Photoionization Models

- How photoionization codes work (simplified)
- Calculating a specific model
- Additional complications/considerations
- Unresolved emission-line regions
- Cloudy

Photoionization Codes

Equations for calculating a model:

1) $$\frac{dI_\nu}{ds} = -I_\nu \frac{d\tau_\nu}{ds} + j_\nu$$ (radiative transfer)

where $$\frac{d\tau_\nu}{ds} = \sum n_j a_{\nu_j}$$ (sum over all ions)

2) $$n(X^i)\int_{\nu_i}^{\infty} \frac{4\pi J_\nu}{h\nu} a_\nu(X^i)\, d\nu = n(X^{i+1}) n_e \alpha(X^i, T)$$ (ion. equil.)

where $\sum n(X^i) = n(X)$ and Abundance $= n(X)/n(H)$

3) $$G = L_R + L_{FF} + L_C$$ (conservation of energy)

Procedure:

- Assume a geometry (spherical, plane-parallel, etc.)
- Determine the ionizing flux at the incident face of the cloud (PN – inner face of shell, filled H II region – surface of star, AGN – ionized face of discrete cloud (usually a slab)
- Divide the cloud into zones and calculate the reduction of photons as you move into the cloud
- Use the on-the-spot approximation (all diffuse ionizing photons are absorbed locally) in the first series of calculations to determine: temperature, ionization fractions, emissivities, and reduction of ionizing photons in each zone
- In subsequent iterations, determine the diffuse field as you go to deeper zones in the cloud

Calculating a Specific Model

- Estimate the initial input parameters:

  1) Geometry (sphere, shell, slab, other?)

  2) n_e (or n_H) - from [O II], [S II], critical densities, etc.

  - is density a function of distance: n(r) ?

  3) Ionizing spectrum (spectral energy distribution)

  - clues from type of source, Zanstra method, etc.

  4) Flux of ionizing source (star, AGN, etc.) at surface of cloud

  5) Abundances (normally assume solar to begin with)
- Calculate the model
- Compare model spectrum to observed spectrum (usually line ratios relative to Hβ)
- Iterate

Additional Considerations

- Optical depth of cloud (when to terminate the integration?)

  Extremes:

  1) matter bounded – optically thin to ionizing radiation

  2) radiation bounded – optically thick to ionizing radiation

- Filling factor (ε): percentage of volume that is filled

  – are there discrete clouds?

- Covering factor (C): fraction of ionizing flux that is intercepted by the gas: $C = \Omega/4\pi$
- Multicomponent models (when one component just won't do!)

  Ex) Condensations in a diffuse medium (two densities)

  Ex) Two or more clouds at different distances from source

- Many other games you can play!

Unresolved Emission-Line Regions

- Ex) broad-line region (BLR) of AGN
- Problem: don't know distance from source to cloud(s)
- Assume a slab (discrete cloud, large distance from source)
- Use the ionization parameter (U):

$$U = \frac{\int_{\nu_0}^{\infty} \frac{L_\nu}{h\nu} d\nu}{4\pi r^2 c n_e} = \frac{\#\ \text{ionizing photons / vol}}{\#\ \text{electrons / vol}} \text{ at the incident face}$$

From the ionization equilibrium equation:

$$U = \frac{Q_{ion}}{4\pi r^2 c n_e} \approx \frac{\alpha(X^i, T)}{a_\nu(X^i)\ c} \frac{n(X^{i+1})}{n(X^i)}$$

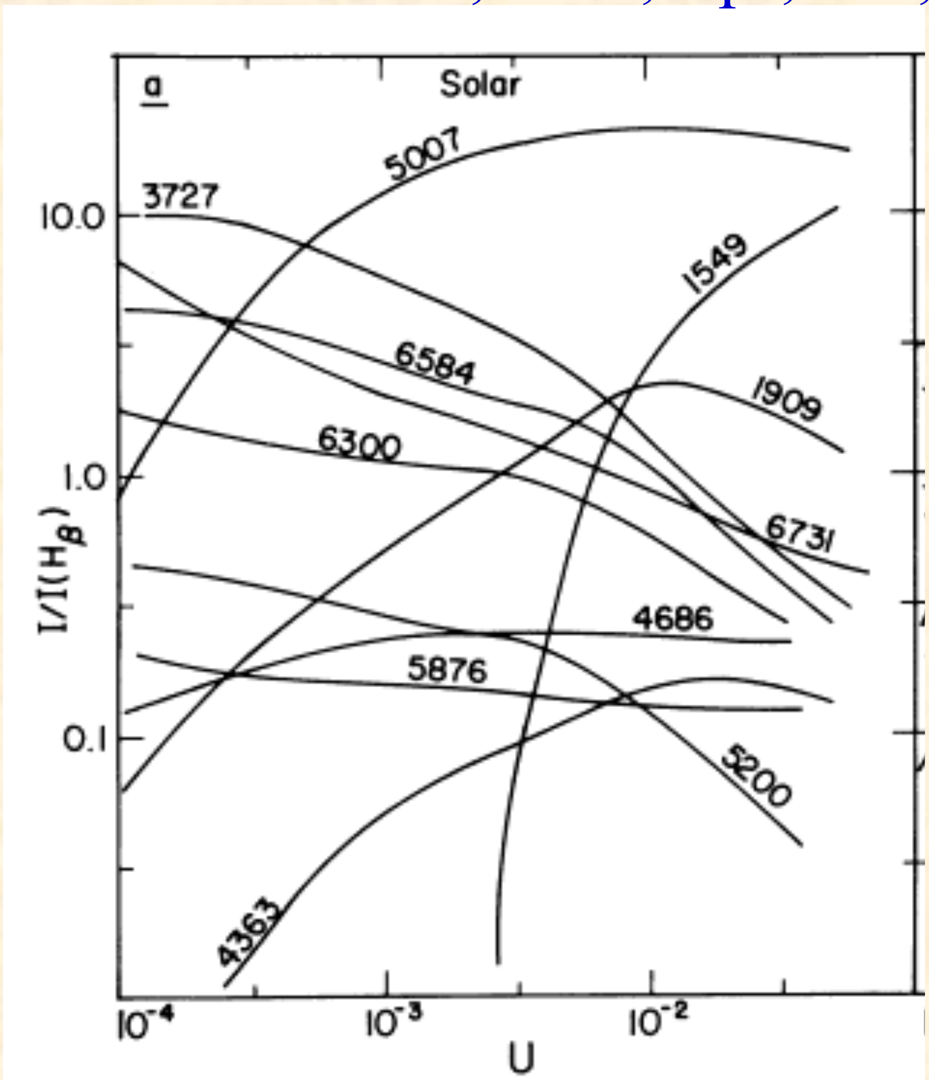
$\rightarrow$ U is a dimensionless parameter that specifies the ionization fractions

$\rightarrow$ U is the most important factor in determining line ratios

(n_e is next most important)

Emission-Line Ratios as a Function of U

(Ferland & Netzer, 1983, ApJ, 264, 105)



[O III] 5007, [O II] 3727, [N II] 6584, [O I] 6300, [S II] 6731, [N I] 5200, C III] 1909, C IV 1549, He I 5876, He II 4686

- So for AGN models, the typical input parameters are:

  1) U – Guess from ratios: C IV/C III], etc.

  2) n_H – presence of lines with certain critical densities

     Ex) [O III] not present in BLR, so $n_H > 10^8$ cm^{-3}

  3) SED – from X-ray, UV, and optical observations (don't know EUV!)

  4) N_H – integrate model until lines that form deep in cloud are matched – usually very optically thick

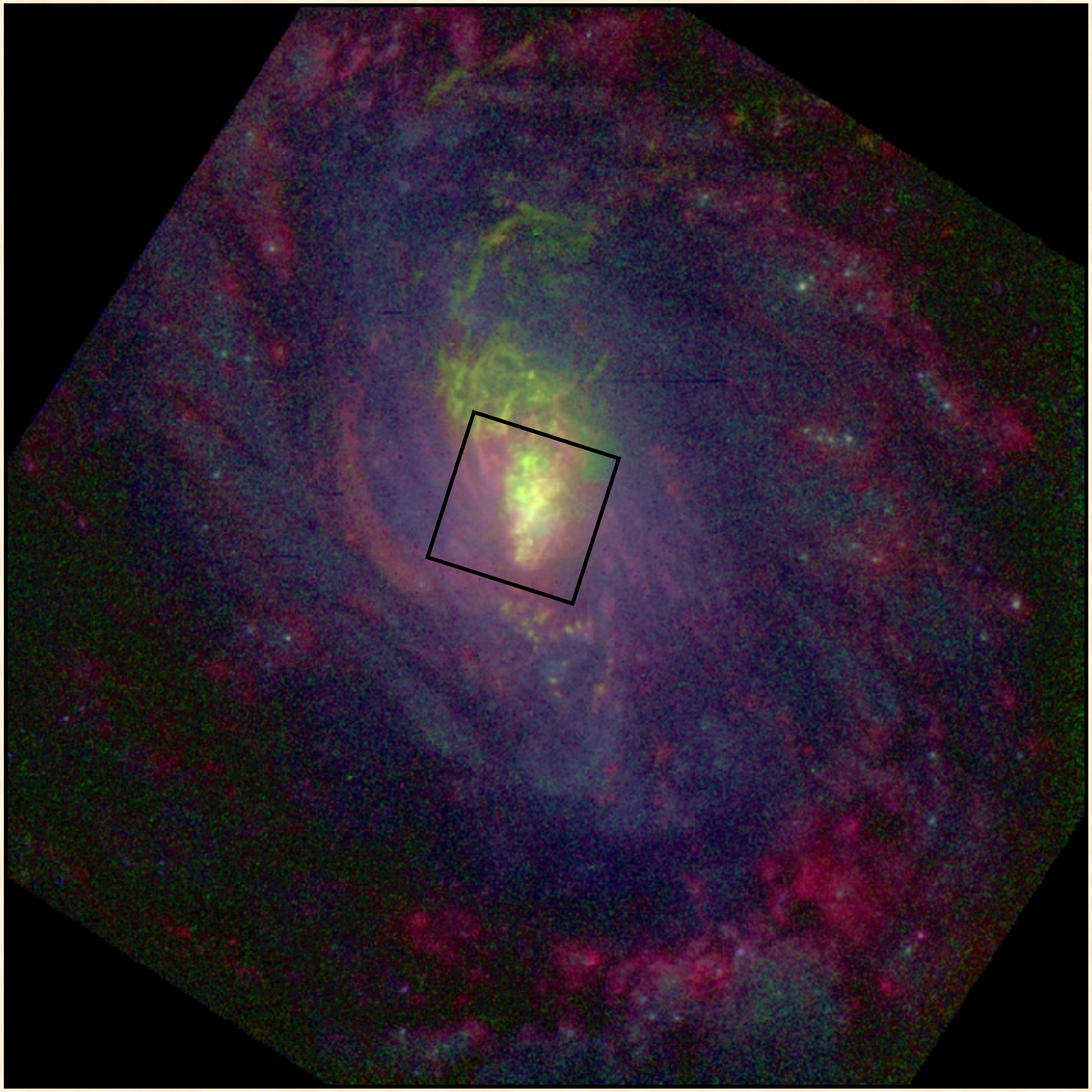
  5) Abundances (last resort!)

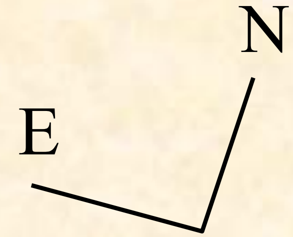
- Usually, at least 2 components with different U, n_e needed
- Can derive distances of clouds from U, n_e

Cloudy - State of the Art

- Main web page (downloads, documentation, discussion, etc.):
  http://www.nublado.org/
- Status of numerical simulations of photoionized gas:
  Ferland, G.J. 2003, ARAA, 41, 517
- To reference cloudy in your published paper:
  Ferland, G.J., et al. 2013, RMxAA, 49, 137

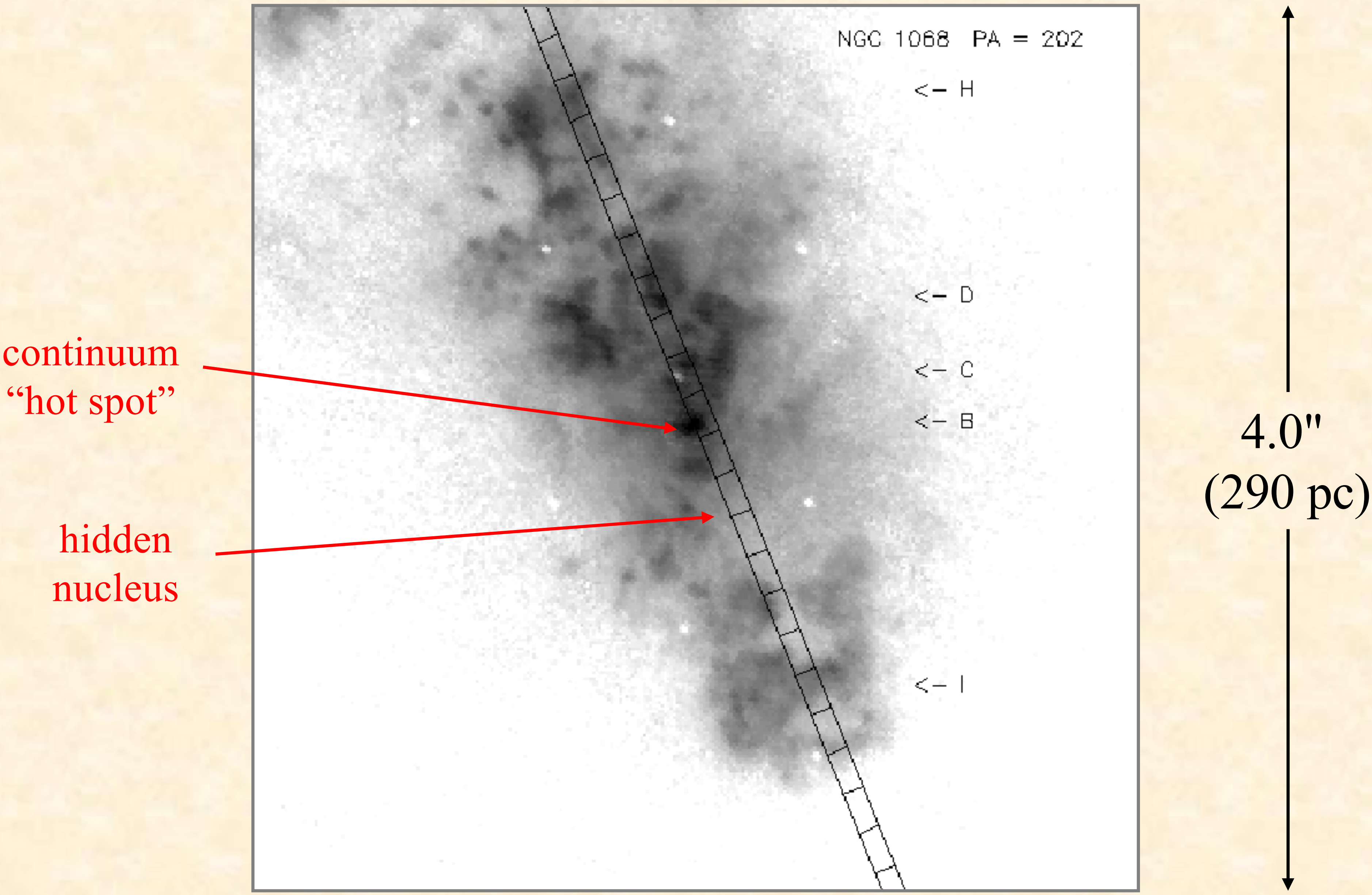
Ex) HST/STIS Spectra of the Narrow-Line Region in NGC 1068 (Seyfert 2 Galaxy)



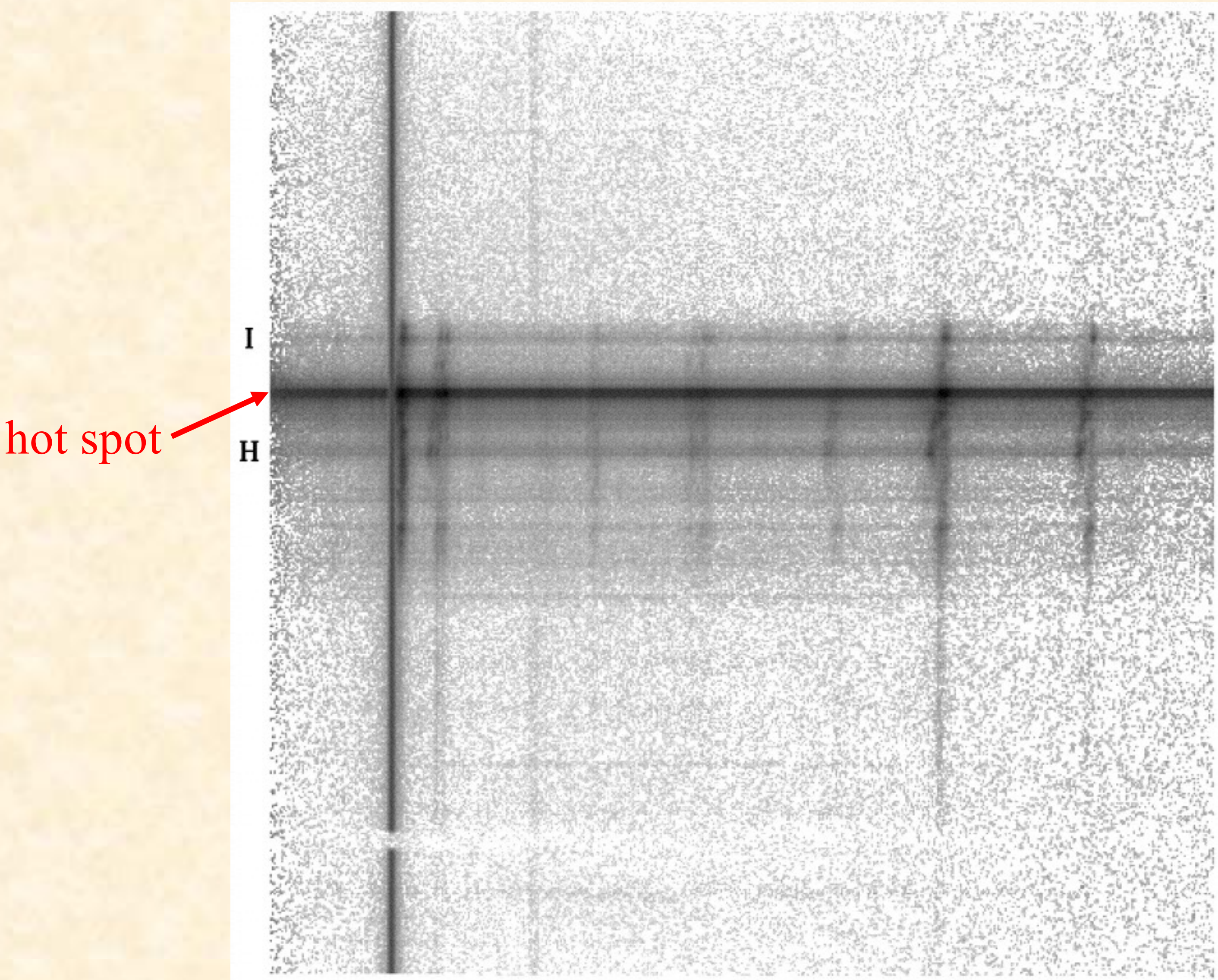


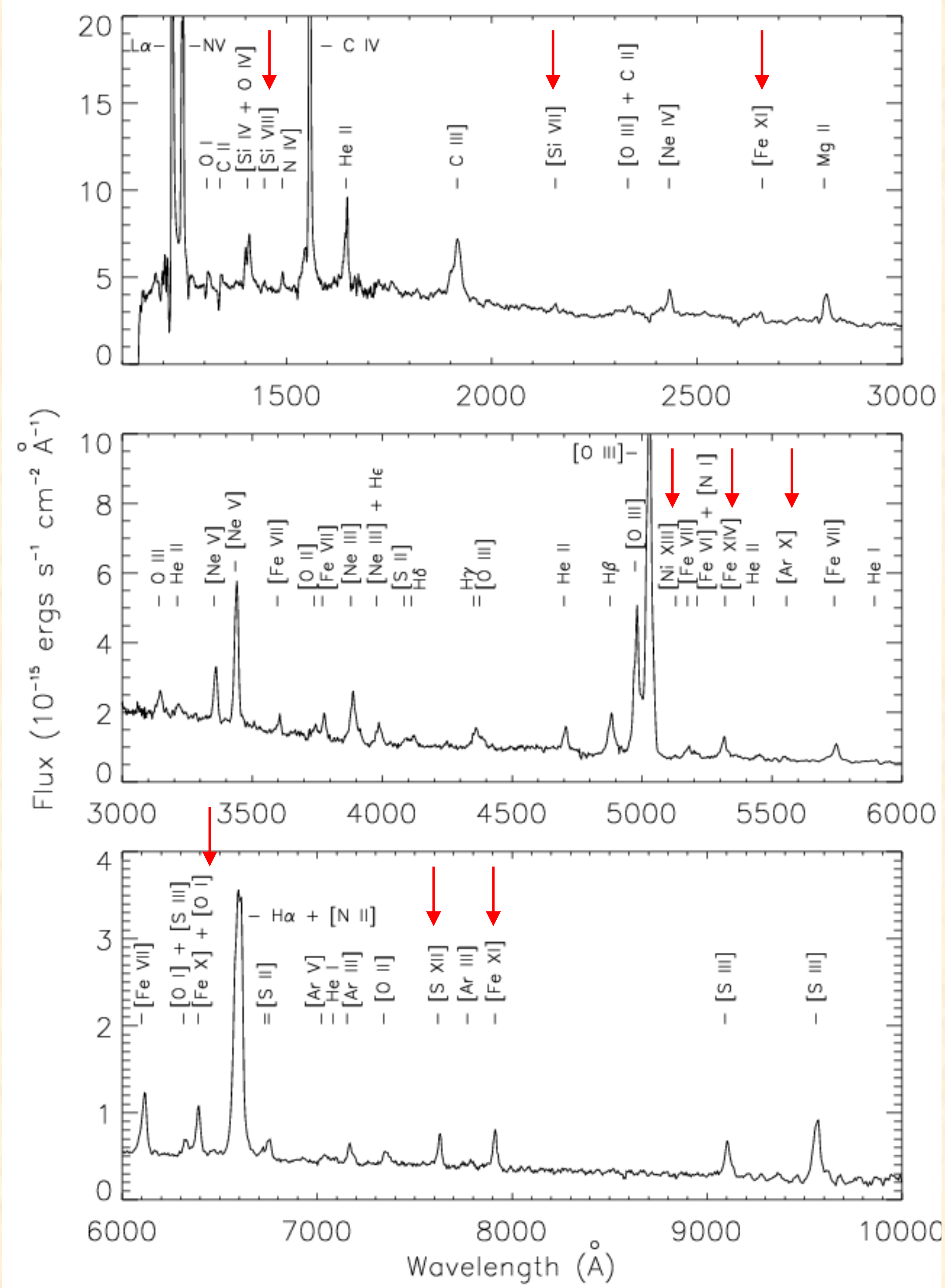
WFPC 2 image
blue - stellar
red - Hα
green - [O III]

NGC 1068: NLR – [O III] Image



STIS Raw UV Spectrum

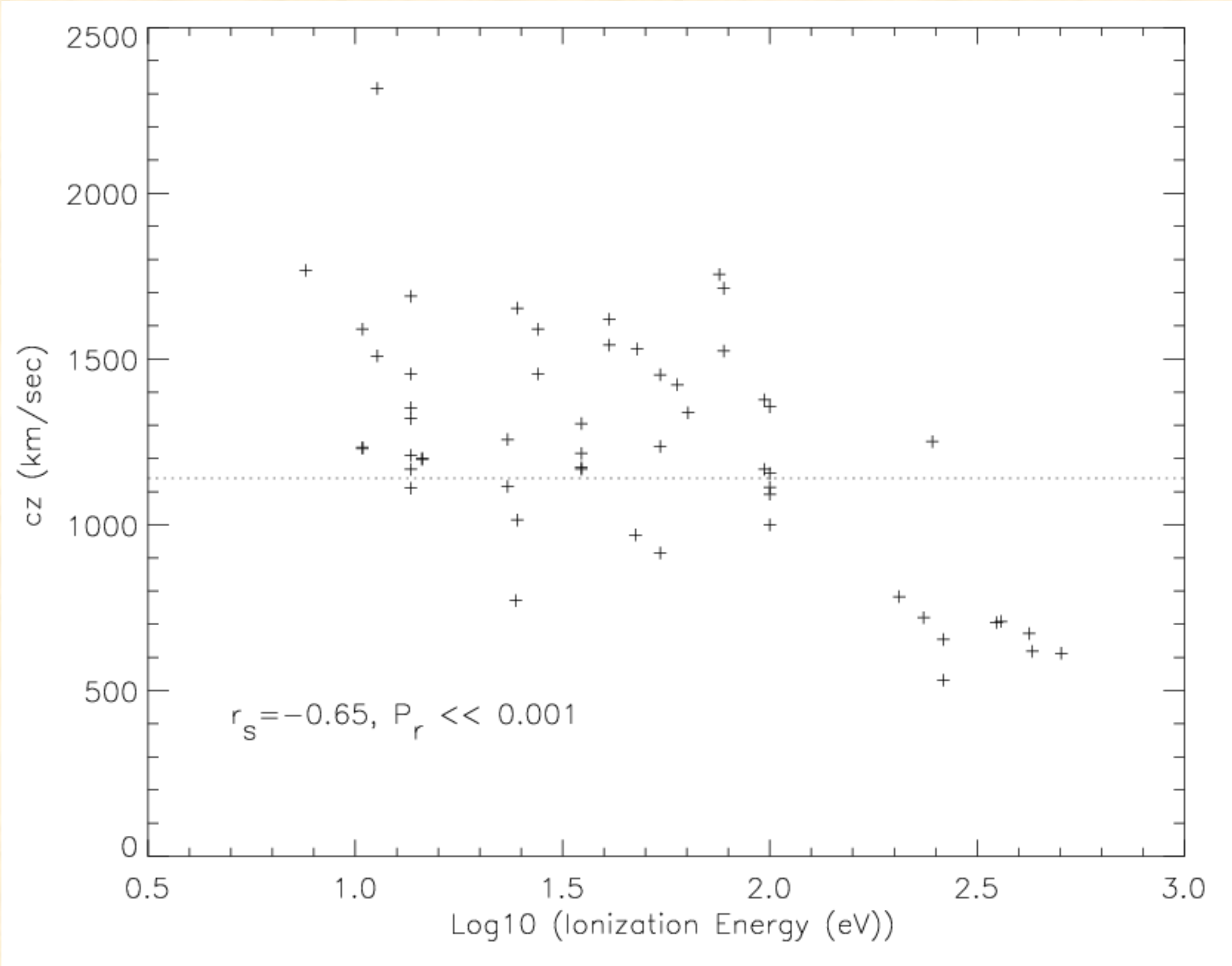




NGC 1068 - Hot Spot
STIS Spectrum of NLR
(Kraemer & Crenshaw, 2000, ApJ, 532, 256)

Huge range in ionization:
- Low: O I, Mg II, C II
- High: C IV, [O III], etc.
- Coronal: [Fe XI], [Fe XIV], [S XII] (IP_C = 504 eV)

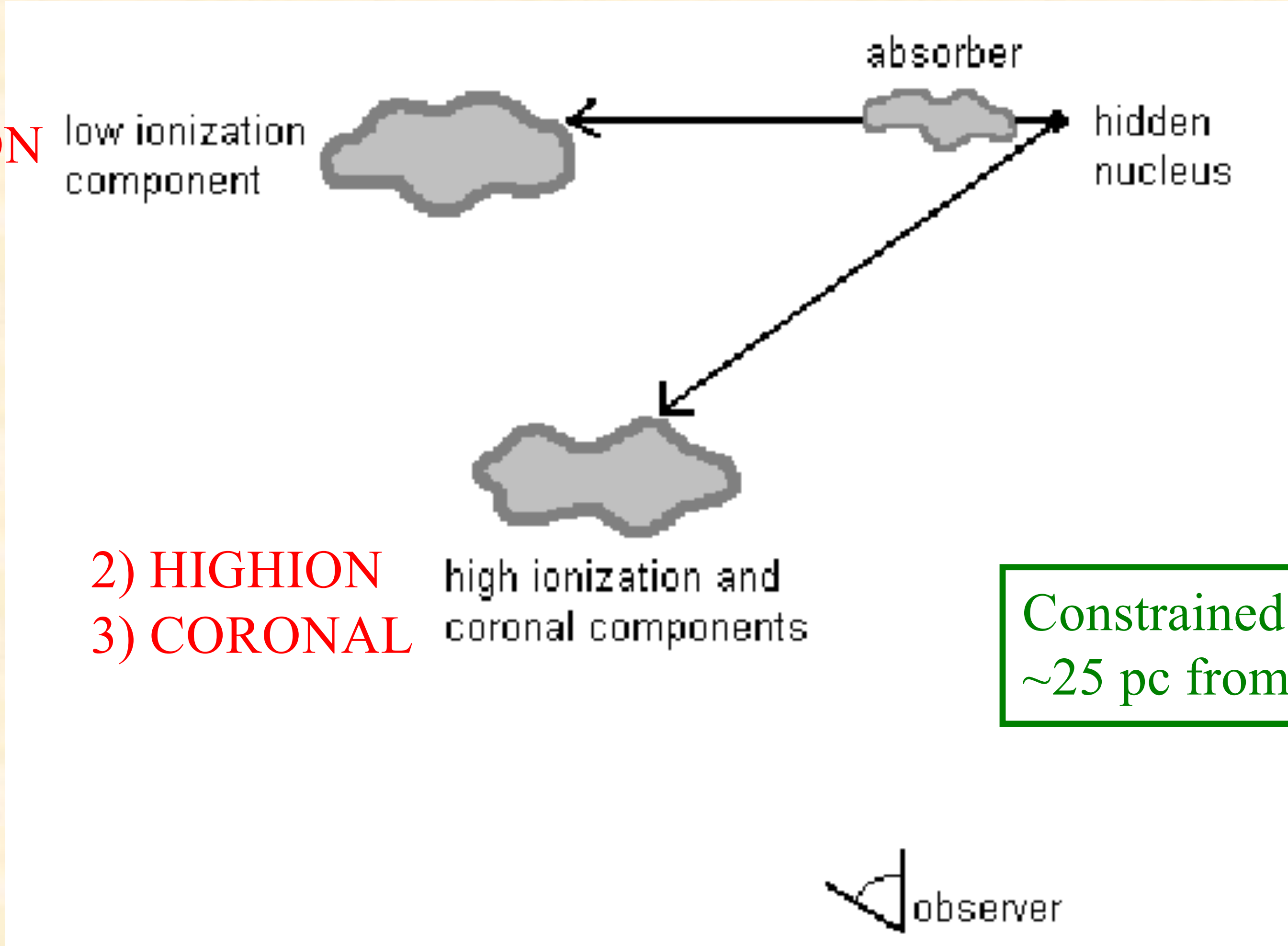
Redshift vs. Ionization Potential



- kinematic evidence for distinct components

NLR Photoionization Models – 3 components

1) LOWION

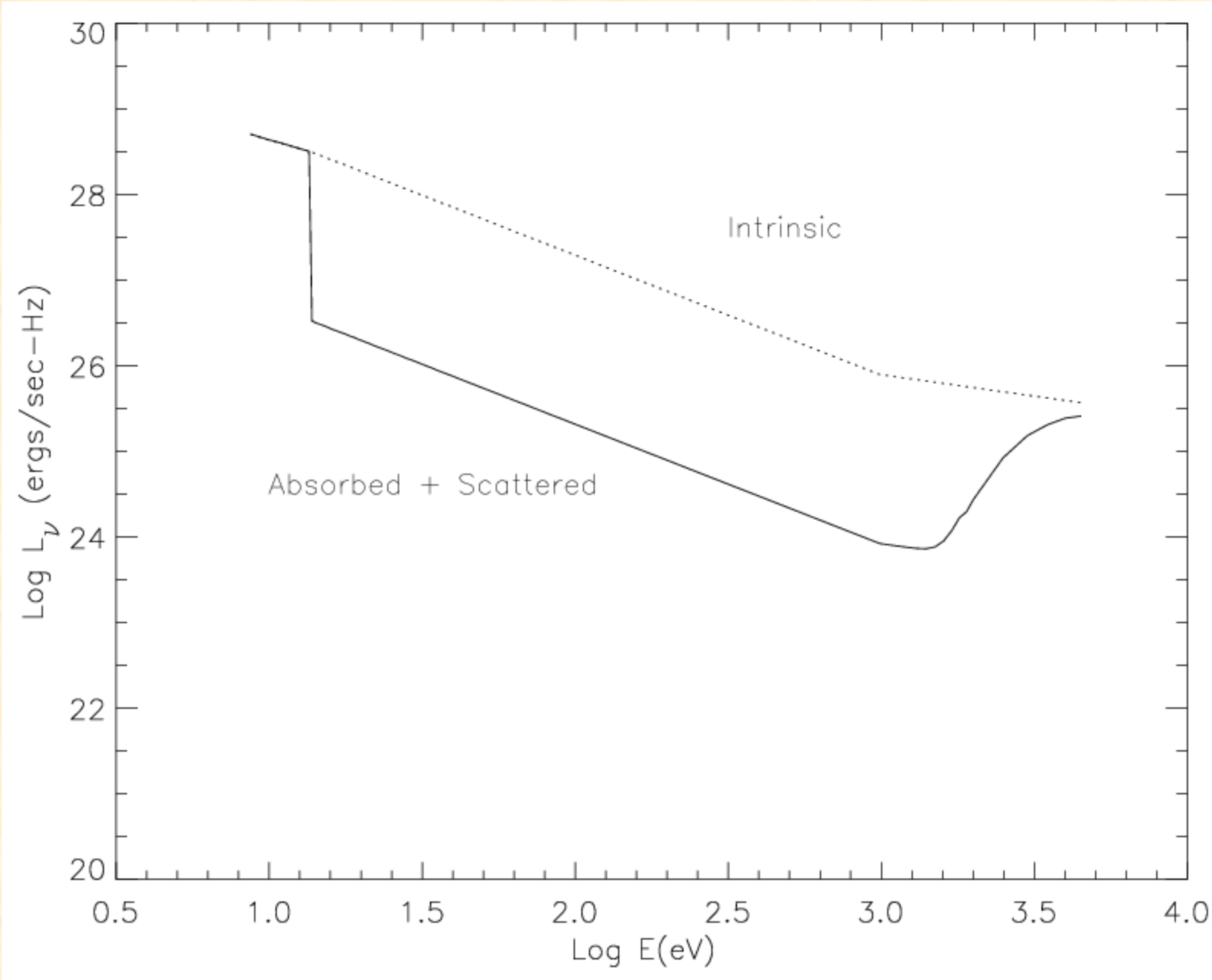


2) HIGHION
3) CORONAL

Constrained to be ~25 pc from nucleus

1) LOWION: $U = 10^{-3.2}$, $n_H = 3 \times 10^4$ cm^{-3}, $N_H = 1 \times 10^{21}$ cm^{-2}
2) HIGHION: $U = 10^{-1.5}$, $n_H = 6 \times 10^4$ cm^{-3}, $N_H = 1 \times 10^{21}$ cm^{-2}
3) CORONAL: $U = 10^{0.2}$, $n_H = 7 \times 10^2$ cm^{-3}, $N_H = 4 \times 10^{22}$ cm^{-2} (?)

Intrinsic and Filtered Continua (for LOWION)



(Absorber: $U = 10^{-1.0}$, $N_H = 7 \times 10^{22}$ cm^{-2})

Line Ratios from Model Components, Composite, and Observations (Relative to Hβ)

Emission Line	HIGHION[a]	LOWION[b,c]	Composite[d]	Observed[e]
C III λ977	(1.47)	(1.08)	(1.37)	...
N III λ990	(0.64)	(0.78)	(0.68)	...
Lyα λ1216	34.18	40.44	35.74	30.17 $\pm$ 5.65
N V λ1240	3.33	0.00	2.50	16.19 $\pm$ 2.86
C II λ1335	0.03	0.09 (4.02)	1.01	0.98 $\pm$ 0.19
O IV] λ1402 + Si IV λ1398	4.74	0.00	3.56	4.99 $\pm$ 0.19
N IV] λ1486	2.99	0.00	2.24	0.76 $\pm$ 0.13
C IV λ1550	32.52	0.03	24.40	19.83 $\pm$ 2.53
He II λ1640	6.30	1.29	5.05	4.34 $\pm$ 0.57
O III λ1663	1.71	0.09	1.31	...
N III λ1750	0.81	0.05	0.62	...
C III] λ1909 + Si III] $\lambda\lambda$1883, 1892	6.66	1.04	5.25	7.16 $\pm$ 0.96
C II] λ2326 + O III] λ2321	0.24	1.96	0.67	0.47 $\pm$ 0.09
[Ne IV] λ2423	1.62	0.01	1.22	1.44 $\pm$ 0.20
[O II] λ2470	0.00	0.77	0.19	...
Mg II λ2800	0.00	3.05 (8.54)	2.13	1.91 $\pm$ 0.21
He II λ3204	0.36	0.08	0.29	0.89 $\pm$ 0.21
[Ne V] λ3346	1.83	0.00	1.38	1.74 $\pm$ 0.17
[Ne V] λ3426	4.99	0.00	3.74	4.94 $\pm$ 0.36
[Fe VII] λ3588	0.46	0.00	0.34	0.44 $\pm$ 0.07
[O II] λ3727	0.00	2.81	0.70	0.56 $\pm$ 0.08
[Fe VII] λ3760	0.63	0.00	0.48	0.85 $\pm$ 0.07
[Ne III] λ3869	1.12	1.67	1.26	2.35 $\pm$ 0.19
[Ne III] λ3967 + Hϵ	0.50	0.68	0.55	0.86 $\pm$ 0.10
[S II] λ4072	0.00	0.87	0.22	0.33 $\pm$ 0.05
Hδ λ4100	0.26	0.26	0.26	0.33 $\pm$ 0.05
Hγ λ4340	0.47	0.47	0.47	0.66 $\pm$ 0.06
[O III] λ4363	0.63	0.07	0.49	0.43 $\pm$ 0.05
He II λ4686	0.87	0.19	0.70	0.60 $\pm$ 0.05
Hβ	1.00	1.00	1.00	1.00
[O III] λ4959	6.60	2.85	5.66	4.96 $\pm$ 0.38
[O III] λ5007	19.80	8.56	16.99	15.12 $\pm$ 0.98
[Fe VII] λ5721	0.79	0.00	0.60	0.83 $\pm$ 0.07
He I λ5876	0.02	0.13	0.05	0.25 $\pm$ 0.12
[Fe VII] λ6087	1.18	0.00	0.88	1.08 $\pm$ 0.10
[O I] λ6300 + [S III] λ6312	0.00	2.29	0.57	0.27 $\pm$ 0.03
[O I] λ6364 + [Fe X] λ6374	1.17	0.71	1.06	0.80 $\pm$ 0.07
[N II] λ6548	0.00	2.65	0.66	0.98 $\pm$ 0.22
Hα λ6563	2.78	2.94	2.82	2.81 $\pm$ 0.51
[N II] λ6584	0.00	7.65	1.91	2.94 $\pm$ 0.66
[S II] λ6716	0.00	1.03	0.26	0.17 $\pm$ 0.03
[S II] λ6731	0.00	1.22	0.30	0.21 $\pm$ 0.04
[O II] λ7325	0.00	0.98	0.24	0.24 $\pm$ 0.04
[S III] λ9069	0.00	1.17	0.30	0.51 $\pm$ 0.09
[S III] λ9532	0.01	3.08	0.72	1.28 $\pm$ 0.17

"CORONAL" Model

PREDICTED MEAN IONIZATION FRACTIONS (FROM CORONAL MODEL)

Element	VII	VIII	IX	X	XI	XII	XIII	XIV	XV
Si	0.001[a]	0.034[a]	0.191	0.339	0.288	0.099	0.046	0.002	...
S	...	0.019	0.124	0.235	0.261	0.221[a]	0.107	0.025	0.007
Ar	0.001	0.012	0.101	0.179[a]	0.229	0.228	0.150	0.077	0.019
Fe	...[a]	...	0.003	0.020[a]	0.076[a]	0.188	0.252	0.193[a]	0.160
Ni	...	...	0.001	0.022	0.106	0.180	0.181[a]	0.170	0.144[a]

[a] Observed in hot spot spectrum.

Atomic Data Needed

- "Toy model" generated to match the ionization states seen
- To get a real model of the emission lines, we need:
  1) Collision strengths for these intermediate ionization states
  2) Accurate dielectronic recombination rates
     (over a temperature range 40,000 – 100,000 °K)