

# User wishes to VAMDC

**Volker Ossenkopf**

**I. Physikalisches Institut, Universität zu Köln**



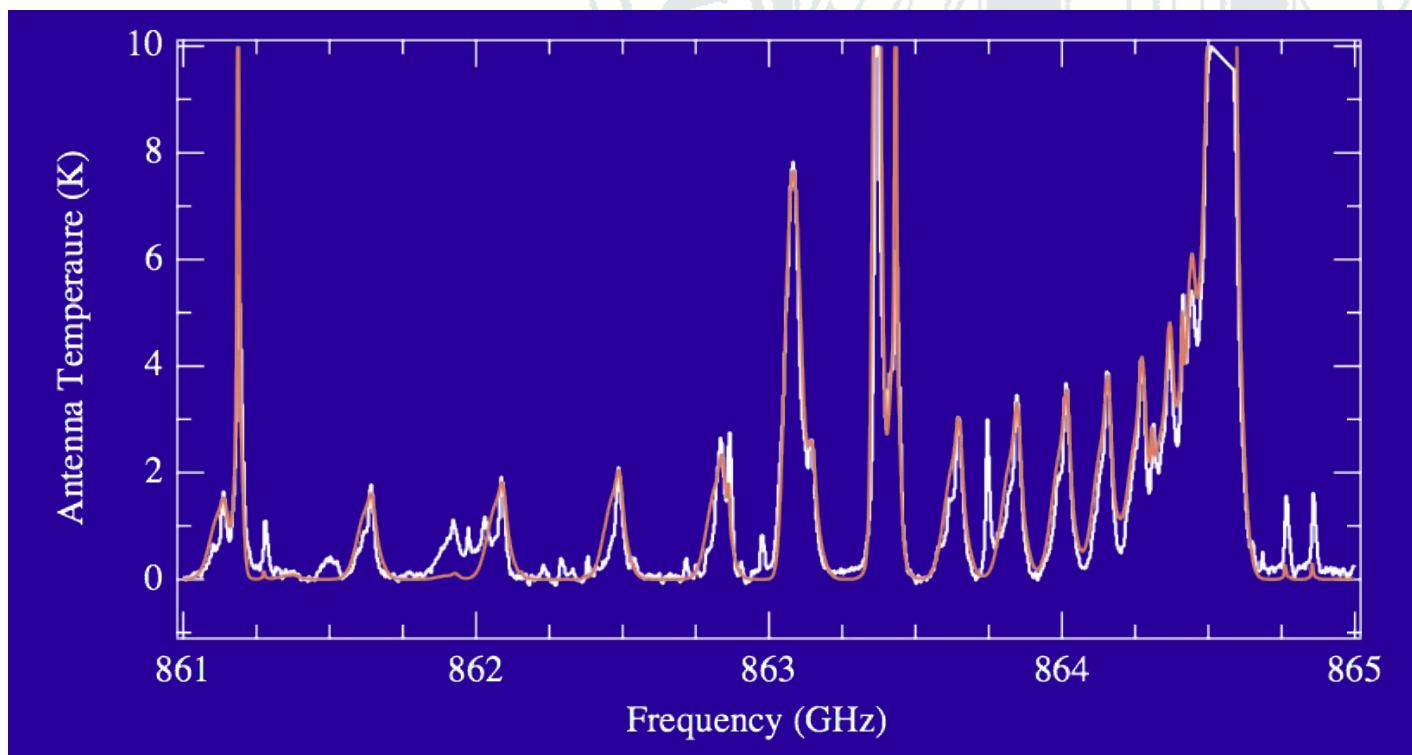
- **Line identification**
- **Radiative transfer**
- **Chemical networks**
- **Summary: clients count**



# Line identification

## Typical usage:

- ◆ Get line identification file
  - Start from CDMS files or splatalogue to have most complete data set
  - Use built-in catalogues: XCLASS, CASSIS, ...
- ◆ Combined identification and LTE fit of multiple transitions



Lines of  $\text{CH}_3\text{OH}$  and  $\text{SO}_2$  in Orion KL spectrum (Crocket & Bergin 2011)

# Line identification

## Typical questions/problems:

- ◆ Which of the catalogues should I trust?
- ◆ How do I have to read the error bars and how can I exploit the information from multiple lines?
  - If transition A of a molecule fits within 0.1MHz but transition B deviates by 2.0MHz (within the error bars) does this still provide a reliable identification?
  - How far can the LTE line intensity fit deviate between two lines for reasonable parameters to still provide a reliable identification?
- ◆ How can I extrapolate frequencies not covered in current catalogue file?
- ◆ Minor annoyance:
  - Statistical weights or  $f$  ground states not directly contained in CDMS files

## Requirements to VAMDC:

- ◆ **Give me everything!** → Easy access to latest “valid” entries for all documented species
  - Continued quality management
- ◆ Characterize mutual dependence of uncertainties covering multiple transitions
- ◆ Extrapolation rules

# Radiative transfer computations – collision rates

LAMDA data base is most used reference:

- ❖ Covers only few species
- ❖ Often not up-to-date

Atomic datafiles		
C	C <sup>+</sup>	O
Molecular datafiles		
CO	CS	HCl
OCS	SO	SO <sub>2</sub>
SiO	SiS	SiC <sub>2</sub>
HCO <sup>+</sup>	N <sub>2</sub> H <sup>+</sup>	HCS <sup>+</sup>
HC <sub>3</sub> N	HCN	HNC
C <sub>3</sub> H <sub>2</sub>	H <sub>2</sub> O	H <sub>2</sub> CO
OH	CH <sub>3</sub> OH	NH <sub>3</sub>
HDO	H <sub>3</sub> O <sup>+</sup>	HNCO
NO	CN	CH <sub>3</sub> CN
O <sub>2</sub>	HF	
Radiative transfer		
RADEX Benchmarking		
Development		
Update history		
Future updates		

## LAMDA

### Leiden Atomic and Molecular Database

[Atomic datafiles](#) | [Molecular datafiles](#) | [Data format](#) | [RADEX](#)

The aim of this project is to provide users of radiative transfer codes with the basic atomic and molecular data needed for the excitation calculation. Line data of a number of astrophysically interesting species are summarized, including energy levels, statistical weights, Einstein A-coefficients and collisional rate coefficients. Available collisional data from quantum chemical calculations and experiments are in some cases extrapolated to higher energies.

Currently the database contains atomic data for 3 species and molecular data for 29 different species. In addition, several isotopomers and deuterated versions are available. Work is currently underway to add more datafiles. We encourage comments from the users in order to improve and extend the database.

This database should form an important tool in analyzing observations from current and future infrared and (sub)millimetre telescopes. Databases such as these rely heavily on the efforts by the chemical physics community to provide the relevant atomic and molecular data. We strongly encourage further efforts in this direction, so that the current extrapolations of collisional rate coefficients can be replaced by actual calculations in future releases.

RADEX, a computer program for performing statistical equilibrium calculations is made publically available as part of the data base.

**NEWS (17 June 2011): Updated datafile for atomic oxygen.**

If you use the data files in your work please refer to the [publication](#) by **Schöier, F.L., van der Tak, F.F.S., van Dishoeck E.F., Black, J.H. 2005, A&A 432, 369-379** introducing this data base. When individual molecules are considered, references to the original papers providing the spectroscopic and collisional data are encouraged.

This website is dedicated to Fredrik Schöier, who initiated this database. Unfortunately, Fredrik passed away on 14 January 2011, at the age of 41. We remember Fredrik as a dedicated and inspiring scientist. See also [this obituary](#).

*Floris van der Tak, Ewine van Dishoeck, John Black*

*This research is supported by the Netherlands Organization for Scientific Research (NWO), the Netherlands Research School for Astronomy (NOVA) and the Swedish Research Council.*

Last update on 06/20/2011 11:08:05. Send comments to [moldata@strw.leidenuniv.nl](mailto:moldata@strw.leidenuniv.nl)



# Example: LAMDA

LAMDA files can be read  
by most RT codes

- ◆ Mixes general molecule description with spectroscopy data and collision rates
- ◆ Unusable for line identification

## Example molecular data file: HCO<sup>+</sup>

```
!MOLECULE HCO+
!MOLECULAR WEIGHT
29.0
!NUMBER OF ENERGY LEVELS
21
!LEVEL + ENERGIES(cm-1) + WEIGHT + J
1 0.000000000 1.0 0
2 2.975008479 3.0 1
(etc)
21 624.269300464 41.0 20
!NUMBER OF RADIATIVE TRANSITIONS
20
!TRANS + UP + LOW + EINSTEIN(A s-1) + FREQ(GHz)
1 2 1 4.251e-05 89.18839570
2 3 2 4.081e-04 178.37481404
(etc)
20 21 20 4.955e-01 1781.13802857
!NUMBER OF COLL PARTNERS
1
!COLLISIONS BETWEEN
1 H2-HCO+ from Flower (1999)
!NUMBER OF COLL TRANS
210
!NUMBER OF COLL TEMPS
12
!COLL TEMPS
10.0 20.0 30.0 50.0 70.0 100.0 150.0 200.0 250.0 300.0 350.0 400.0
!TRANS + UP + LOW + COLL RATES(cm3 s-1)
1 2 1 2.6e-10 2.3e-10 2.1e-10 2.0e-10 1.9e-10 1.8e-10 2.0e-10 2.2e-10 2.3e-10 2.5e-10 2.7e-10 2.8e-10
2 3 1 1.4e-10 1.2e-10 1.1e-10 1.0e-10 9.2e-11 8.8e-11 8.4e-11 8.2e-11 8.1e-11 8.3e-11 8.1e-11 8.5e-11
(etc)
210 21 20 3.7e-10 3.6e-10 3.6e-10 3.5e-10 3.5e-10 3.5e-10 3.8e-10 4.0e-10 4.4e-10 4.7e-10 5.0e-10 5.2e-10
```





# Radiative transfer computations – collision rates

## Typical questions/problems:

- ◆ How do I extrapolate existing rates to higher levels?
- ◆ How do I scale collision rates for collisions with He to those for H<sub>2</sub>?
- ◆ How do I scale collision rates for a similar molecule to my molecule of interest?

- Example solution:  
**Neural network extrapolation**  
(Neufeld 2010, ApJ 708, 635)

## Requirements to VAMDC:

- ◆ Easy selection of collision partners:  
H, para-H<sub>2</sub>, ortho-H<sub>2</sub>, He, e<sup>-</sup>
  - Combination and common range of conditions
- ◆ “Invent” non-measured rates

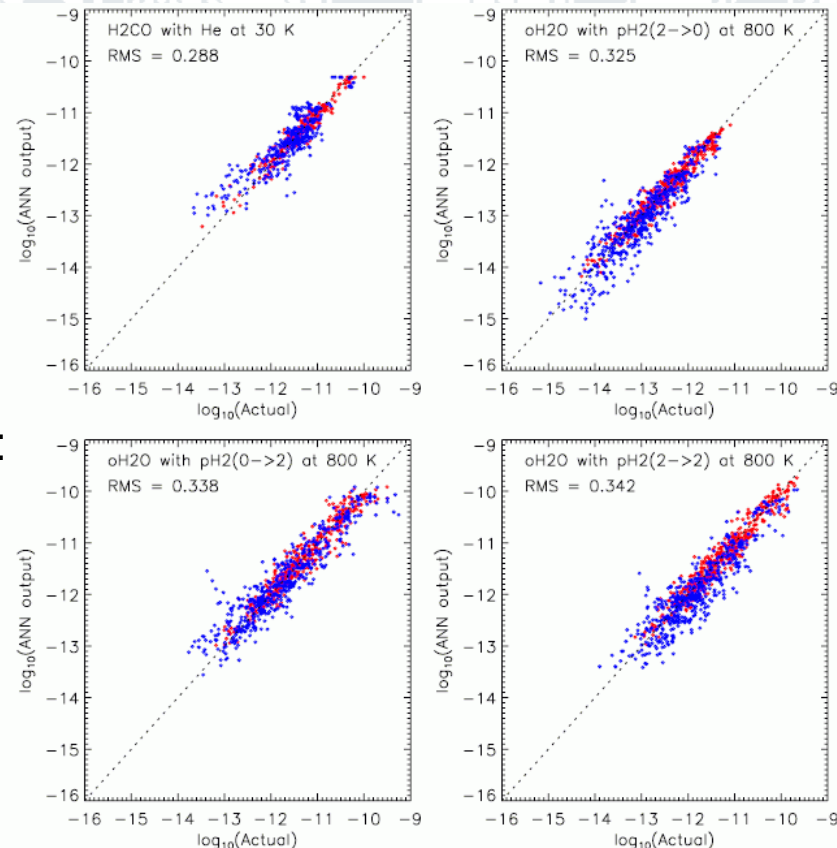


Figure 6. Results obtained for excitation of ortho-H<sub>2</sub>CO (Green 1991) in collisions with He and ortho-H<sub>2</sub>O in collisions with para-H<sub>2</sub> (Dubernet et al. (2009) for cases in which the initial and/or final state of H<sub>2</sub> is  $J = 2$ .

# Chemical models – reaction rates

## Typical use:

- ◆ Parametrization in udfa and Ohio data bases
- ◆ Reliability very opaque

**udfa<sup>6</sup>**   or  or

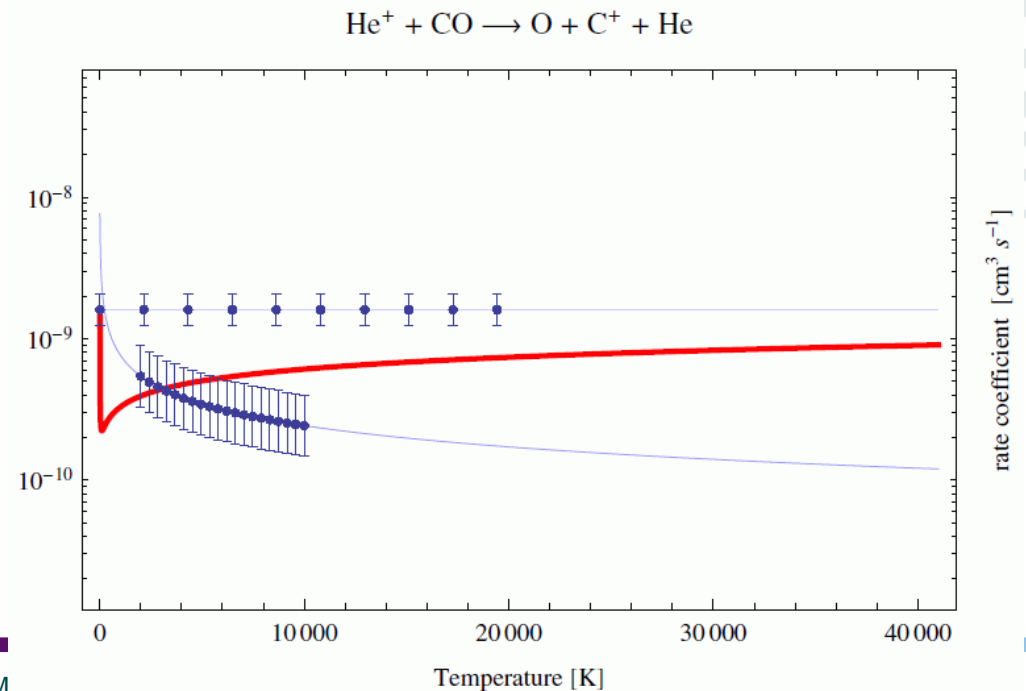
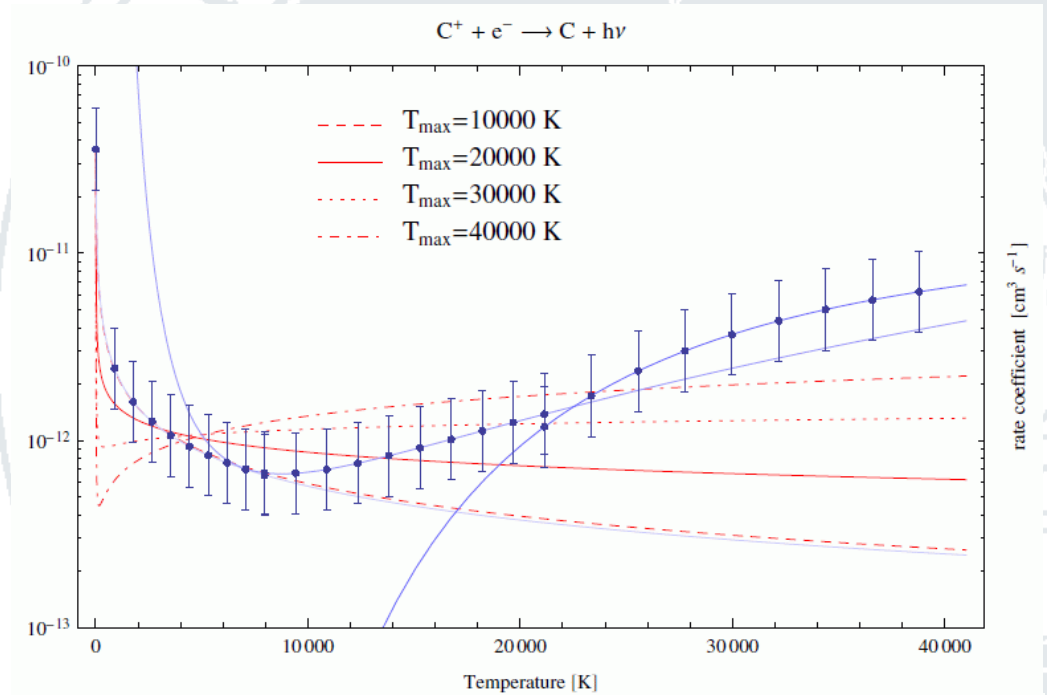
Found 248 'HCO+' reactions, showing 1 - 50 [next 50](#)

	Reaction	$\alpha$	$\beta$	$\gamma$	$T_l - T_u$ (K)	Accuracy	Source
1	$C + H_3O^+ \rightarrow HCO^+ + H_2$	1.00E-11	0.00	0.0	10 - 41000	factor 2	Lit. Search
2	$C + HCO^+ \rightarrow CO + CH^+$	1.10E-09	0.00	0.0	10 - 41000	factor 2	Lit. Search
3	$C^+ + H_2CO \rightarrow HCO^+ + CH$	7.80E-10	0.00 / -0.50	0.0	10 - 41000	within 25%	Measurement
4	$C^+ + H_2O \rightarrow HCO^+ + H$	9.00E-10	0.00 / -0.50	0.0	10 - 41000	within 25%	Measurement
5	$C^+ + HCO \rightarrow HCO^+ + C$	4.80E-10	0.00 / -0.50	0.0	10 - 41000	factor 2	Lit. Search
6	$C_2 + HCO^+ \rightarrow CO + C_2H^+$	8.30E-10	0.00	0.0	10 - 41000	factor 2	Lit. Search
7	$C_2^+ + HCO \rightarrow HCO^+ + C_2$	3.80E-10	0.00 / -0.50	0.0	10 - 41000	factor 2	Lit. Search
8	$C_2H + CO^+ \rightarrow HCO^+ + C_2$	3.90E-10	0.00	0.0	10 - 41000	factor 2	Lit. Search
9	$C_2H + HCO^+ \rightarrow CO + C_2H_2^+$	7.80E-10	0.00	0.0	10 - 41000	factor 2	Lit. Search
10	$C_2H_2 + HCO^+ \rightarrow CO + C_2H_3^+$	1.40E-09	0.00	0.0	10 - 41000	within 25%	Measurement
11	$C_2H_2 + O_2^+ \rightarrow HCO^+ + H + CO$	6.50E-11	0.00	0.0	10 - 41000	within 50%	Measurement
12	$C_2H_2^+ + HCO \rightarrow HCO^+ + C_2H_2$	5.00E-10	0.00 / -0.50	0.0	10 - 41000	factor 2	Lit. Search
13	$C_2H_3 + HCO^+ \rightarrow C_2H_4^+ + CO$	1.40E-09	0.00 / -0.50	0.0	10 - 41000	factor 2	Lit. Search
14	$C_2H_4 + HCO^+ \rightarrow C_2H_5^+ + CO$	1.40E-09	0.00	0.0	10 - 41000	factor 2	Lit. Search
15	$CH + CO^+ \rightarrow HCO^+ + C$	3.20E-10	0.00 / -0.50	0.0	10 - 41000	factor 2	Lit. Search
16	$CH + HCO^+ \rightarrow CO + CH_2^+$	6.30E-10	0.00 / -0.50	0.0	10 - 41000	factor 2	Lit. Search
17	$CH + O \rightarrow HCO^+ + e^-$	2.00E-11	0.44	0.0	10 - 1750	within 50%	Calculation
18	$CH + O_2^+ \rightarrow HCO^+ + O$	3.10E-10	0.00 / -0.50	0.0	10 - 41000	factor 2	Lit. Search
19	$CH + SiO^+ \rightarrow HCO^+ + Si$	5.90E-10	0.00 / -0.50	0.0	10 - 41000	factor 2	Lit. Search
20	$CH^+ + CO_2 \rightarrow HCO^+ + CO$	1.60E-09	0.00	0.0	10 - 41000	within 25%	Measurement
21	$CH^+ + H_2CO \rightarrow HCO^+ + CH_2$	9.60E-10	0.00 / -0.50	0.0	10 - 41000	within 25%	Measurement
22	$CH^+ + H_2O \rightarrow HCO^+ + H_2$	2.90E-09	0.00 / -0.50	0.0	10 - 41000	within 25%	Measurement
23	$CH^+ + HCO \rightarrow HCO^+ + CH$	4.60E-10	0.00 / -0.50	0.0	10 - 41000	factor 2	Lit. Search
24	$CH^+ + O_2 \rightarrow HCO^+ + O$	9.70E-10	0.00	0.0	10 - 41000	within 25%	Measurement

# Chemical models – reaction rates

## Typical use:

- ◆ Parametrization in udfa and Ohio data bases
- ◆ Reliability very opaque
- ◆ Arrhenius parametrization often inappropriate
- ◆ Contradicting entries



Röllig (2011)

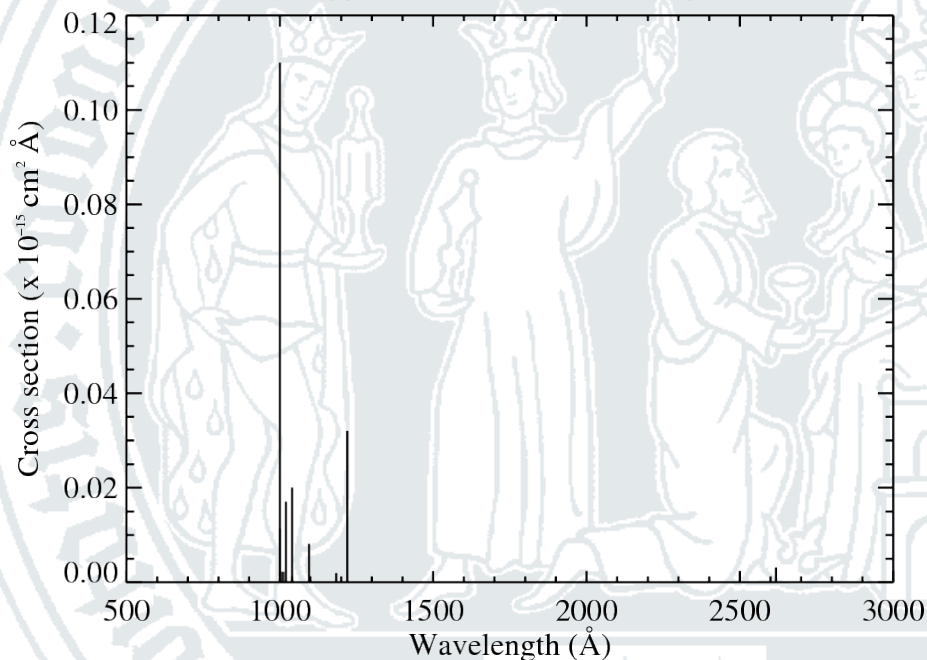


# Chemical models – photo-reactions

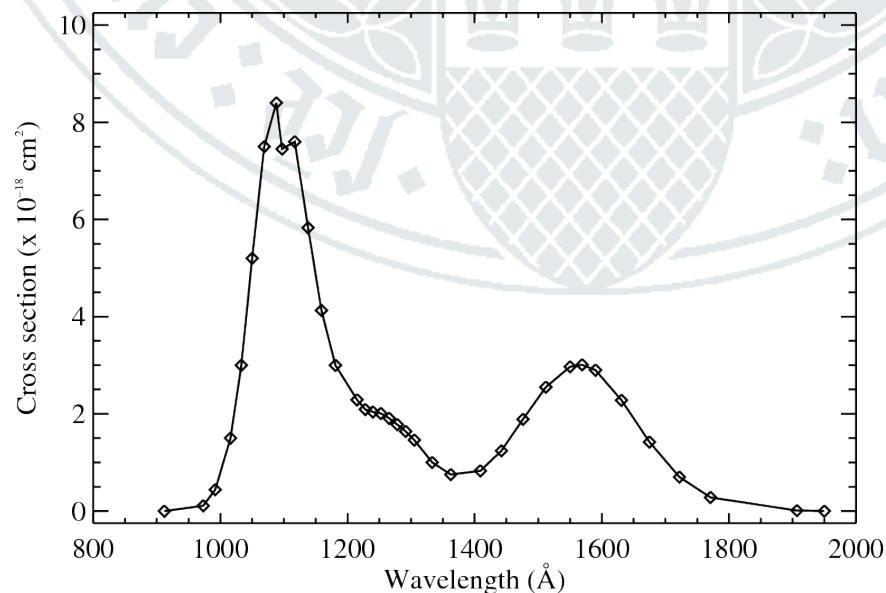
## Typical use:

- ◆ Translation of cross sections to rates for particular spectral shape
- ◆ Original cross sections hardly available
- ◆ Integration bounds often not clear
- ◆ Reaction rates wrong for other spectral shapes!

Photodissociation line channels of OH



Photodissociation continuum data of OH



van Dishoeck et al. (1988)

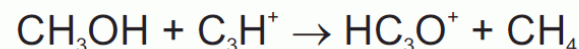
# Chemical models – reaction rates

## Typical questions/problems:

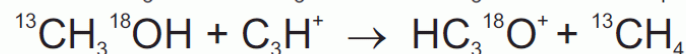
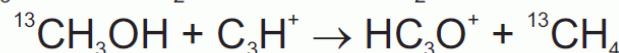
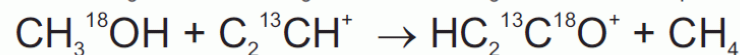
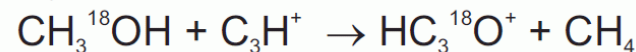
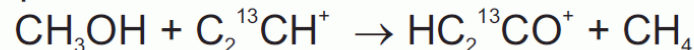
### ◆ How do I expand my network to isotopologues?

- Example:  
(Röllig & Ossenkopf 2010)

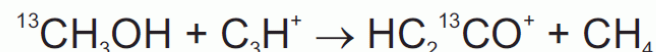
Introducing  $^{13}\text{C}$  and  $^{18}\text{O}$  into the reaction:



gives the possible reactions:



but not the reaction:



because the carbon atom in the methyl group ( $\text{CH}_3$ ) reacts to  $\text{CH}_4$  and must keep its isotopic status.

- ◆ Which reaction dominates the uncertainties in the abundance of a selected species for given conditions?
- ◆ How do I scale my photo-rates under some real physical conditions?

# Summary: What astronomers want of VAMDC

## Can we trust the entries?

- ◆ Provide an easy way to errors, history and mutual dependencies.
  - Continued quality assessment in data base → **throw away outdated entries!**

## We always want more than you can ever provide!

- ◆ **Capability to extrapolate is essential**
  - More transitions, other isotopologues
  - Collision rates for higher levels, other partners, other species
  - On the fly reaction rate prediction (isotopologues, photo-rates, non-Arrhenius, ...)
  - **Error estimates for extrapolation**
- ◆ Extrapolation could be integrated on client side
  - Grey area of where extrapolation “pollutes” the data base

# Summary: What astronomers want of VAMDC

## We do not care about internals:

- ◆ The internal data format is irrelevant, **clients matter!**
  - Allow for easy export to common used file formats
  - **Provide libraries for VAMDC access that can be easily incorporated in user code!**
  - Common routines for online data and offline usage needed
- ◆ Data volume is usually small
  - Local storage often preferred
- ◆ User-acceptance is typically driven by ease-of-use, not quality
  - Clients and user interfaces can be more important than the data base content
  - One shop for everything: Common interface/client for all data types

**VAMDC is a perfect foundation,  
but astronomers want the house.**