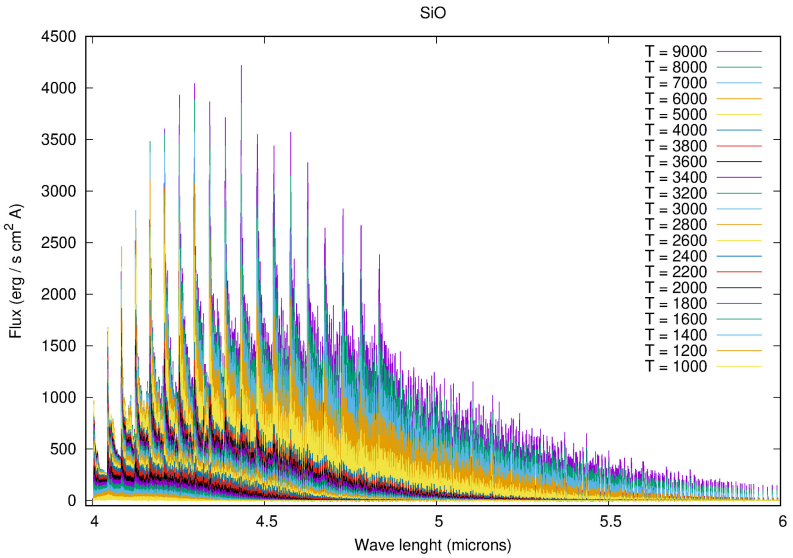
Silicon monoxide (SiO).

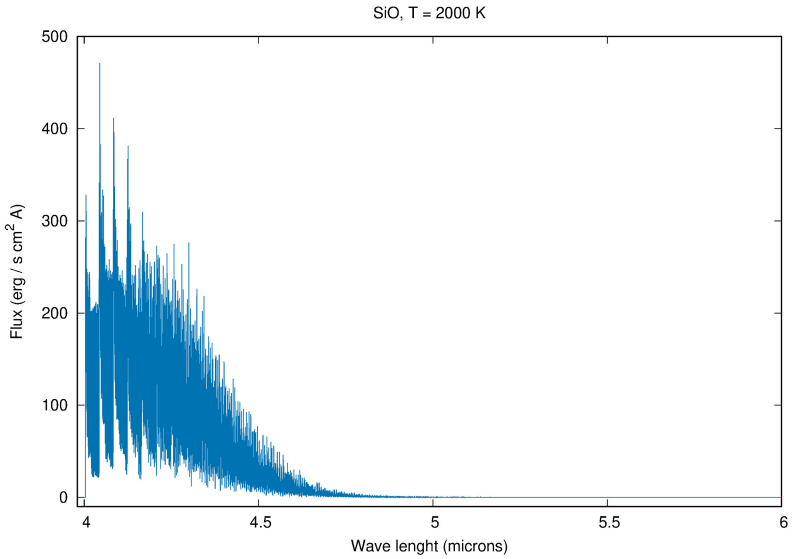
10920 transitions, (4.00 - 6.00 μ).

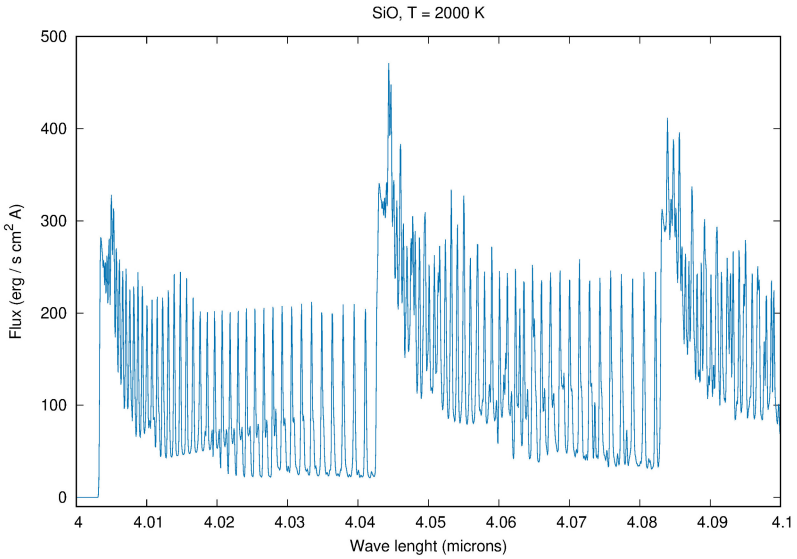
2961 energy levels.

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

$^{28}Si^{16}O$, **$^{29}Si^{16}O$**, **$^{30}Si^{16}O$**, $^{28}SiC^{17}O$, $^{28}Si^{18}O$.







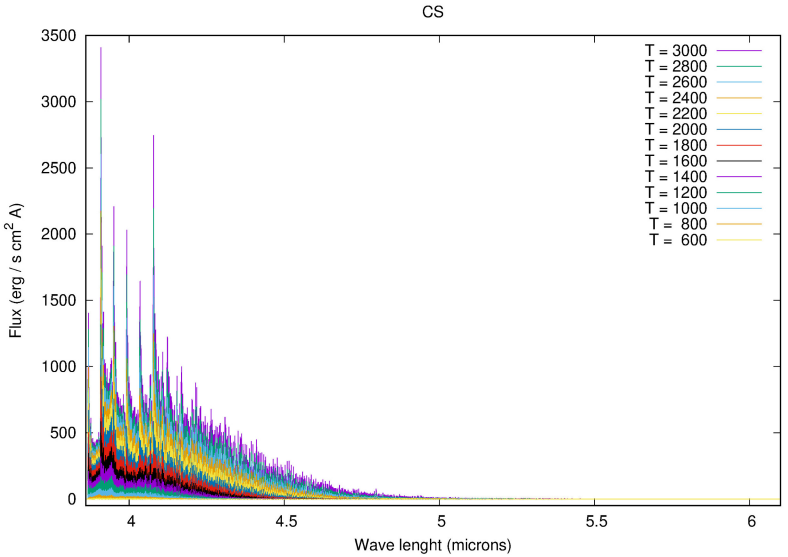
Carbon sulfide (CS).

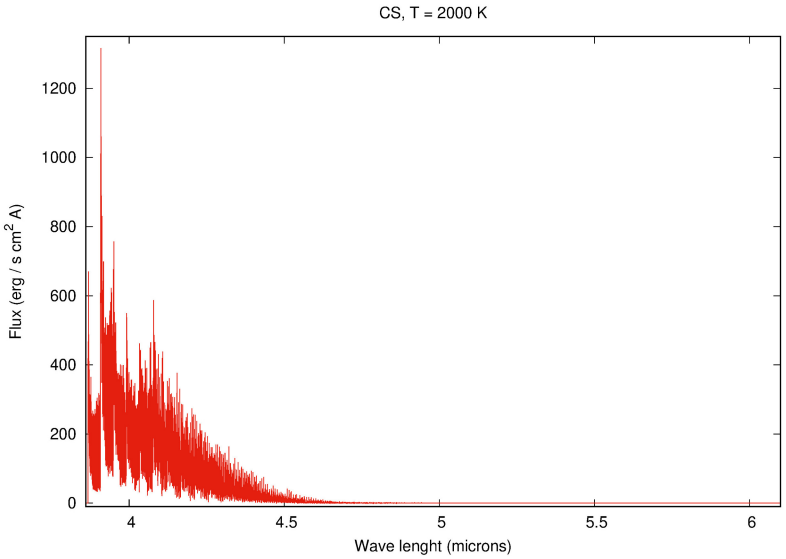
11480 transitions, (3.86 - 6.10 μ).

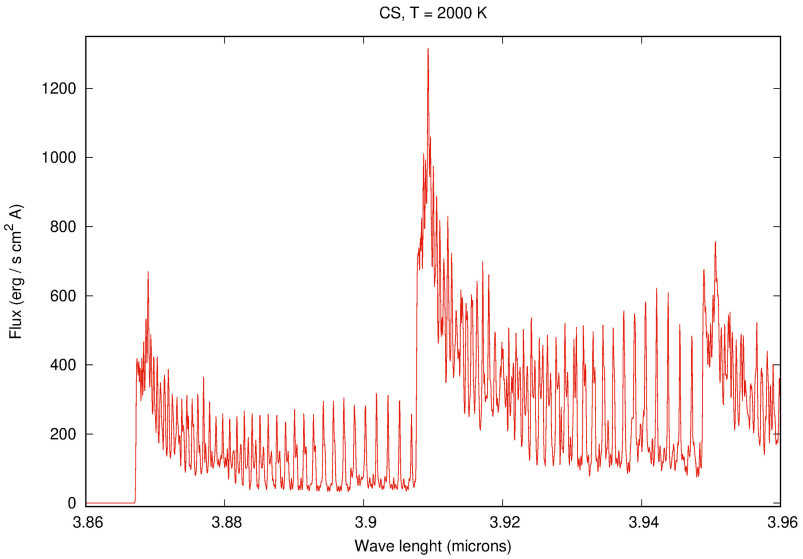
2961 energy levels.

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

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







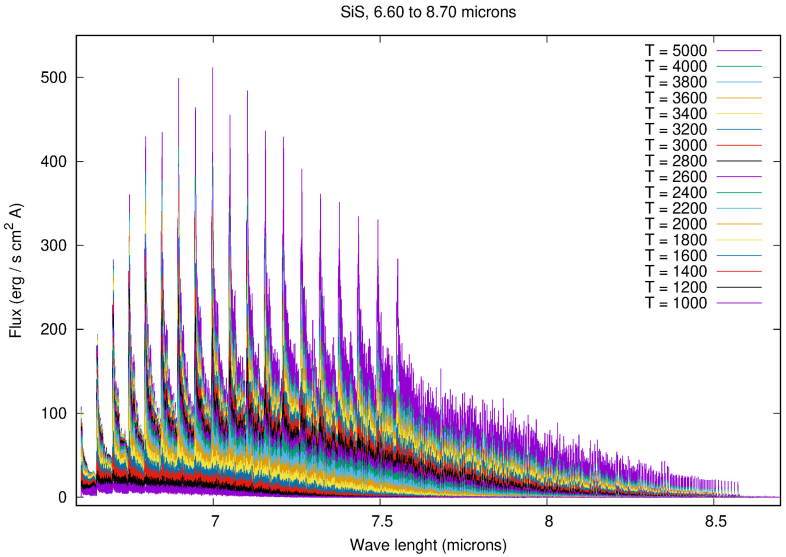
Silicon sulfide (SiS).

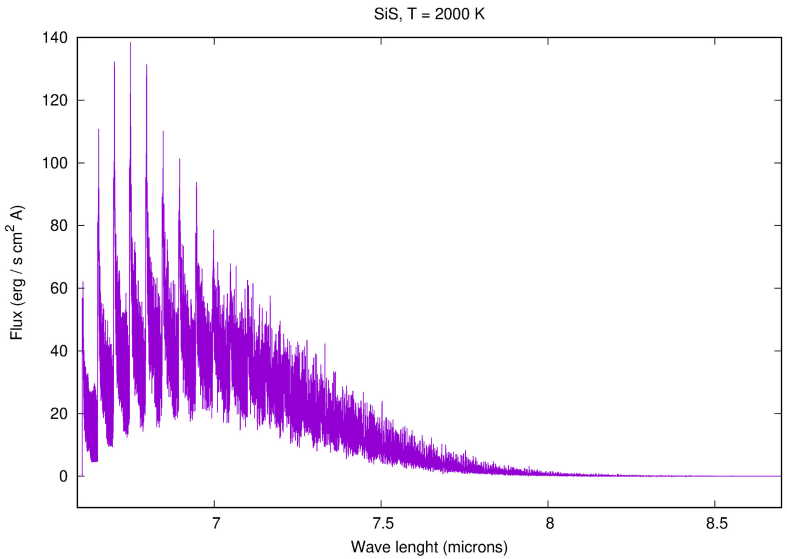
10920 transitions, (6.60 - 8.70 μ).

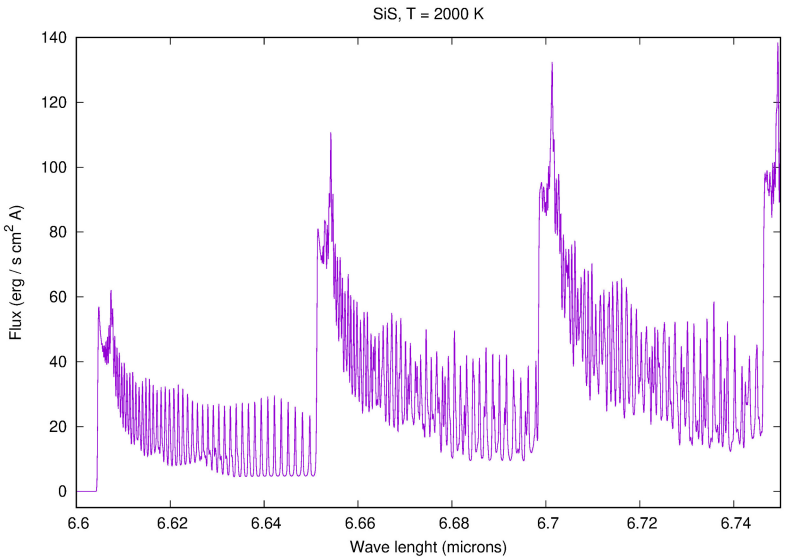
2961 energy levels.

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

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







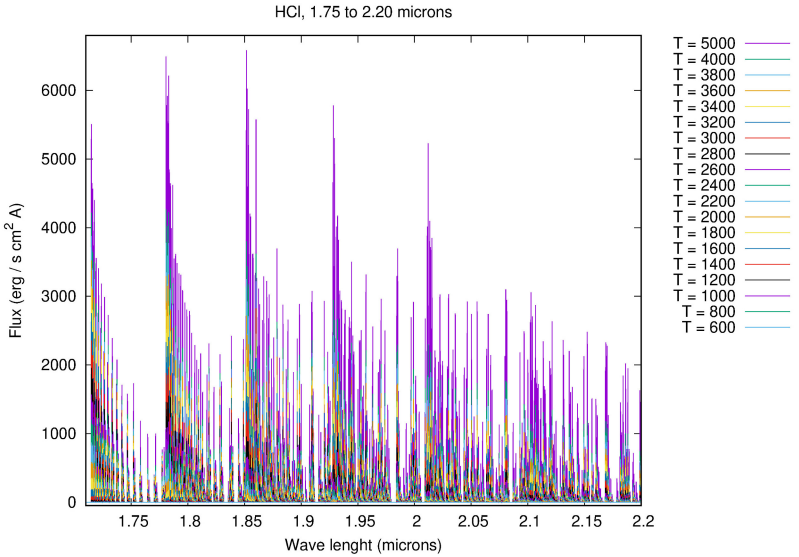
Chlorine hydride (HCl).

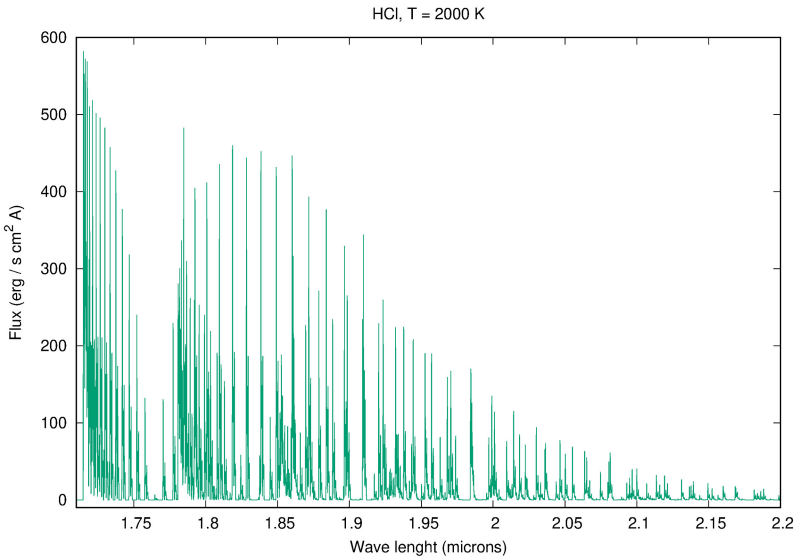
2509 transitions, (1.71 - 2.20 μ).

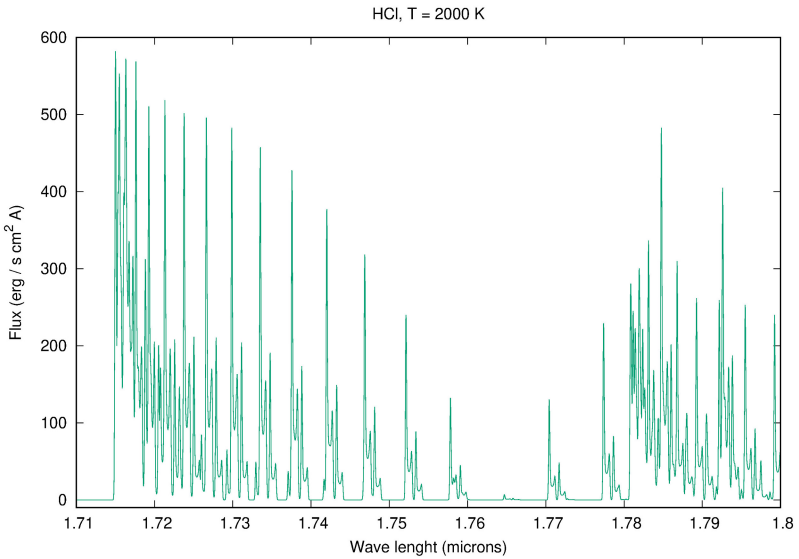
710 energy levels.

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

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







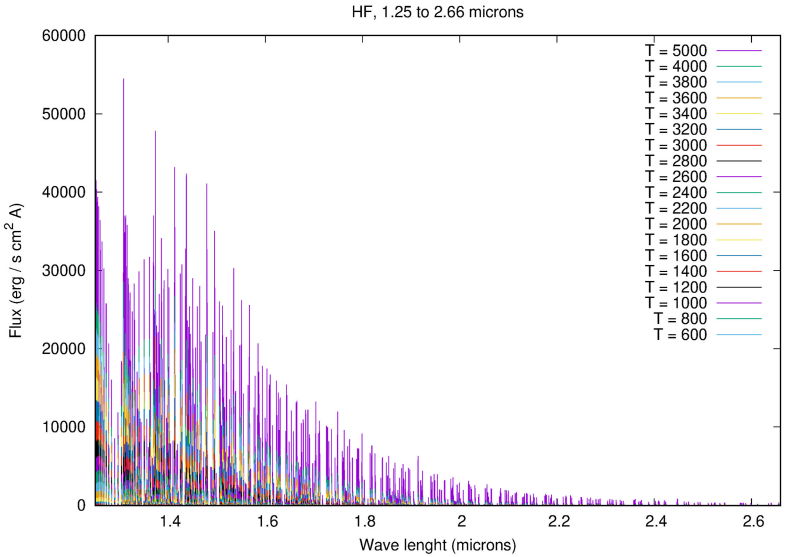
Fluorine hydride (HF).

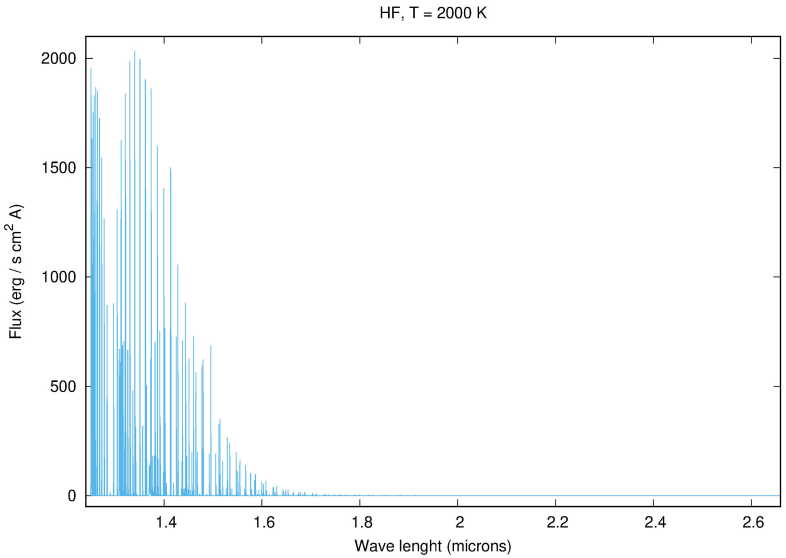
1457 transitions, (1.25 - 2.66 μ).

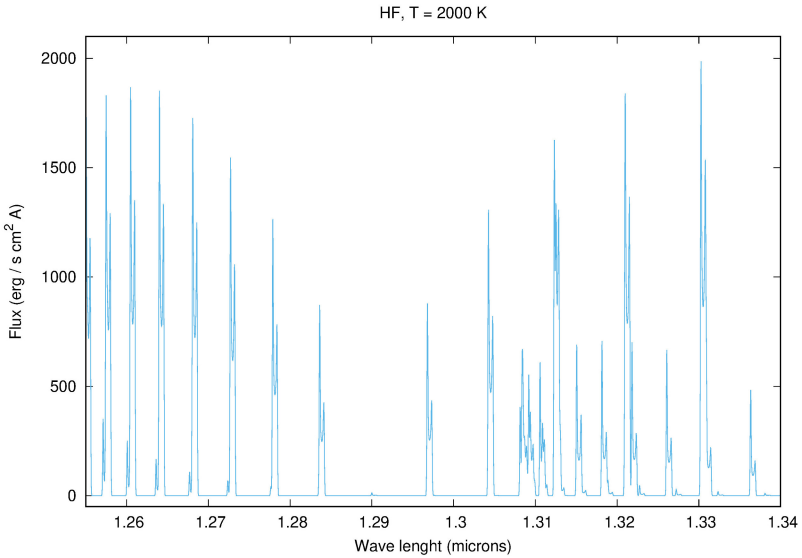
468 energy levels.

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

$^{1}H^{19}F$.







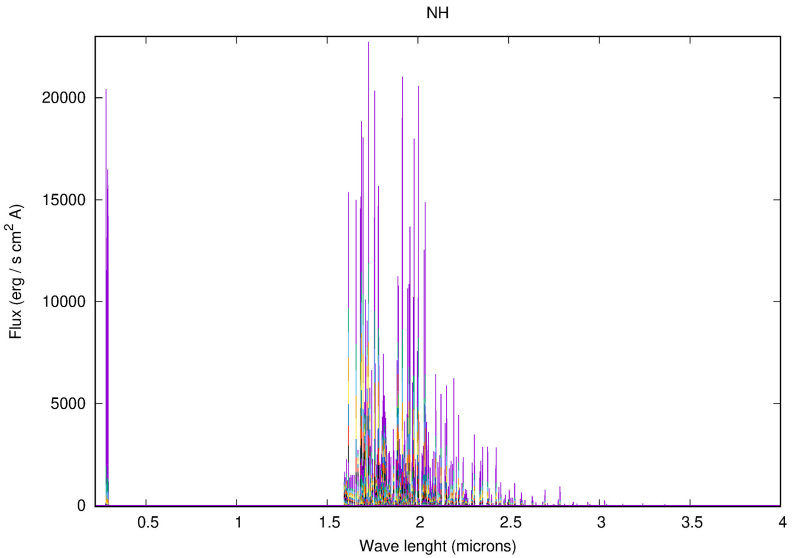
Nitrogen hydride (NH).

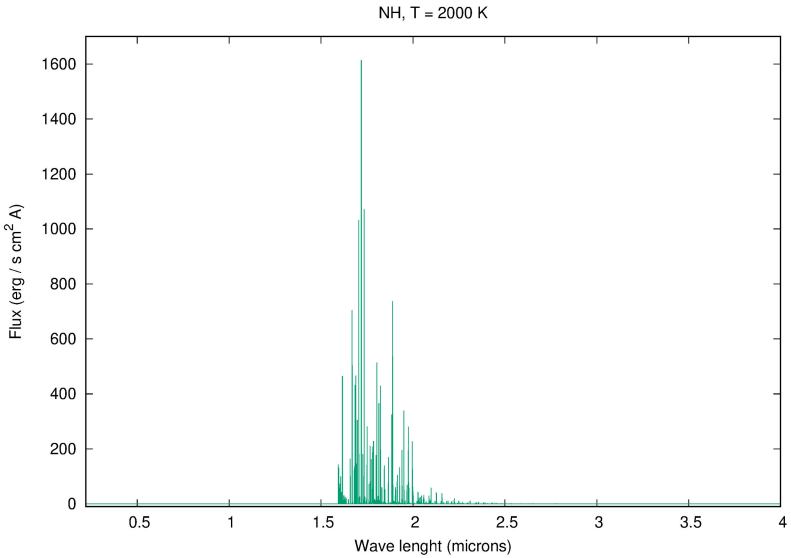
7561 transitions, (1.57 - 2.90 μ).

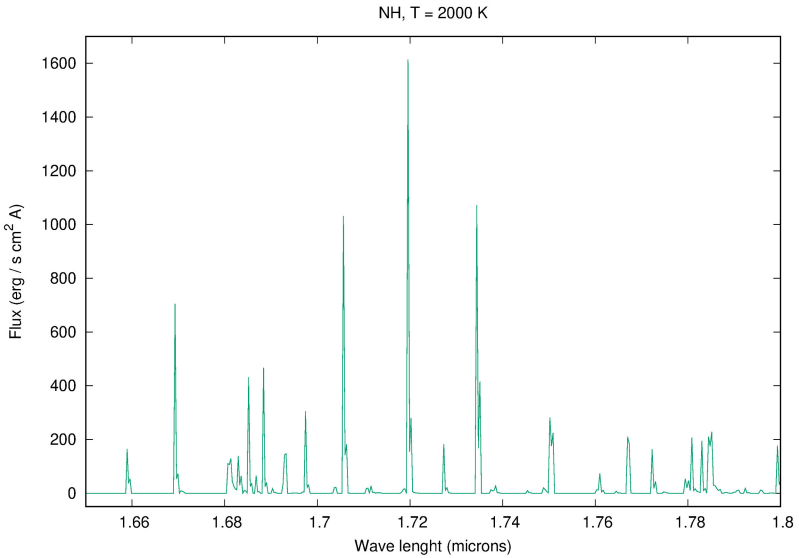
1285 energy levels.

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

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







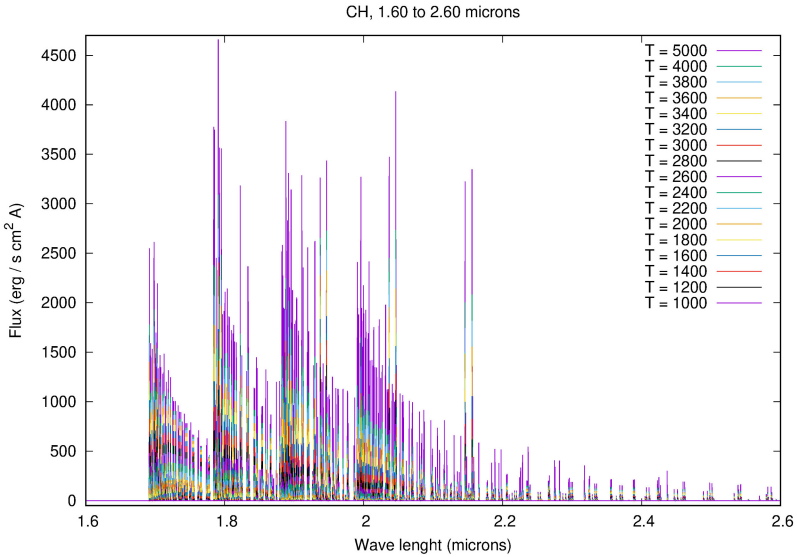
Carbon hydride (CH).

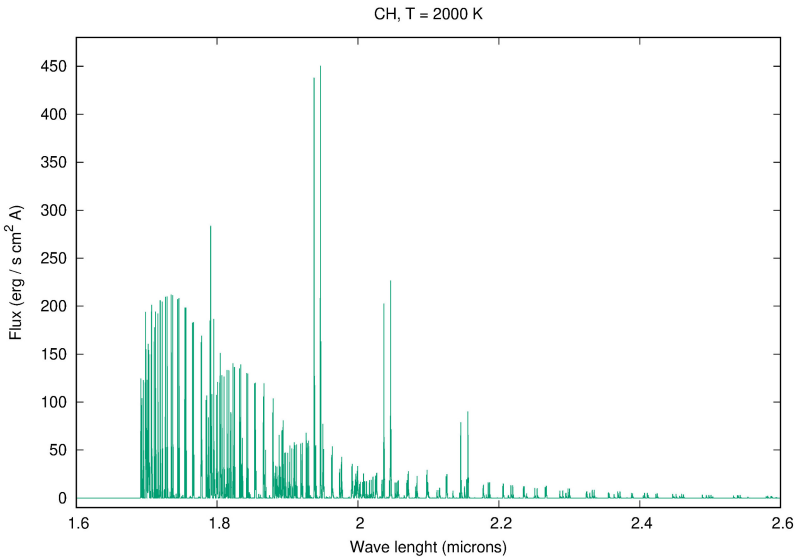
20080 transitions, (1.60 - 2.60 μ).

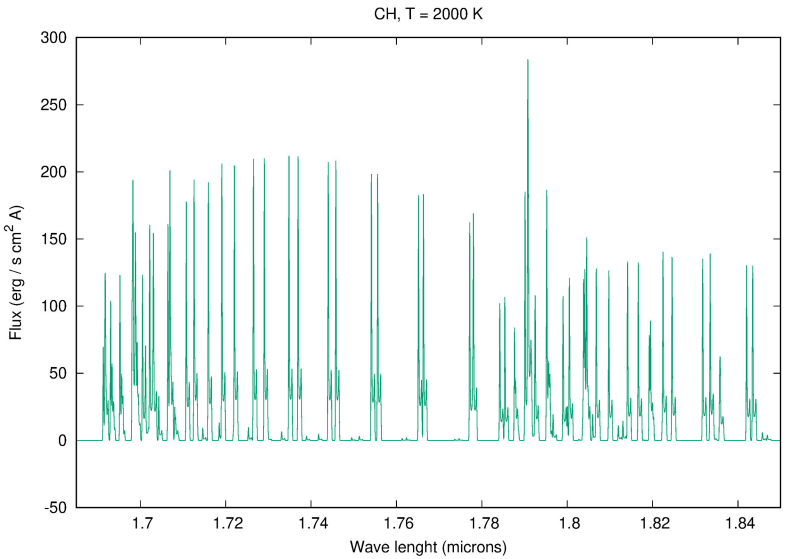
1596 energy levels.

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

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







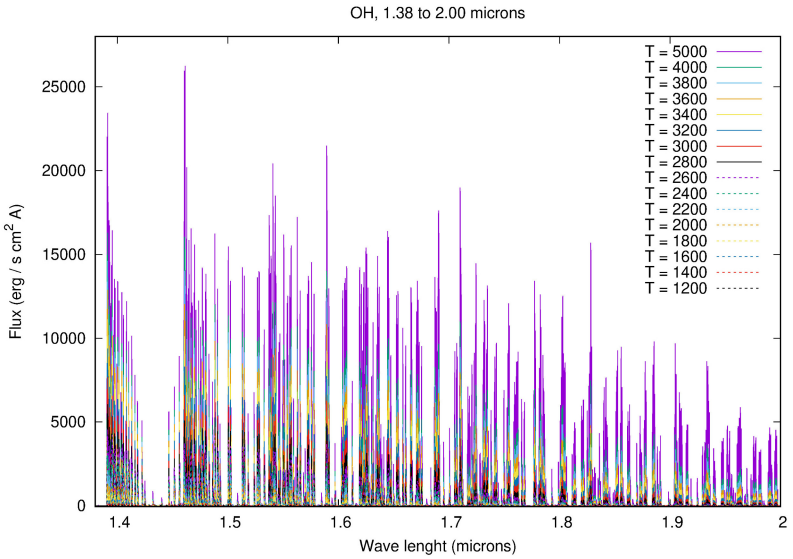
Hydroxyl (OH).

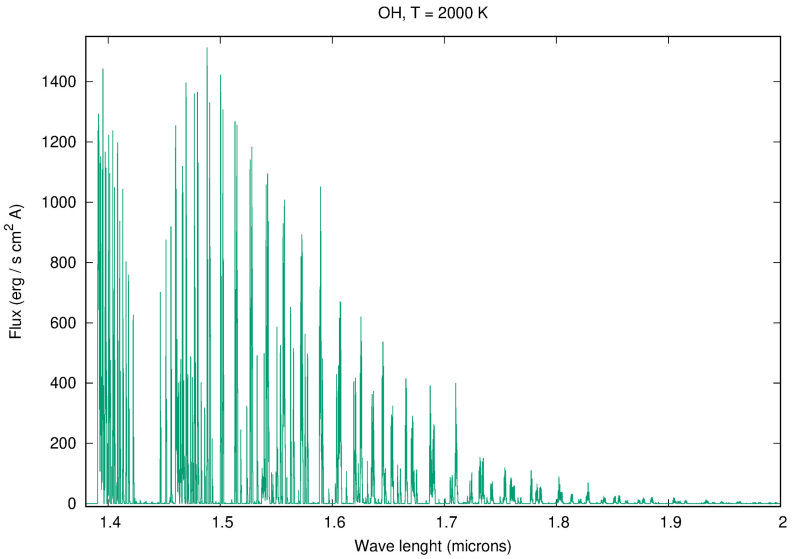
12306 transitions, (1.38 - 2.00 μ).

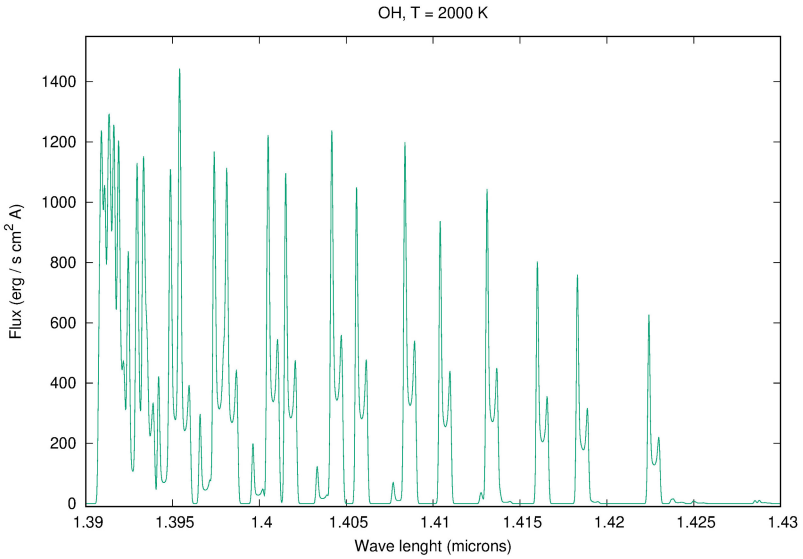
1878 energy levels.

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

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







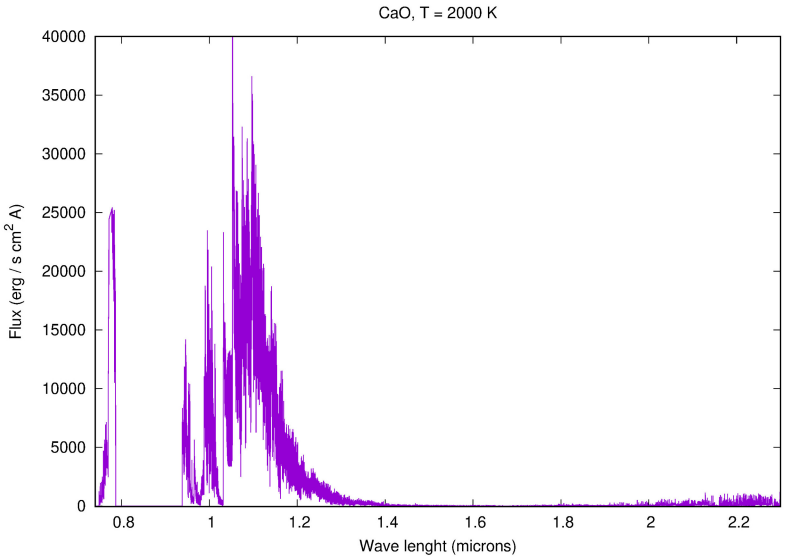
Calcium monoxide (CaO).

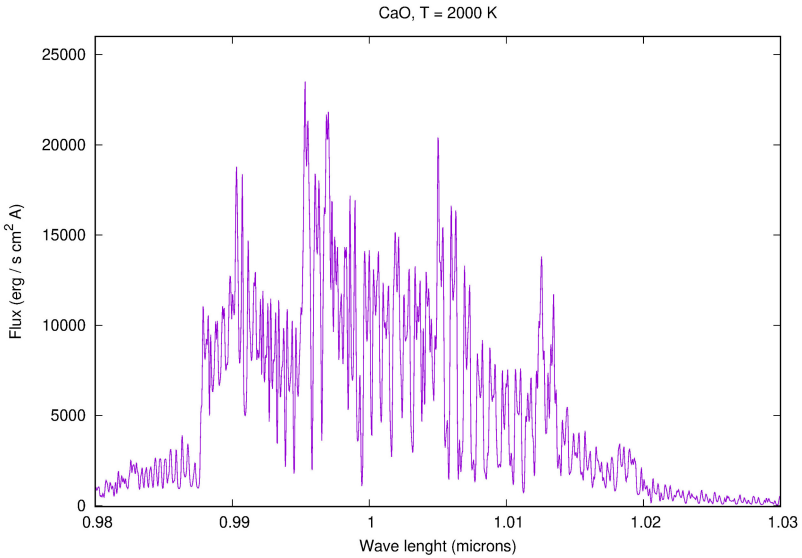
453331 transitions, (0.74 - 2.30 μ).

19113 energy levels.

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

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





Iron hydride (FeH).

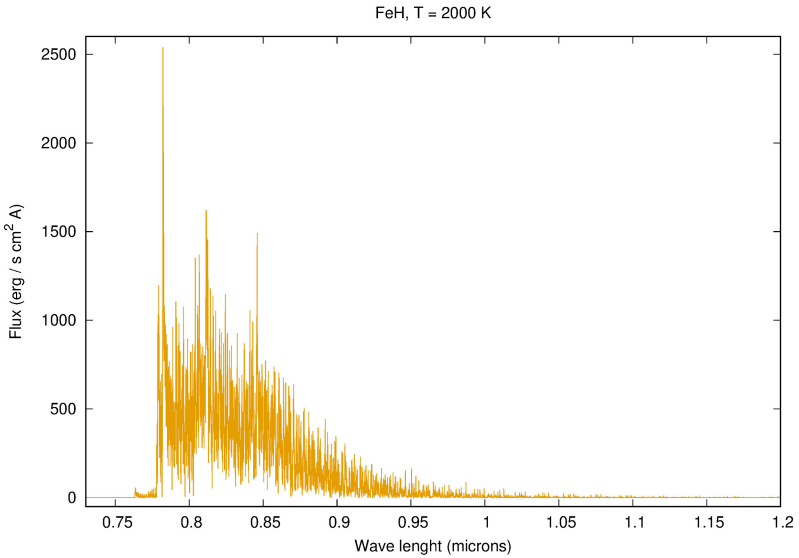
45232 transitions, (0.73 - 1.20 μ).

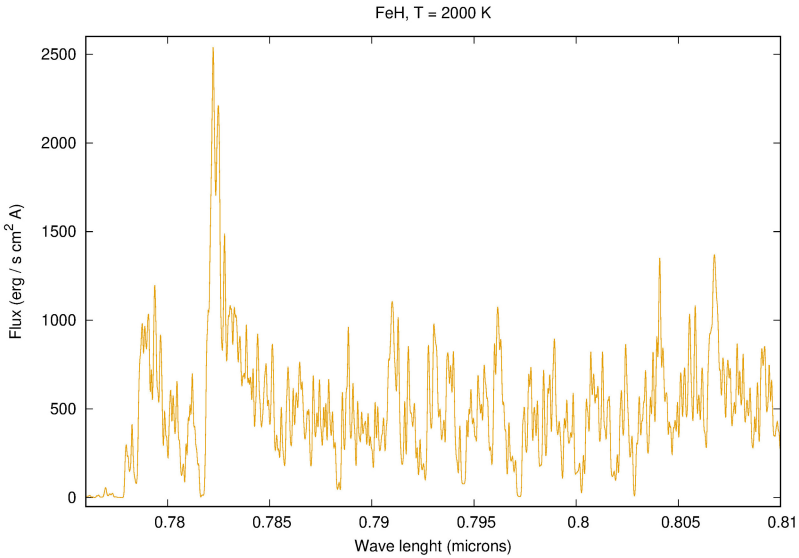
3960 energy levels.

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

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

Column density = 10^{17} cm^{-2}





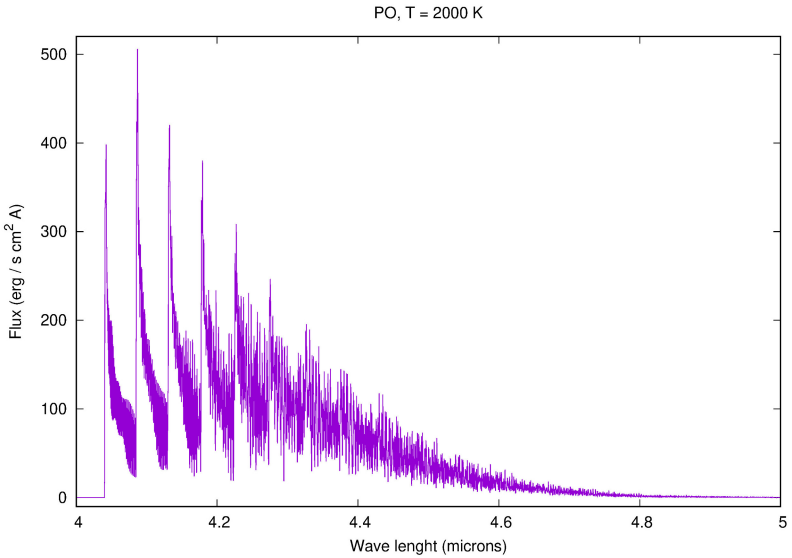
Phosphorus monoxide (PO).

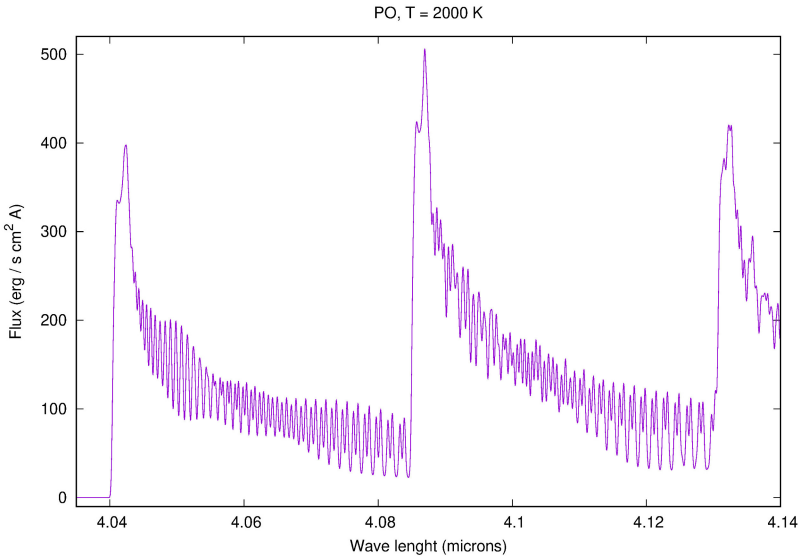
79353 transitions, (4.00 - 5.00 μ), (7.60 - 8.60 μ).

11278 energy levels.

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

$^{31}P^{16}O$.





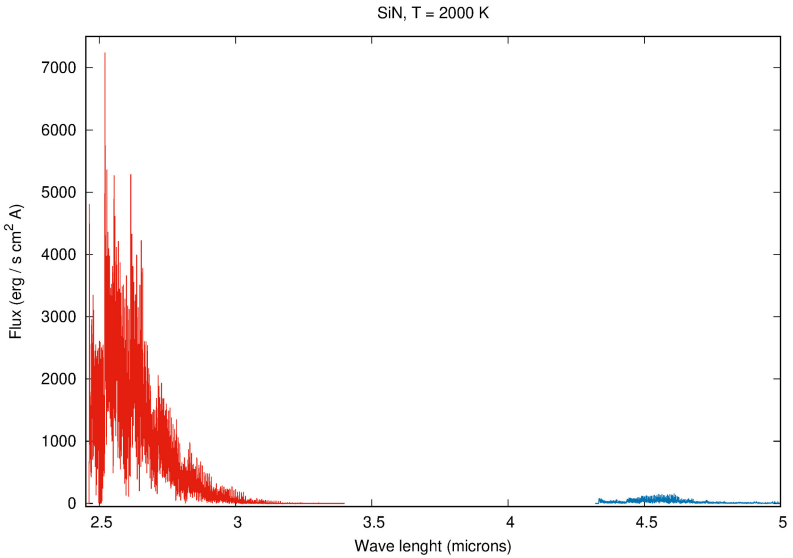
Silicon nitride (SiN).

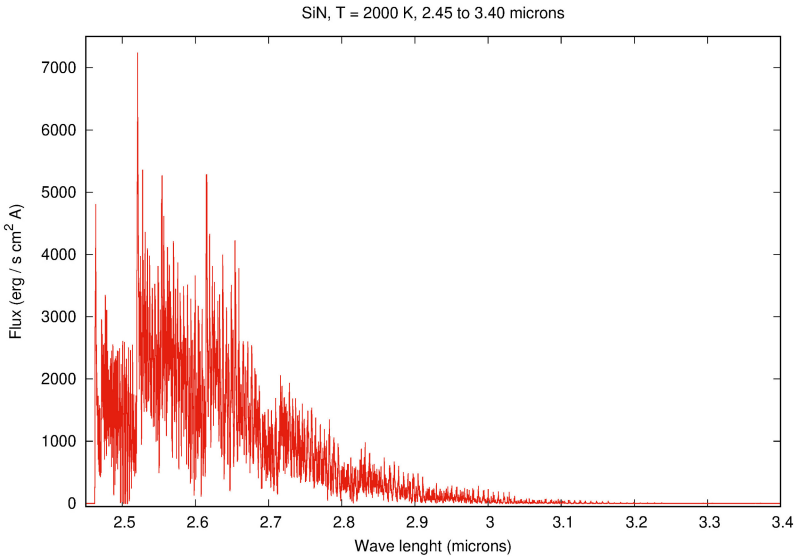
1051315 transitions, (2.45 - 3.40 μ), (4.32 - 5.00 μ).

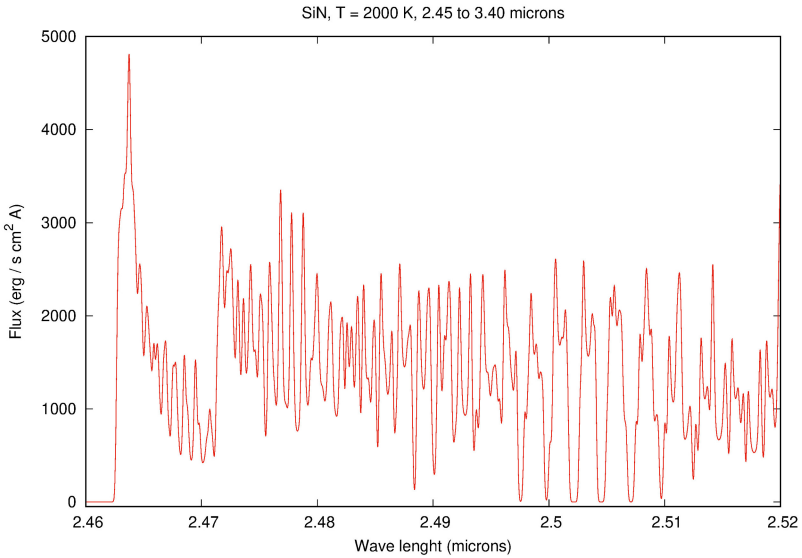
24764 energy levels.

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

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







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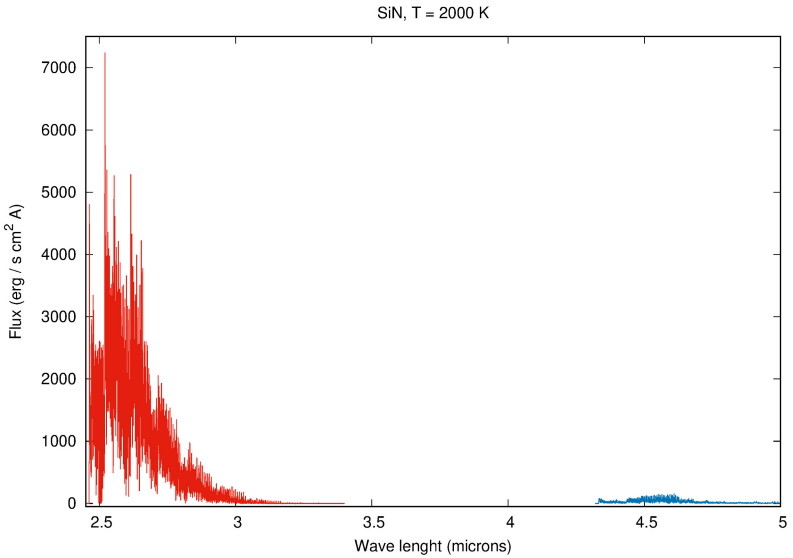
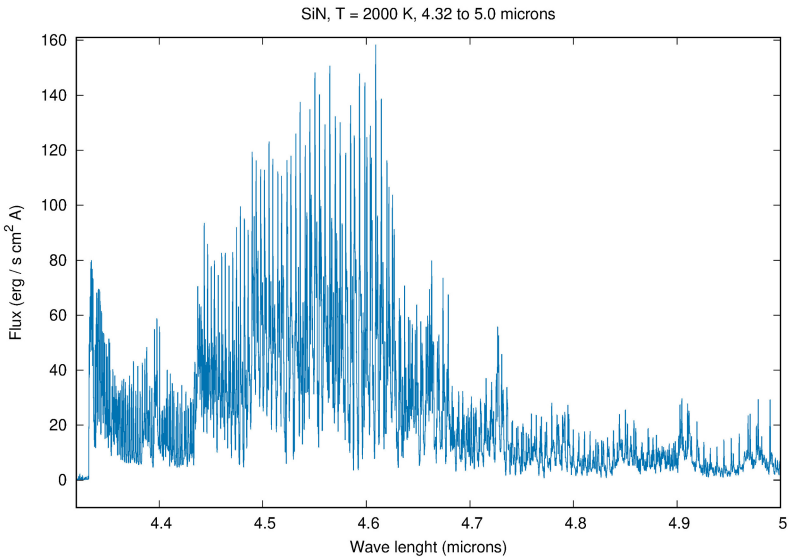
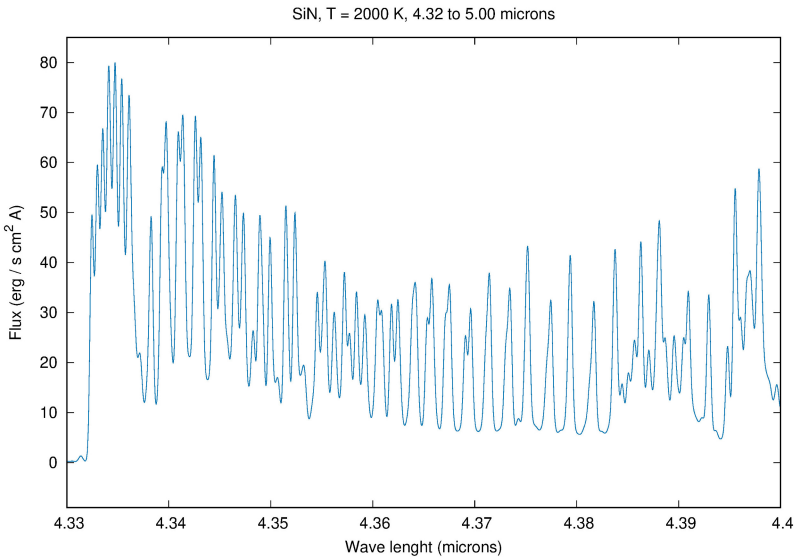
24764 energy levels.

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

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







Molecular carbon (C_2).

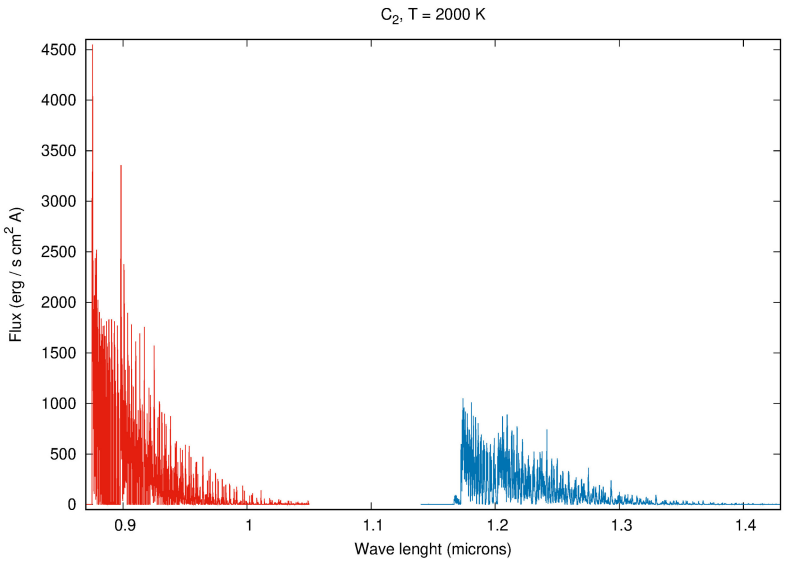
429843 transitions, (0.87 - 1.05 μ), (1.14 - 1.43 μ).

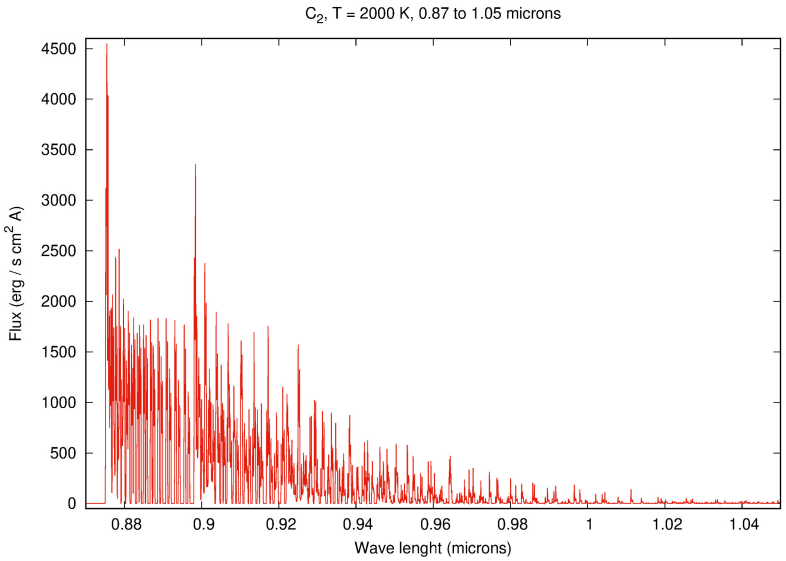
31353 energy levels.

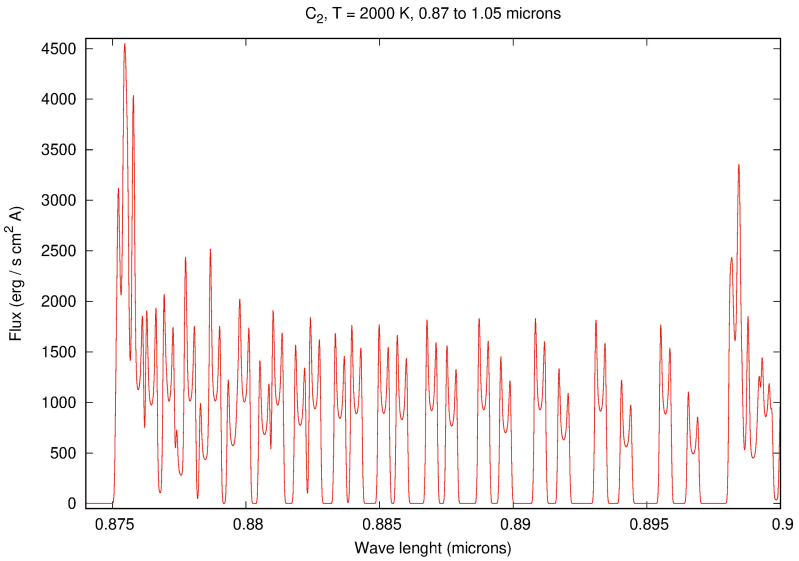
$v_{max} = 20$, $J_{max} = 140$.

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

Column density = 10^{17} cm^{-2}







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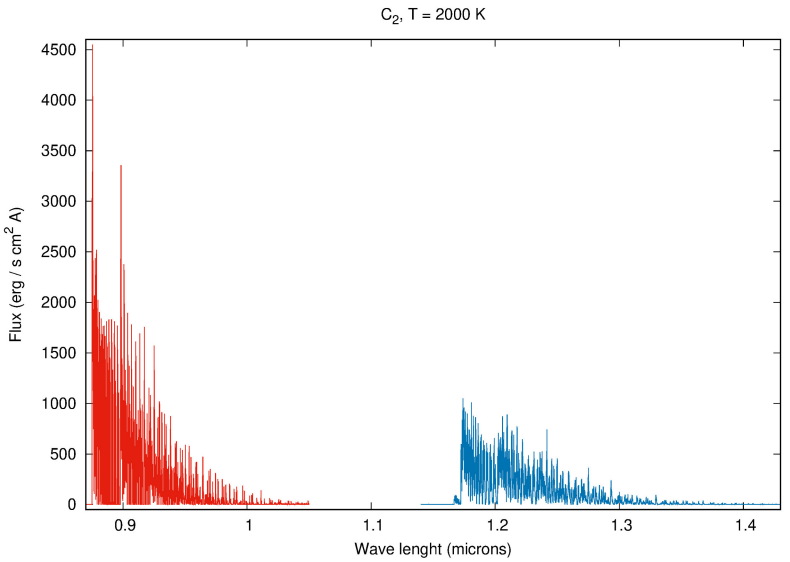
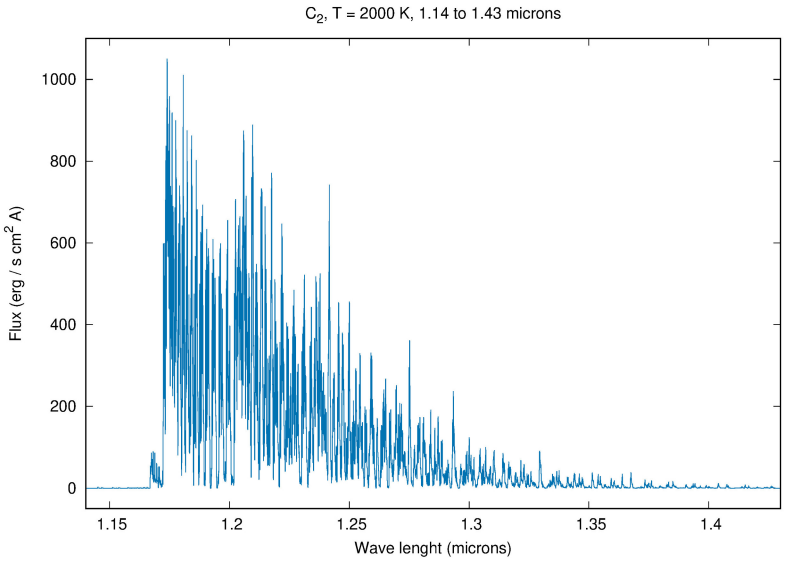
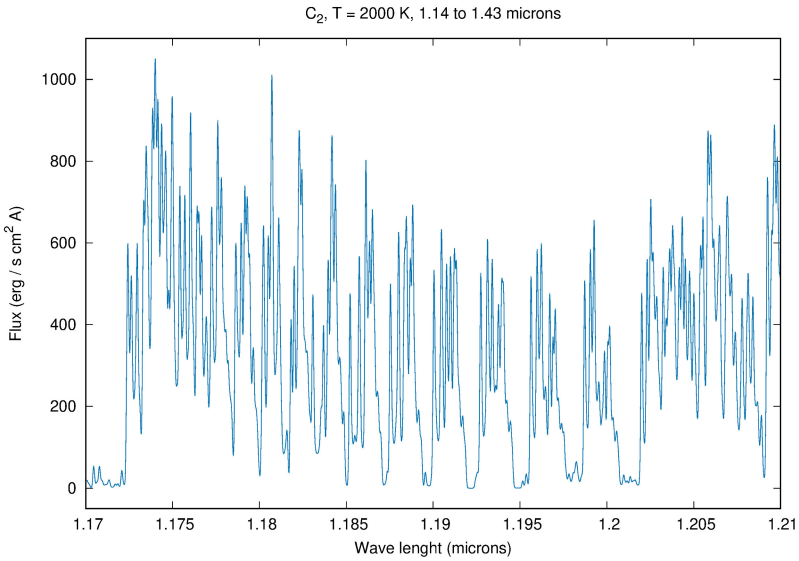
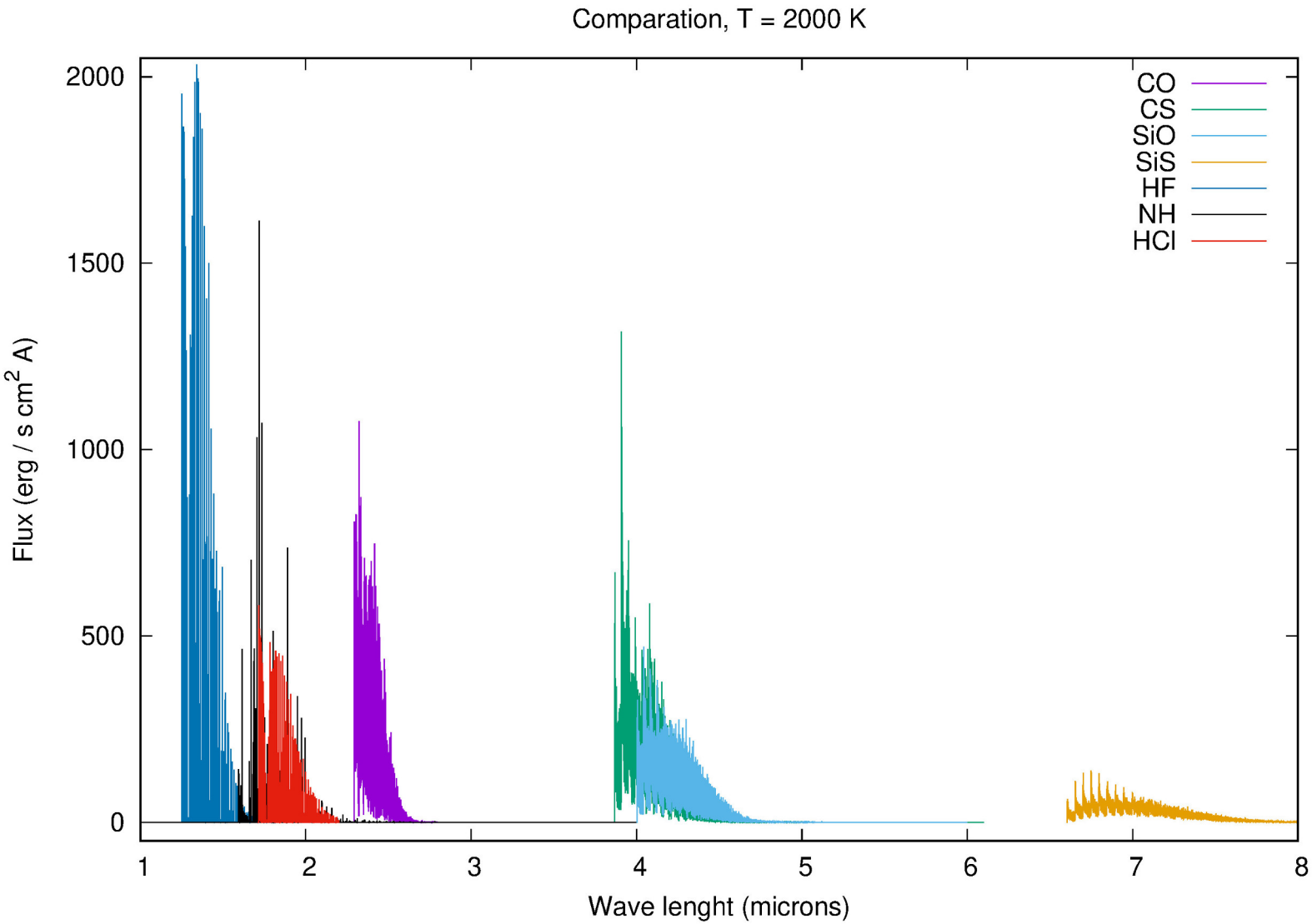
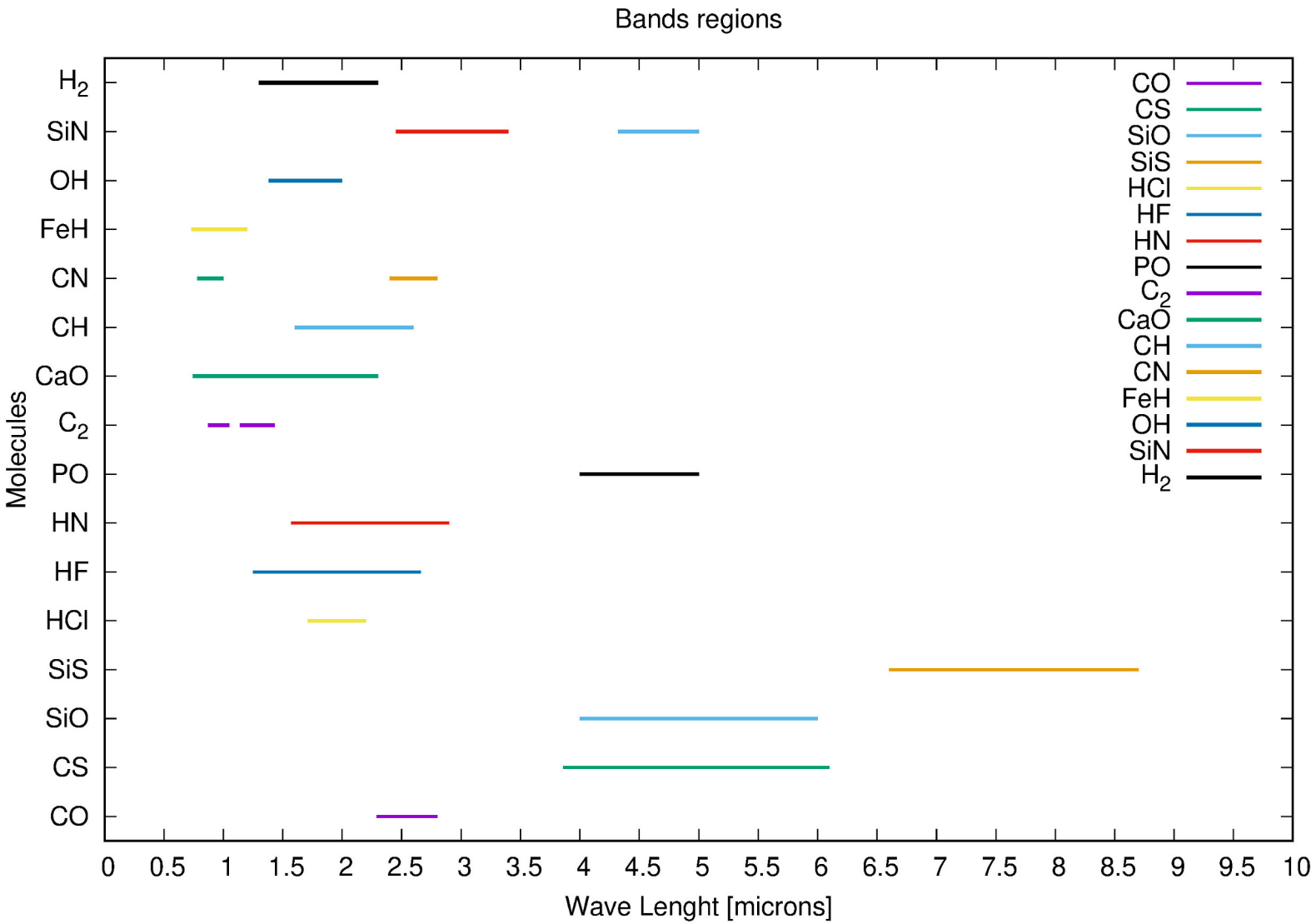
Column density = 10^{17} cm^{-2}








Comparation, T = 2000 K
Flux (erg / s cm^2 A)
Wave lenght (microns)
CO
CS
SiO
SiS
HF
NH
HCl
2000
1500
1000
500
0
1
2
3
4
5
6
7
8


Bands regions
Molecules
H2
SiN
OH
FeH
CN
CH
CaO
C2
PO
HN
HF
HCl
SiS
SiO
CS
CO
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
6
6.5
7
7.5
8
8.5
9
9.5
10
Wave Lenght [microns]
CO
CS
SiO
SiS
HCl
HF
HN
PO
C2
CaO
CH
CN
FeH
OH
SiN
H2

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_2	N_2
AlH	TiO	CP	SiN
CrH	NaO	PS	LiH^+
CaH	LaO	NS	H2+
BeH	ZrO	NaF	HeH^+
TiH	O_2	AlCl	OH^+

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.

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Muchas gracias

Thank you very much

Děkuji moc