# Fine-structure Excitation of Atomic Ions:

*Astrophysical applications, status, and needs*

Phillip C. Stancil

Department of Physics and Astronomy
Center for Simulational Physics
University of Georgia

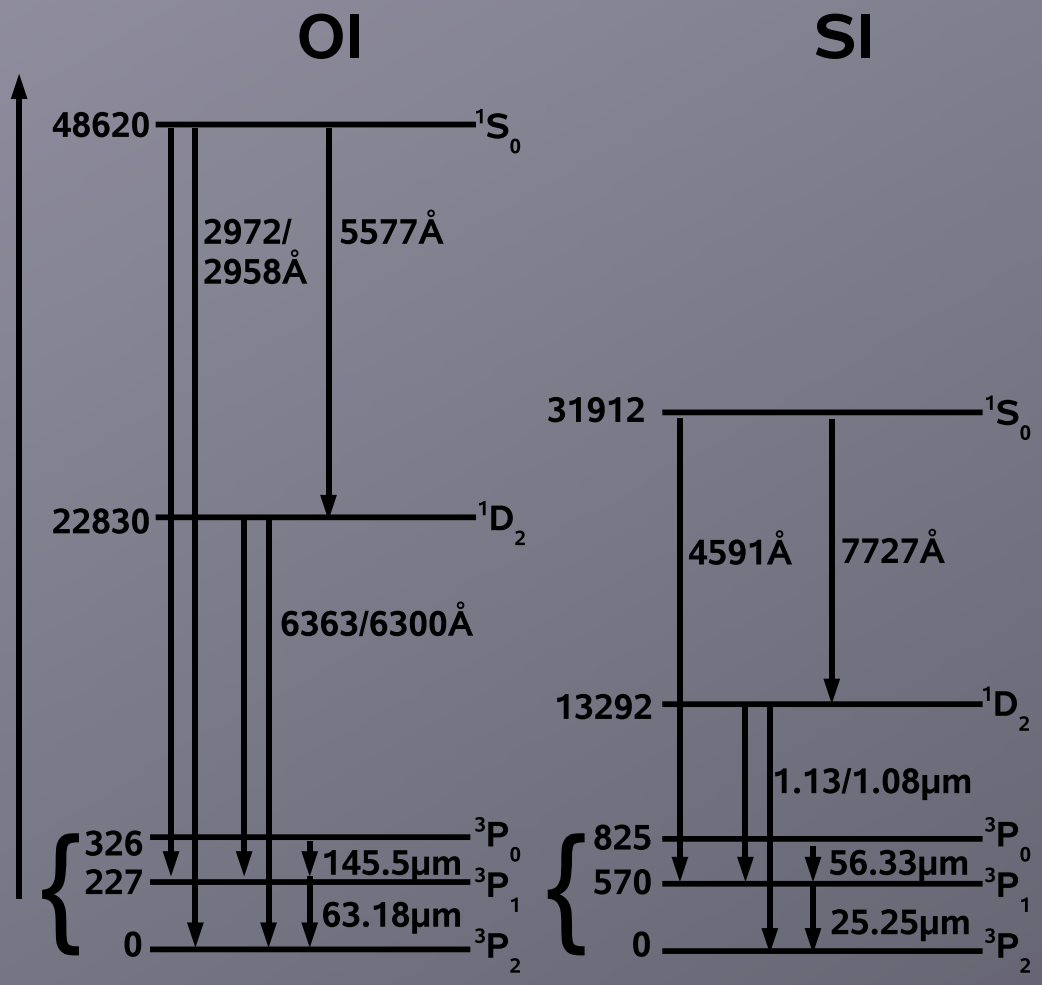
# UGA Theoretical Atomic and Molecular Astrophysics Group

- Charge exchange
- Molecular rovibrational excitation
- Photodissociation
- Radiative association
- Molecular (diatomics) line lists
- Applications: astrophysics, cold collisions, quantum simulation

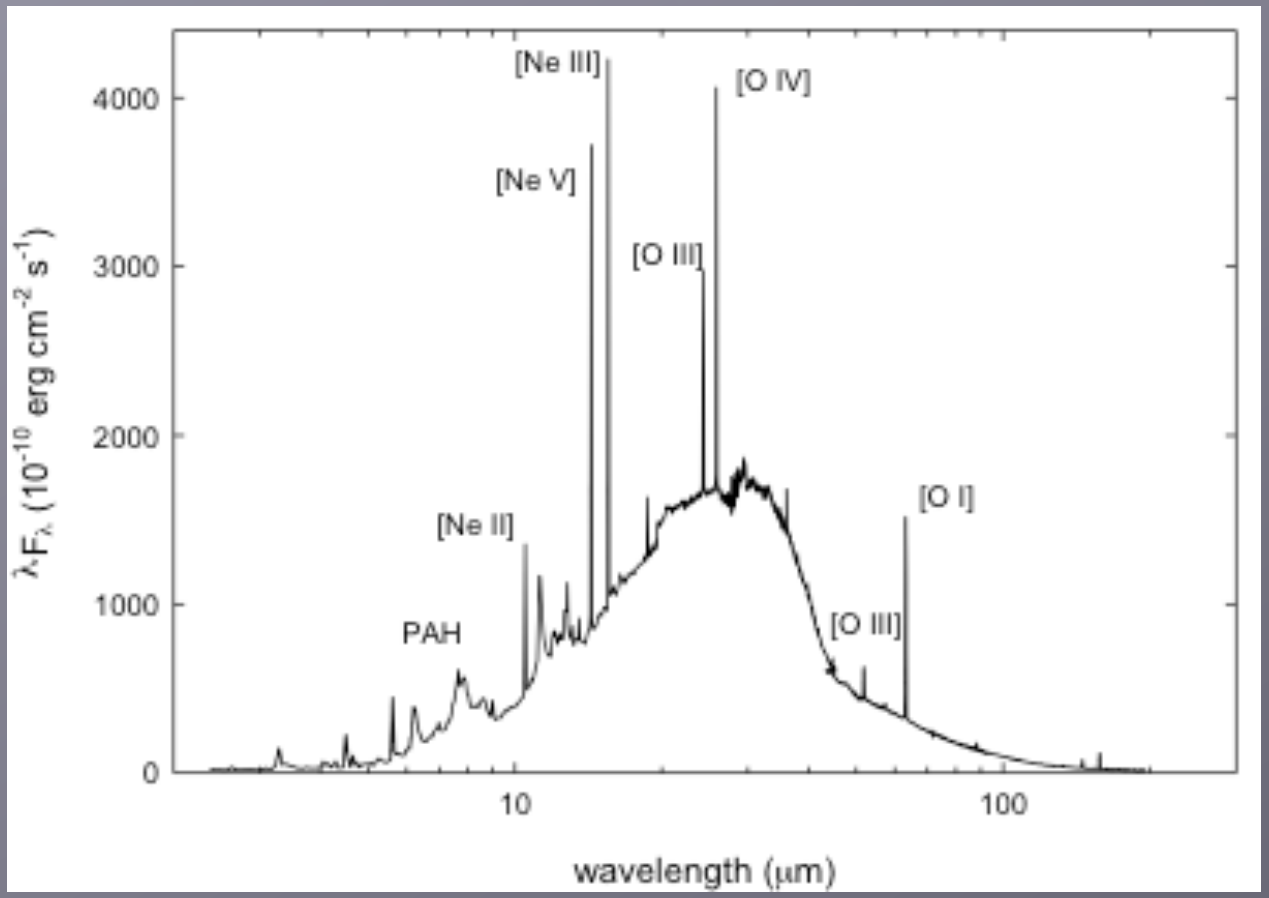
# Fine-Structure Excitation

- Collision of an ion X of charge q (or a neutral) with $e^-$ or heavy particle
$$X(nlLJ) + Y \rightarrow X(nlLJ') + Y$$
- Important in a variety of cool and molecular environments:
  - Level populations (non-LTE emission spectra)
  - Radiative cooling
  - Temperature, density, radiation diagnostics
  - Many lines observable by *Spitzer, SOFIA, Herschel*
- No comprehensive data compilation

# Energy Diagram



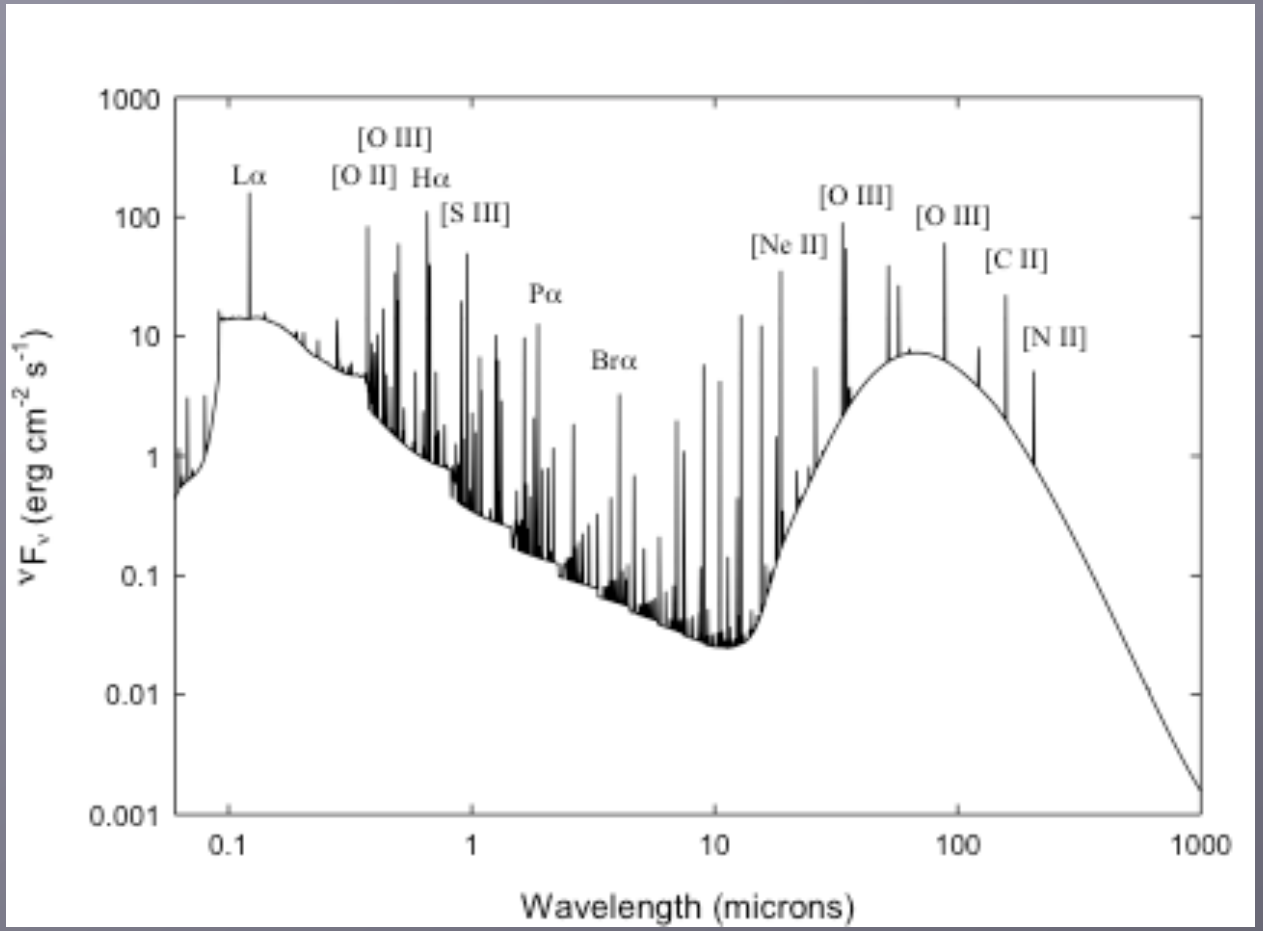
# Example Spectra




- Observed spectra of planetary nebula NGC 7027

Osterbrock & Ferland (2006)

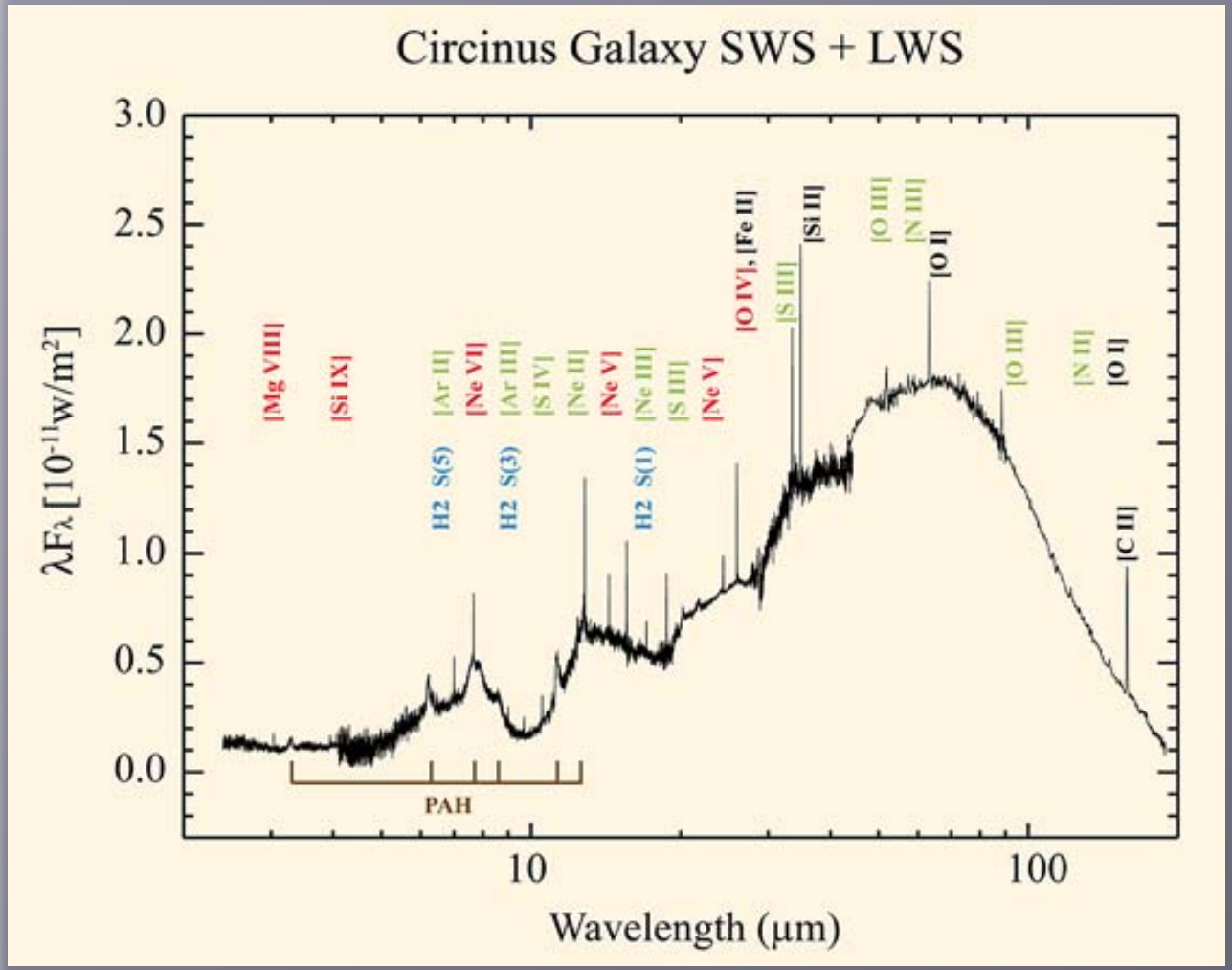
# Example Spectra




- Model spectra of a photo-dissociation region (Orion Nebula)

Osterbrock & Ferland (2006)

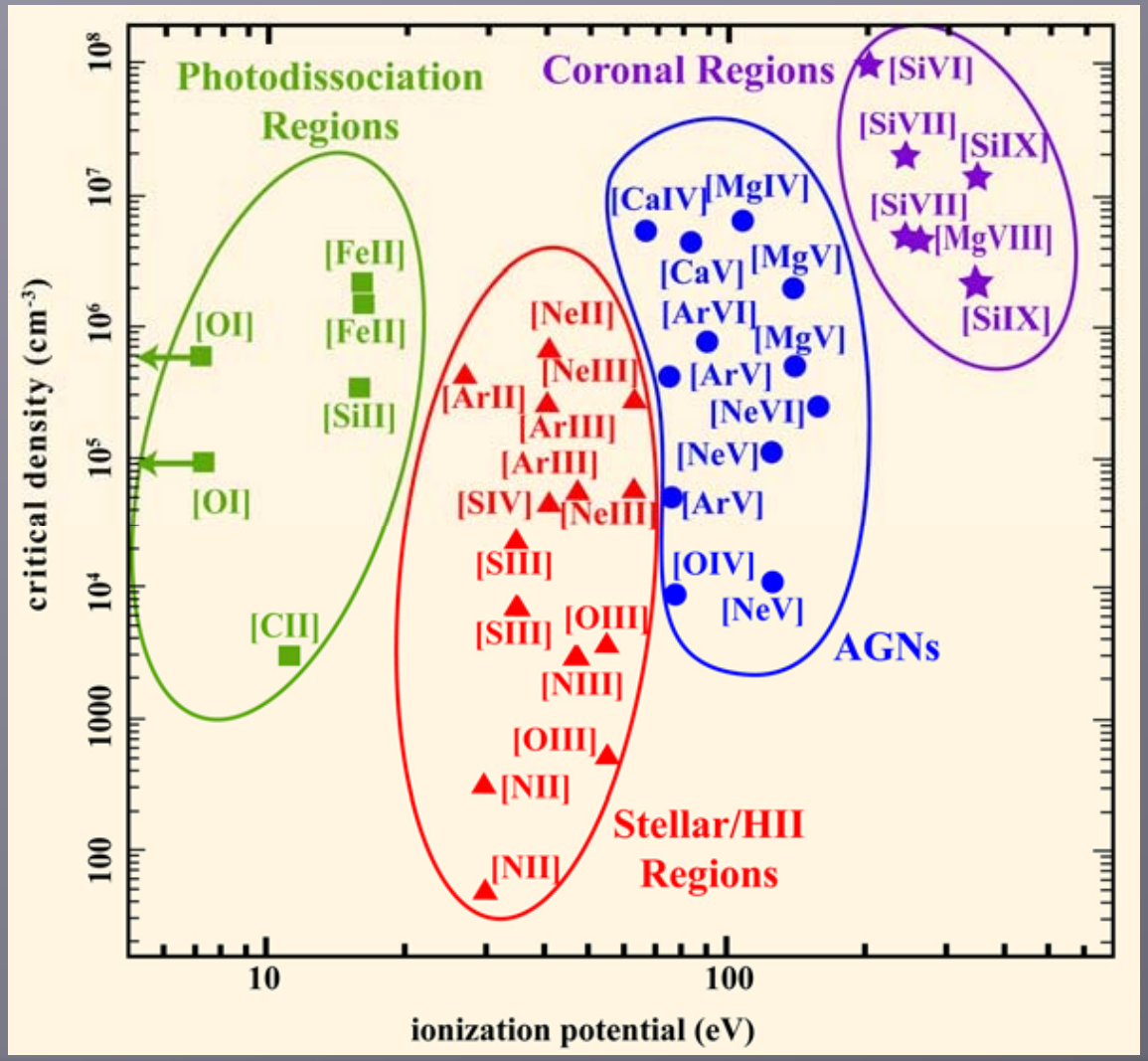
# Example Spectra




- Observed spectra of a galaxy

Harwit et al., white paper (2010)

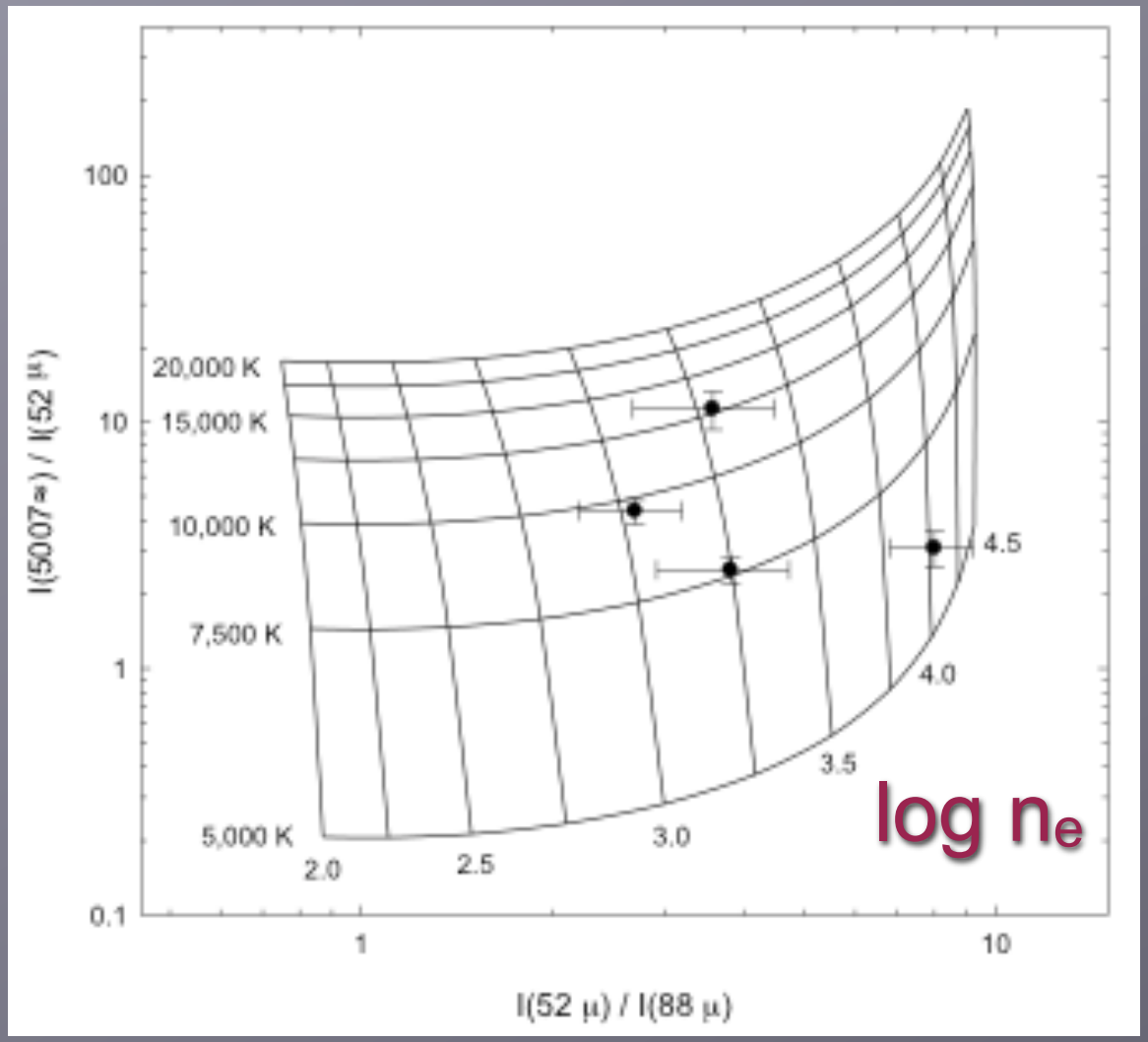
# Key Fine-structure Diagnostics




- Diagnostic lines versus ionization potential for various environments

Harwit et al., white paper (2010)

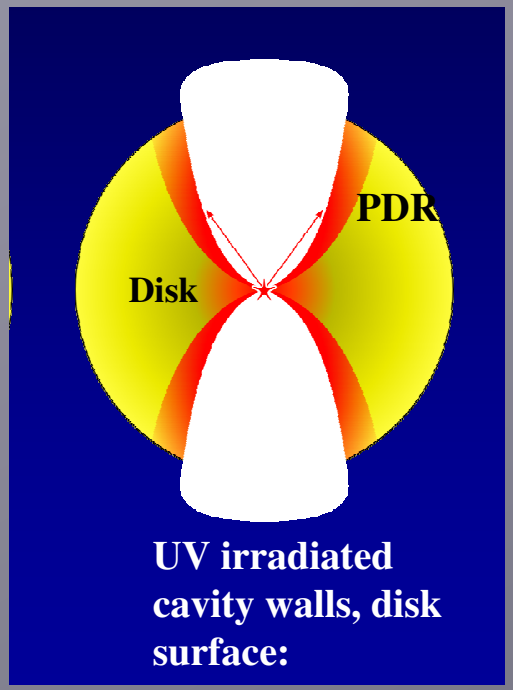
# Temperature-Density Diagnostic




- $O^{2+}$ line ratios combined with forbidden lines
- Comparison to planetary nebulae observations

Osterbrock & Ferland (2006)

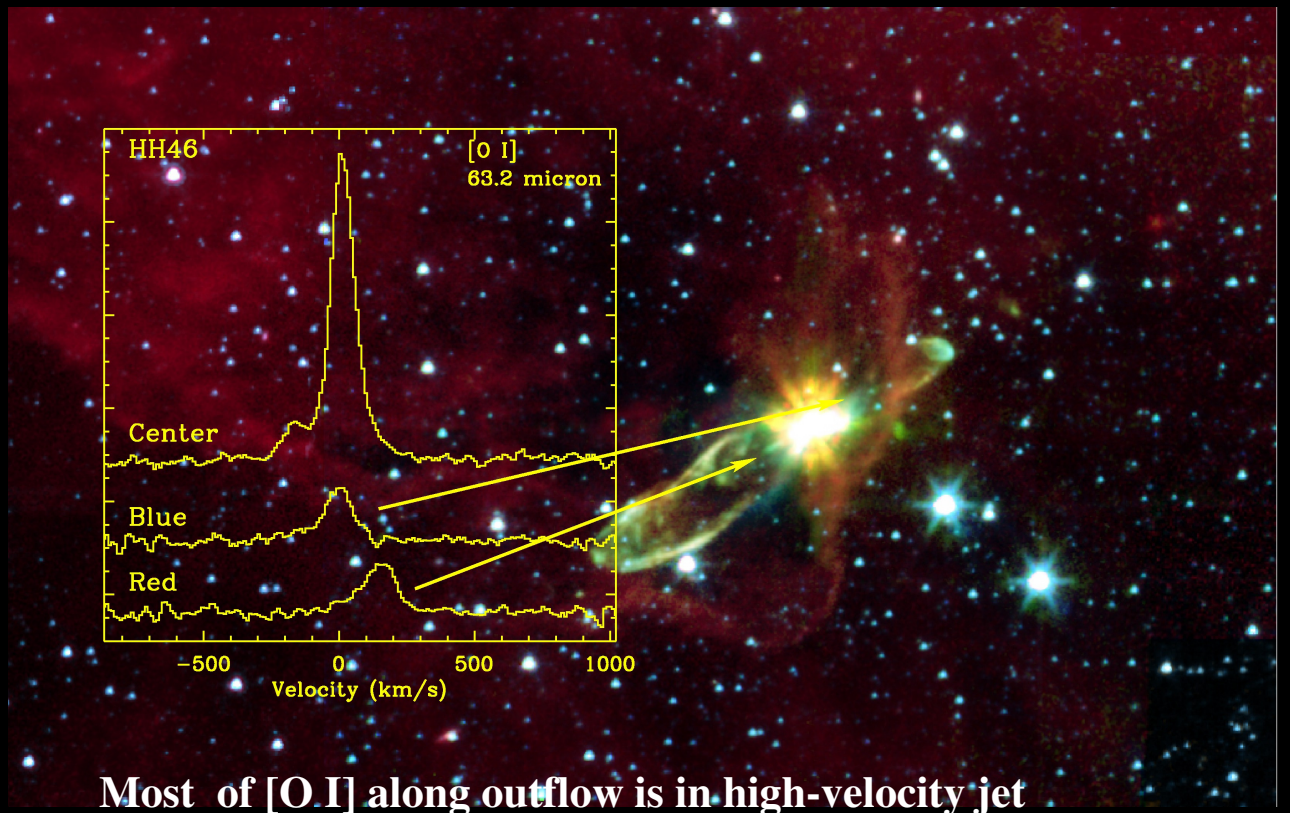
# YSO Disks



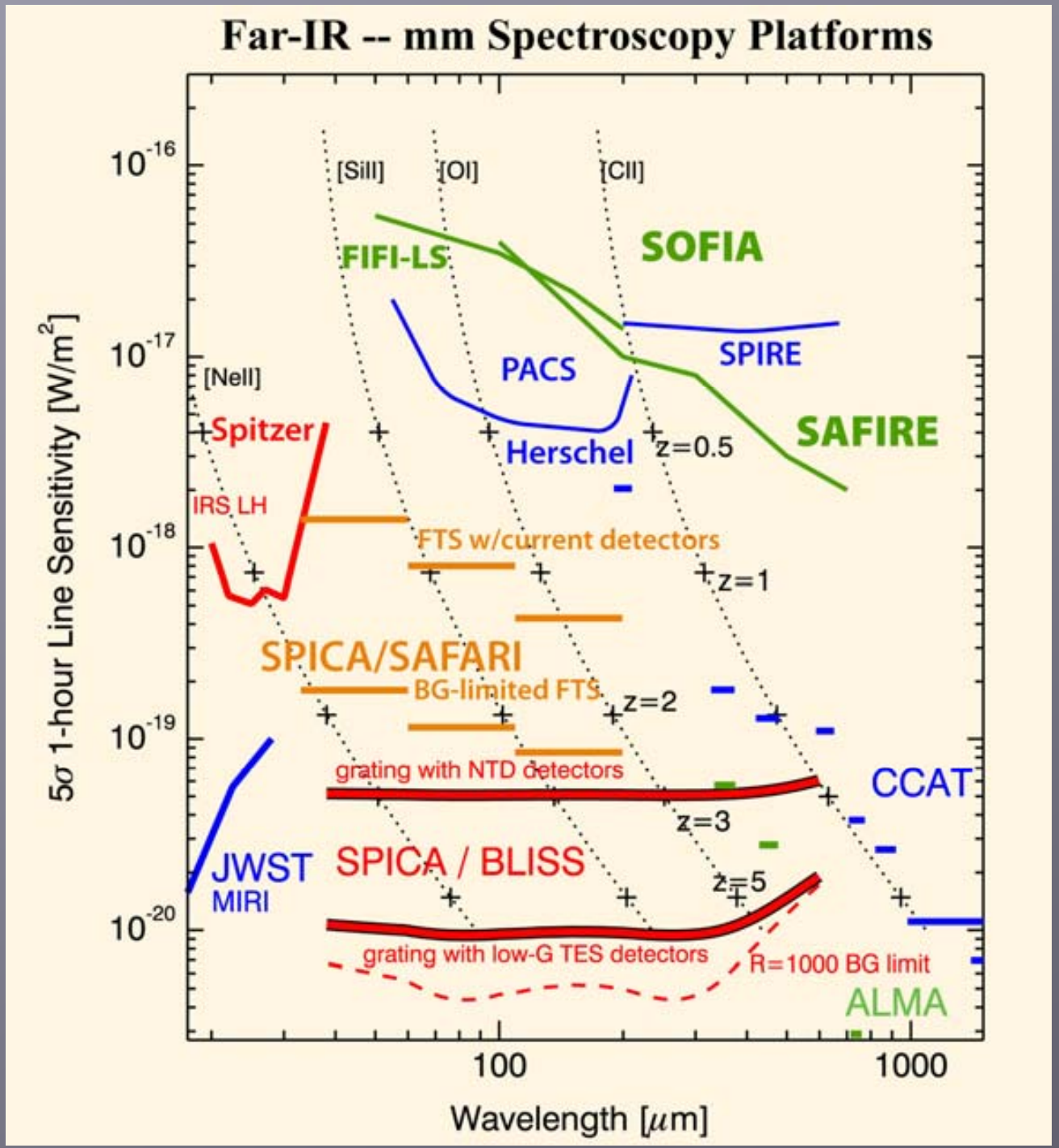

UV irradiated cavity walls, disk surface:

van Dishoeck (2009)

## HH 46 [O I]




Most of [O I] along outflow is in high-velocity jet


Far-IR -- mm Spectroscopy Platforms
5σ 1-hour Line Sensitivity [W/m²]
Wavelength [μm]
[SiII]
[OI]
[CII]
[NeII]
FIFI-LS
SOFIA
PACS
SPIRE
SAFIRE
Herschel
Spitzer
IRS LH
FTS w/current detectors
z=0.5
z=1
z=2
z=3
z=5
SPICA/SAFARI
BG-limited FTS
grating with NTD detectors
CCAT
JWST
MIRI
SPICA / BLISS
grating with low-G TES detectors
R=1000 BG limit
ALMA
100
1000

# Databases?

## LAMDA

### Leiden Atomic and Molecular Database

Atomic datafiles | Molecular datafiles | Data format | RADEX

**Atomic datafiles**

CI CII OI

**Molecular datafiles**

| | | |
|---|---|---|
| CO | CS | HCl |
| OCS | SO | $SO_2$ |
| SiO | SiS | $SiC_2$ |
| $HCO^+$ | $N_2H^+$ | $HCS^+$ |
| $HC_3N$ | HCN | HNC |
| $C_3H_2$ | $H_2O$ | $H_2CO$ |
| OH | $CH_3OH$ | $NH_3$ |
| HDO | $H_3O^+$ | HNCO |
| NO | CN | $CH_3CN$ |
| O2 | HF | |

**Radiative transfer**

RADEX Benchmarking

**Development**

Update history
Future updates

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 (4 January 2011): Minor update of OH datafile.

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.

*Fredrik Schöier, 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.*

```
!MOLECULE
C+ (atomic ion)
!MOLECULAR WEIGHT
12.0
!NUMBER OF ENERGY LEVELS
8
!LEVEL + ENERGIES(cm^-1) + WEIGHT + J
    1      0.000000000   2.0      0.5  ! 2P
    2     63.395087      4.0      1.5  ! 2P
    3   43003.291       2.0      0.5  ! 4P
    4   43025.285       4.0      1.5  ! 4P
    5   43053.568       6.0      2.5  ! 4P
    6   74930.074       6.0      2.5  ! 2D
    7   74932.608       4.0      1.5  ! 2D
    8   96493.727       2.0      0.5  ! 2S
!NUMBER OF RADIATIVE TRANSITIONS
14
!TRANS + UP + LOW + EINSTEINA(s^-1) + FREQ(GHz) + E_u(K)
    1     2     1  2.300E-06        1900.5369        91.21
    2     3     1  5.530E+01     1289206.2        61871.8
    3     3     2  6.550E+01     1287305.7        61871.8
    4     4     1  1.710E+00     1289865.6        61903.4
    5     4     2  5.240E+00     1287965.1        61903.4
    6     4     3  2.390E-07         659.364      61903.4
    7     5     2  4.320E+01     1288813.0        61944.1
    8     5     4  3.670E-07         847.903      61944.1
    9     5     3  3.490E-14        1507.267      61944.1
   10     7     1  2.393E+08     2246423.1       107810.6
   11     7     2  4.773E+07     2244522.5       107810.6
   12     6     2  2.864E+08     2244476.5       107808.4
   13     8     1  7.643E+08     2892809.2       138832.1
   14     8     2  1.526E+09     2890908.6       138832.1
!NUMBER OF COLL PARTNERS
4
!COLLISIONS BETWEEN
2 C+ + pH2  ! Flower & Launay (1977, JPB, 10, 3673); no corr. for Flower (1988)
!NUMBER OF COLL TRANS
1
!NUMBER OF COLL TEMPS
6
!COLL TEMPS
   10.0   20.0   50.0  100.0  200.0  250.0
!TRANS + UP + LOW + COLLRATES(cm^3 s^-1)
    1     2     1  3.0e-10 3.4e-10 3.9e-10 4.3e-10 4.6e-10 4.7e-10
!COLLISIONS BETWEEN
3 C+ + oH2  ! Flower & Launay (1977, JPB, 10, 3673)
!NUMBER OF COLL TRANS
1
!NUMBER OF COLL TEMPS
6
!COLL TEMPS
   10.0   20.0   50.0  100.0  200.0  250.0
!TRANS + UP + LOW + COLLRATES(cm^3 s^-1)
    1     2     1  4.4e-10 4.6e-10 4.9e-10 5.1e-10 5.6e-10 5.7e-10
```

| Ion | $e^-$ | H | $H_2$ | He | $H^+$ | λ(μm) |
|---|---|---|---|---|---|---|
| O | Bell 1998 | Abraham. 2007 | Jaquet 1992 | Monteiro 1987 | Chambau 1980 | 63,145 |
| $O^{2+}$ | McLaugh. 1998 | | | | | 288 |
| $O^{3+}$ | Tayal 2006 | | | | | 26 |
| C | Johnson 1987 | Abraham. 2007 | Schroed. 1991 | Staemml. 1991 | Roueff 1990 | 370 |
| $C^+$ | Tayal 2008 | Barinovs 2005 | Launay 1977 | | | 158 |
| $N^+$ | Hudson 2004 | | | | | 122, 205 |
| $N^{2+}$ | Blum 1992 | | | | | 57 |

| Ion | $e^-$ | H | $H_2$ | He | $H^+$ | λ(μm) |
|---|---|---|---|---|---|---|
| $Ne^+$ | Griffin 2001 | | | | | 12.8 |
| $Ne^{2+}$ | McLaugh. 2000 | | | | | 16, 36 |
| $Ne^{4+}$ | Griffin 2000 | | | | | 14, 24 |
| $Ne^{5+}$ | Mitnik 2001 | | | | | 7.6 |
| $Mg^{3+}$ | Witthoeft (2007) | | | | | 4.5 |
| $Mg^{4+}$ | Butler 1994 | | | | | 5.6, 13.5 |
| $Mg^{6+}$ | Lennon 1994 | | | | | 5.5, 9 |

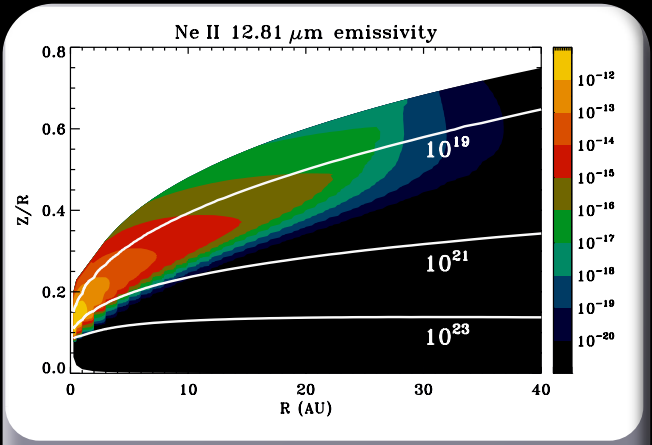
| Ion | $e^-$ | H | $H_2$ | He | $H^+$ | λ(μm) |
|---|---|---|---|---|---|---|
| $Mg^{7+}$ | Zhang 1994 | | | | | 3.0 |
| Al | | | | | | 89 |
| $Al^{4+}$ | Witthoeft (2006) | | | | | 2.9 |
| Si | | | | | | 25, 57 |
| $Si^+$ | Tayal 2008 | Barinovs 2005 | | | | 35 |
| $Si^{5+}$ | Witthoeft (2007) | | | | | 1.96 |
| $Si^{6+}$ | Butler 1994 | | | | | 2.5, 6.5 |

| Ion | $e^-$ | H | $H_2$ | He | $H^+$ | λ(μm) |
|---|---|---|---|---|---|---|
| $Si^{8+}$ | Lennon 1994 | | | | | 2.5, 3.9 |
| $Si^{9+}$ | Zhang 1994 | | | | | 1.43 |
| $P^+$ | Tayal 2003? | | | | | 33, 61 |
| $P^{2+}$ | Krueger 1970 | | | | | 17.9 |
| $P^{6+}$ | Witthoeft (2007) | | | | | 1.37 |
| S | Tayal 2004 | | | | | 25, 57 |
| $S^{2+}$ | Tayal 1999 | | | | | 19, 34 |

| Ion | $e^-$ | H | $H_2$ | He | $H^+$ | λ(μm) |
|---|---|---|---|---|---|---|
| $S^{3+}$ | Tayal 2000 | | | | | 10.5 |
| $S^{7+}$ | Witthoeft (2007) | | | | | 1 |
| $Ar^+$ | Pelan 1995 | | | | | 6.98 |
| $Ar^{2+}$ | Munoz-2009 | | | | | 9, 22 |
| $Ar^{4+}$ | Ludlow 2010 | | | | | 7.9, 13 |
| $Ar^{5+}$ | Ludlow 2010 | | | | | 4.53 |
| $Ca^{3+}$ | Pelan 1995 | | | | | 3.2 |

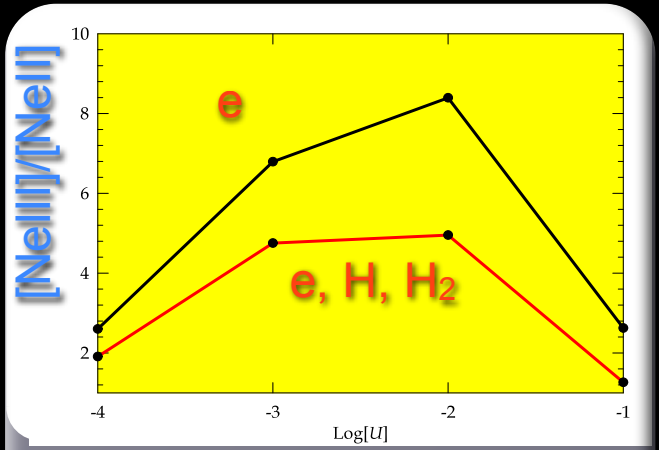
| Ion | $e^-$ | H | $H_2$ | He | $H^+$ | λ(μm) |
|---|---|---|---|---|---|---|
| $Ca^{4+}$ | Galavis 1995 | | | | | 4.1, 11.5 |
| Fe | ? | | | | | 24, 34 |
| $Fe^+$ | ? | | | | | 26, ... |
| $Fe^{2+}$ | ? | | | | | 22.9, ... |
| $Fe^{4+}$ | Ballance (2007?) | | | | | 70, ... |
| $Fe^{5+}$ | Ballance (2008?) | | | | | 20, ... |
| $Fe^{6+}$ | Witthoeft (2007) | | | | | 9.5, 7.8 |

# Fine-structure excitation: Needs



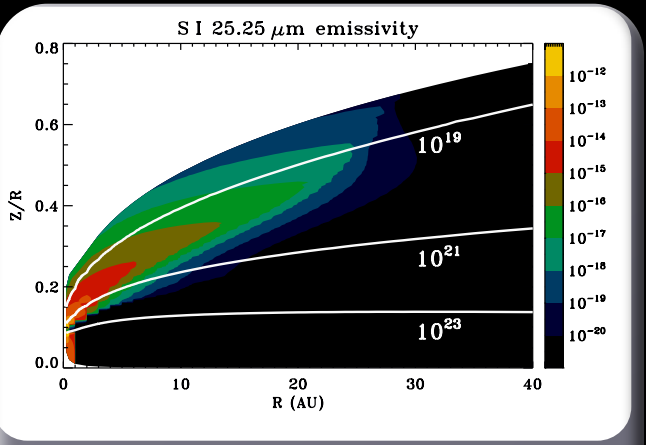

- [NeIII] and [NeII] lines observed in protoplanetary disks with *Spitzer*
- H collisional rates needed

$Ne^+ + H$, $Ne^{2+} + H$ protoplanetary disks (Meijerink et al. 2007)




- [NeIII]/[NeII] ratio used as a diagnostic of AGNs
- Usually only e-collisions considered

$Ne^+ + H, H_2$, $Ne^{2+} + H, H_2$ in XDRs (Abel 2008)




- [SI] observed in proto-planetary disks
- H collisional rates needed

S + H protoplanetary disks (Meijerink et al. 2007)

# Summary - Needs

- Fine-structure excitation by electrons:
  - Calculations for O and C need revisiting
  - Neon ions look in good shape
  - Other possibilities: $N^{2+}$, $Ar^{2+}$, Al, and S
  - Further work on: Fe, $Fe^{+}$, $Fe^{2+}$????
- Fine-structure excitation by heavy particles
  - Calculations for O and C with $H_2$, He, $H^{+}$ need revisiting
  - O + $H^{+}$ (later C + $H^{+}$) in collaboration with David Schultz and Yong Wu
  - $C^{+}$ + $H_2$ should be revisited

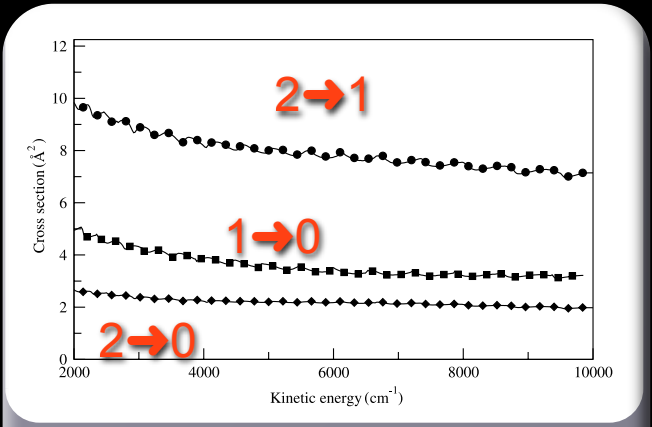
# Summary - Needs

- Fine-structure excitation by heavy particles (cont'd):
  - Calculations of H collisions needed for S, Si, Fe, Al, $Ne^{+}$, $N^{+}$, $Fe^{+}$, $Ne^{2+}$, $O^{2+}$ , $Fe^{2+}$, $S^{2+}$
  - Calculations of He and $H_2$ collisions needed for S, Si, Al ,Fe, $Ne^{+}$, $N^{+}$, $Fe^{+}$, $Ne^{2+}$
  - Calculations of $H^{+}$ collisions needed for S and Fe
  - Consideration of internuclear-dependent spin-orbit coupling
- Compilations needed
- Measurements needed

# Acknowledgements


- Funding from NASA:
  - Astronomy and Physics Research and Analysis (APRA)
  - Origins of Solar Systems Program (OSS)
  - Astrophysics Data Program (ADP)
  - Astrophysics Theory Program (ATP)
- Contributions from collaborators and colleagues:
  - Gary Ferland, Mitch Pindzola, Ryan Porter, David Schultz, Yong Wu

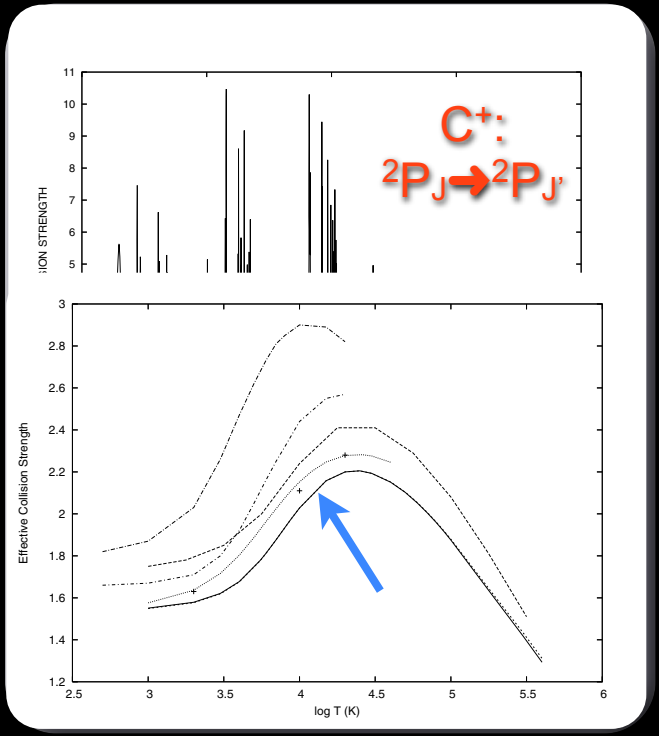
# Fine-structure excitation: Highlights



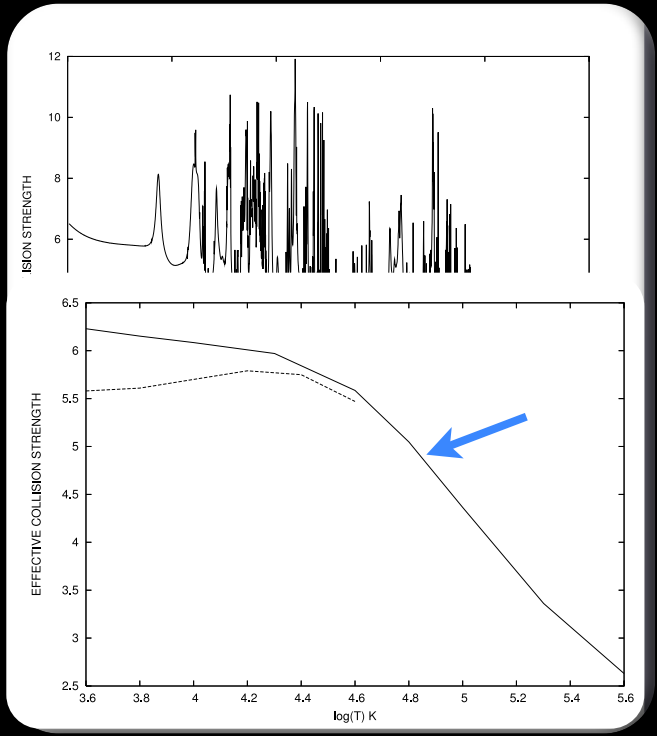

O: $^3P_J \rightarrow {}^3P_{J'}$

- Larger by factors of 2-4 compared to previous calculations

O + H, C+H MOCC Calculations Abrahamsson et al. (2007)




C$^+$ + e R-matrix calculations Tayal (2008)




Si$^+$ + e R-matrix calculations Tayal (2008)