# Atomic and Molecular Physics for Forefront Astronomy


K. Kirby

Harvard-Smithsonian Center for Astrophysics


ICAMDATA, Meudon, 18 October, 2006

# ICAMDATA

- At this meeting, “DATA” is NOT a bad word!
- “DATA” often trivializes the product of challenging theoretical or experimental studies
- Tremendous value in bringing together the data producers/providers/users -- because at the interfaces much can be lost

# Laboratory Astrophysics & Astronomy

- Historically
- Currently, atomic/molec./solid st. data provide the back-bone for much of fundamental astronomical science
  - Interpretation of observations
  - Theoretical models
- A number of interesting talks focusing on particular astrophysical environments/data needs

# Exciting/Challenging Time for Laboratory Astrophysics

- Exciting: New space missions, new ground-based facilities, with higher spectroscopic resolution and greater sensitivities --> New Discoveries. Laboratory Astrophysics will be essential in extracting the science
- Challenging: funding level is very small; the research itself is very difficult.

# Outline

- New Challenges/Opportunities for Laboratory Astrophysics
- Illustrative scientific examples -- x-ray plasma diagnostics, cometary x-rays, WHIM gas around an AGN, DIBs
- Findings of Laboratory Astrophysics Workshop (NASA), Feb. 2006, at UNLV, Las Vegas, NV

# New Challenges for Lab Astro

- There are astronomical observations which are mysteries -- only solvable with Lab Astro capabilities
- New observations at high precision create new demand for highly accurate atomic/molecular/solid state data
- Lab Astro community should engage in the Virtual Observatory development (Dubernet talk)

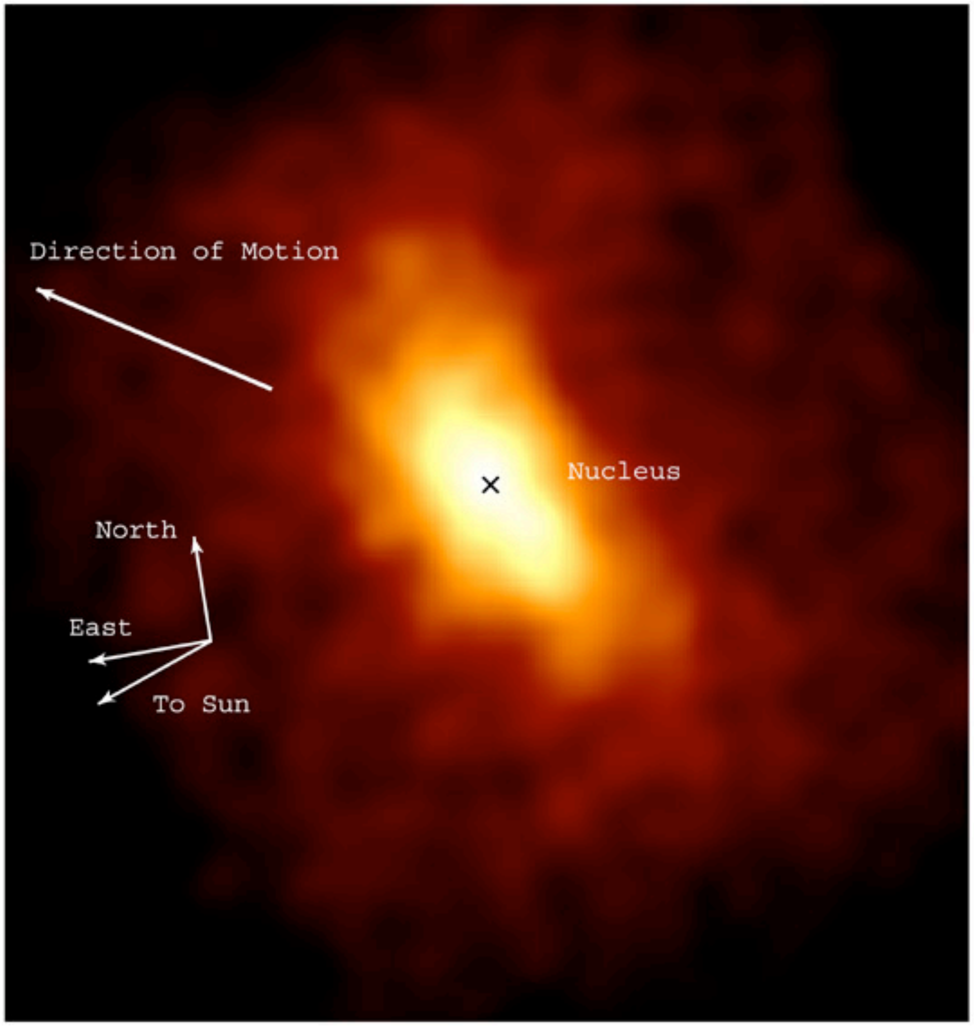
ITAMP

# New Challenges (cont'd)

- Close-coupling of lab astrophysicists ("data"-producers) and astronomers -- essential
- Quality of the atomic/molec/solid state data affects the astrophysics significantly --> astronomers need to be more concerned
- New expts, new theor. methods available to provide data at much higher accuracy than in the past
- Lab Astro needs to gain support for its research in the astronomy community

There will always be astronomical mysteries that can only be solved by Lab. Astro. studies

# Understanding the Origin of Cometary X-rays

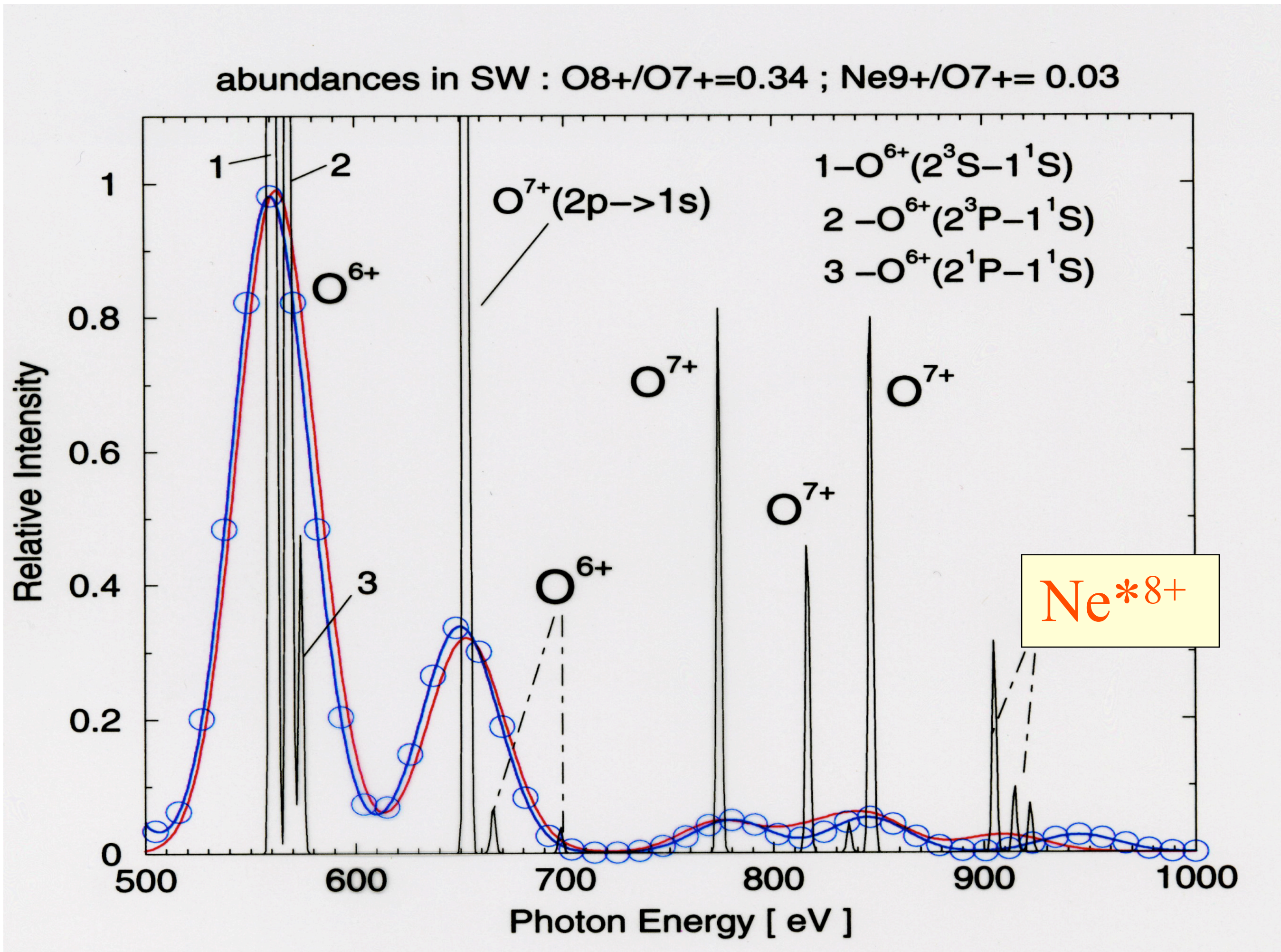


# Mystery!

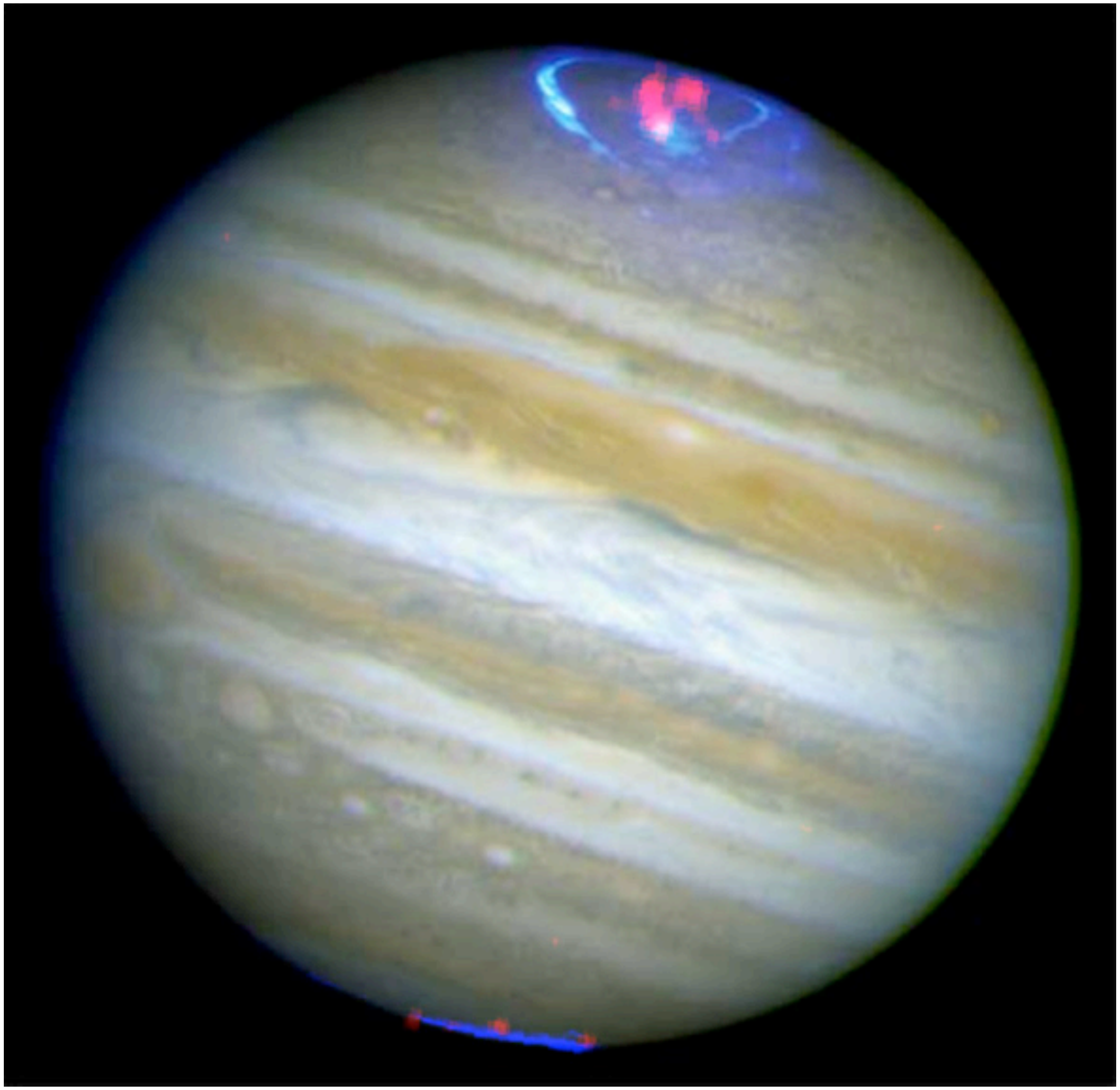
- Many possible mechanisms for x-ray production, (without an adequate spectrum)
- T. Cravens (1997) -- Highly-charged ions in the solar wind colliding with neutral species in the cometary atmosphere --> charge exchange and subsequent EUV and X-ray emission

# X-ray Diagnostics of the Solar Wind Plasma

## Emission Spectra of Comet McNaught Hartley



# Jovian X-rays



ITAMP

# X-rays from Charge Transfer

- Explains many planetary x-ray observations
- Major contributor to the heliospheric diffuse soft x-ray background
- In the future, with higher resolution spectra from new missions, and with improved expt and theory, cometary x-ray spectra could be used as important diagnostics of solar wind composition

# This mechanism does not have to be confined to solar system!

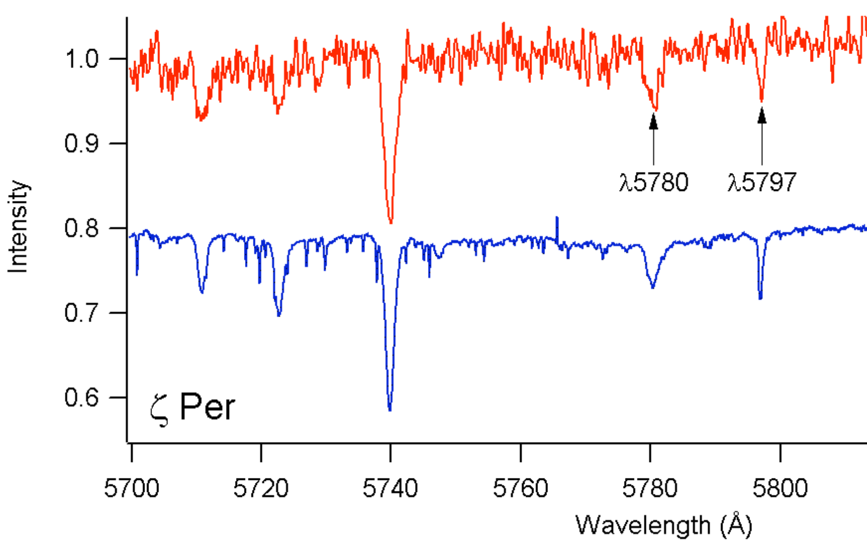
May predict the kind of x-ray spectrum to be expected in detailed observations of Active Galactic Nuclei

Interaction of a highly-ionized plasma with surrounding neutral gas

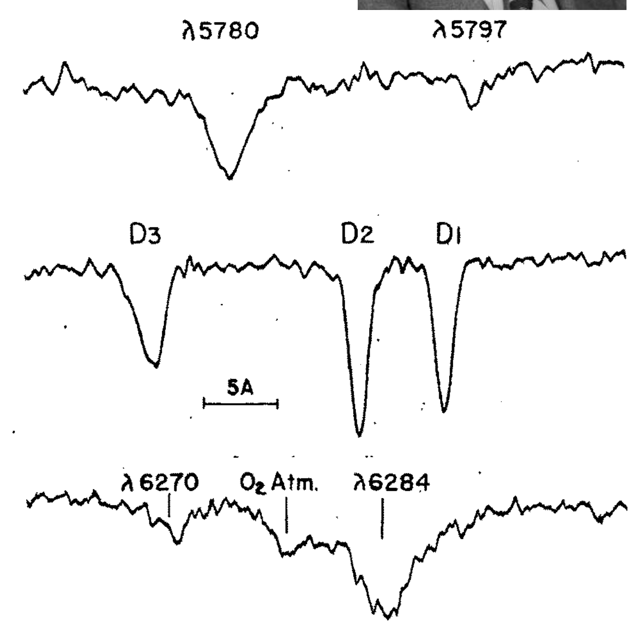
# Mystery #2
# Identity of the Carriers of The Diffuse Interstellar Bands (DIBs)
# Solution will come from Laboratory Spectroscopy!

# Discovery of the DIBs

- λλ5780, 5797 seen as unidentified bands
  - ζ Per, ρ Leo (Mary Lea Heger, Lick, 1919)
- Six bands confirmed as interstellar
  - Merrill & Wilson, Mt. Wilson, 1938
- Broad ("diffuse")

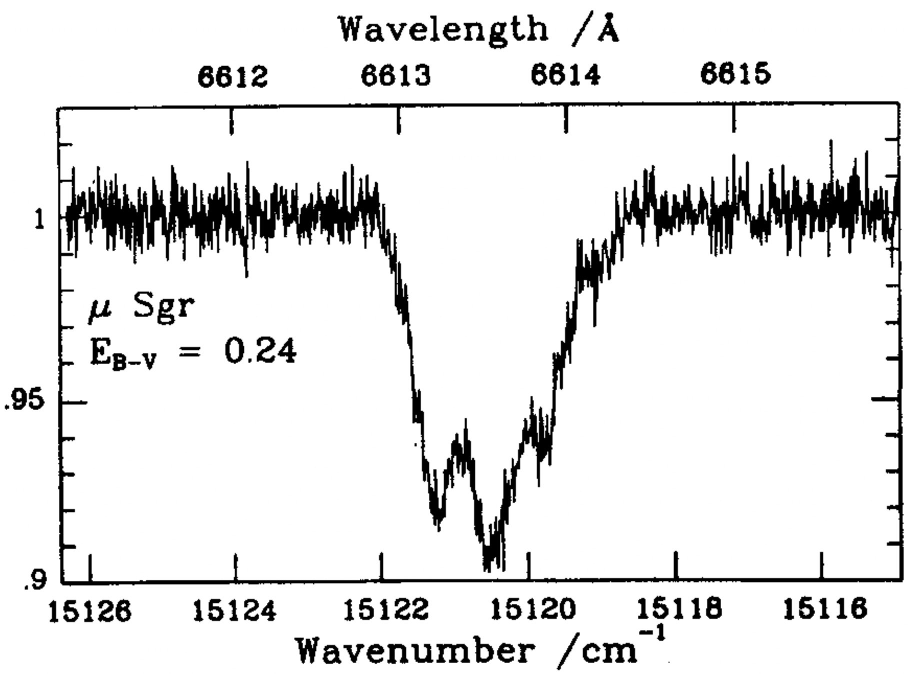



| | |
|---|---|
| 1960 | 10 |
| 1966 | 26 |
| 1975 | 39 |
| 1988 | 50 |
| 1994 | 229 |
| today | 400? |



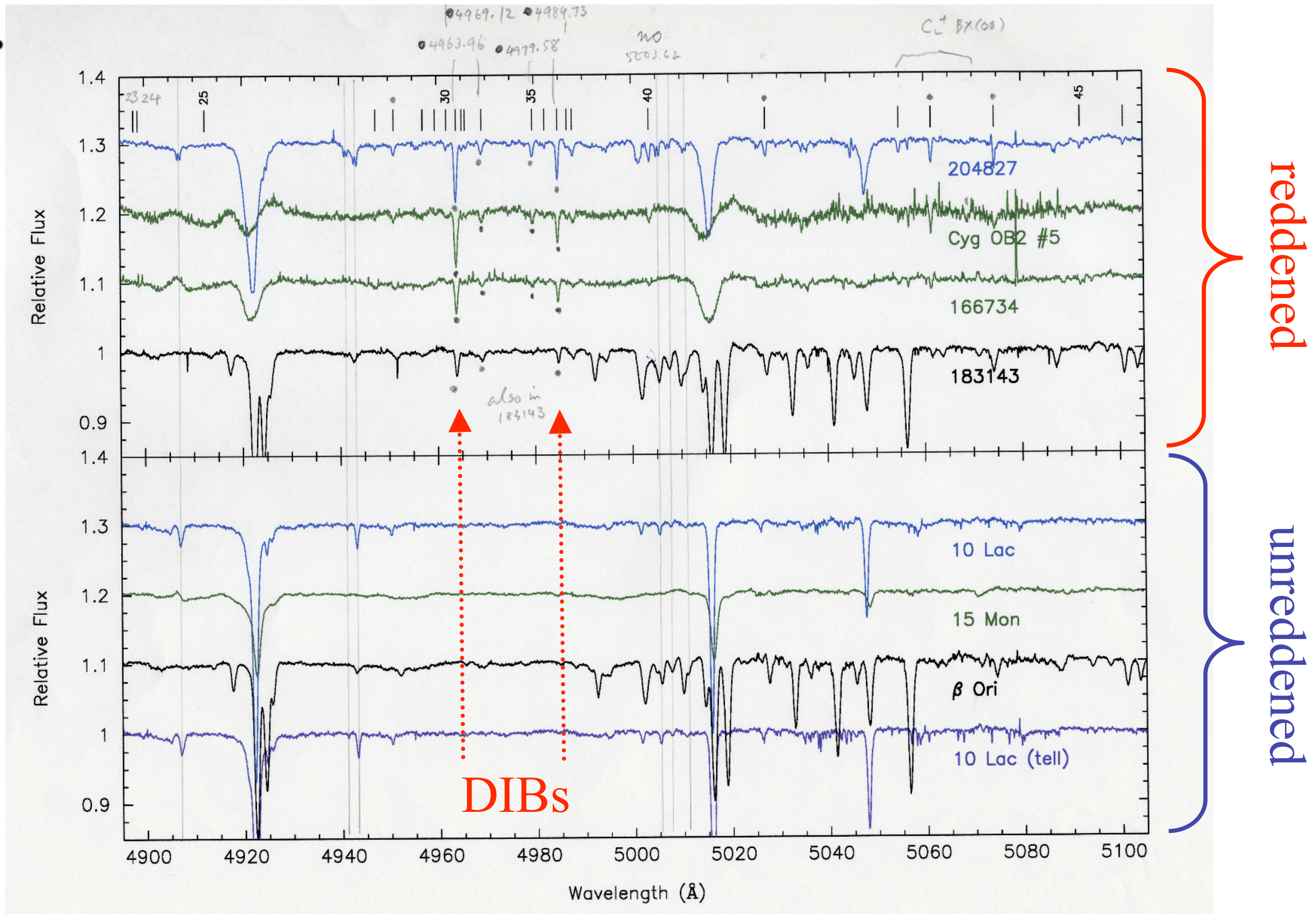
# What are the DIBs?

- Reasonable correlation with dust extinction
  - but “level off” at high $A_V \rightarrow$ diffuse clouds only?
  - for a long time, solid state carriers favored
- Several characteristics argue against dust:
  - constancy of $\lambda$
  - lack of emission
  - fine structure!




- Present consensus:
  - gas-phase molecules
  - probably large
  - likely carbon-based
  - reservoir of organic material
- Greatest unsolved mystery in spectroscopy!

# Stellar Spectra




D. G. York, B. J. McCall, et al., unpublished results

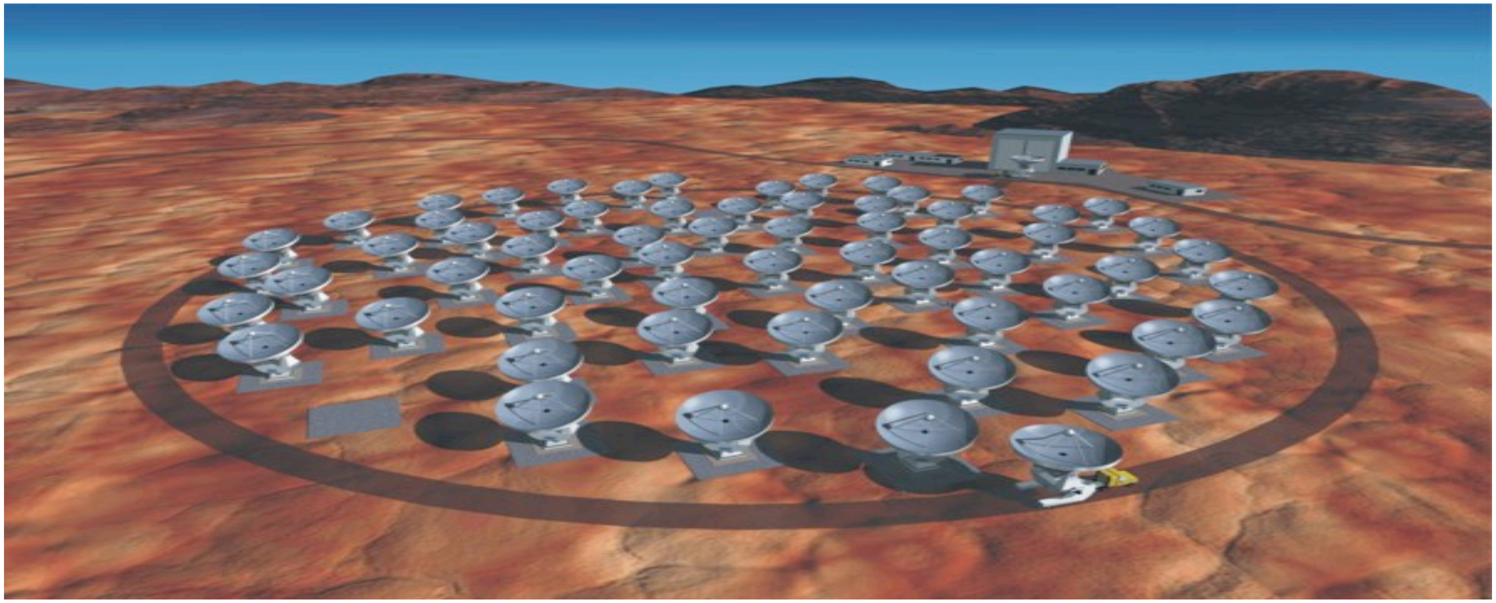
# New observations at high precision create demand for highly accurate Lab Astro data

# ALMA -- Atacama Large Millimeter Array

- Atacama Desert -- one of highest, driest places, ideal for astronomy at mm-wavelengths
- Located in foothills of the Andes in Chile

# ALMA

- International collaboration
- 64 radio-telescope antennas, each 12 m. across
- Frequency uncertainty is the leading uncertainty in the velocities of some molecular lines

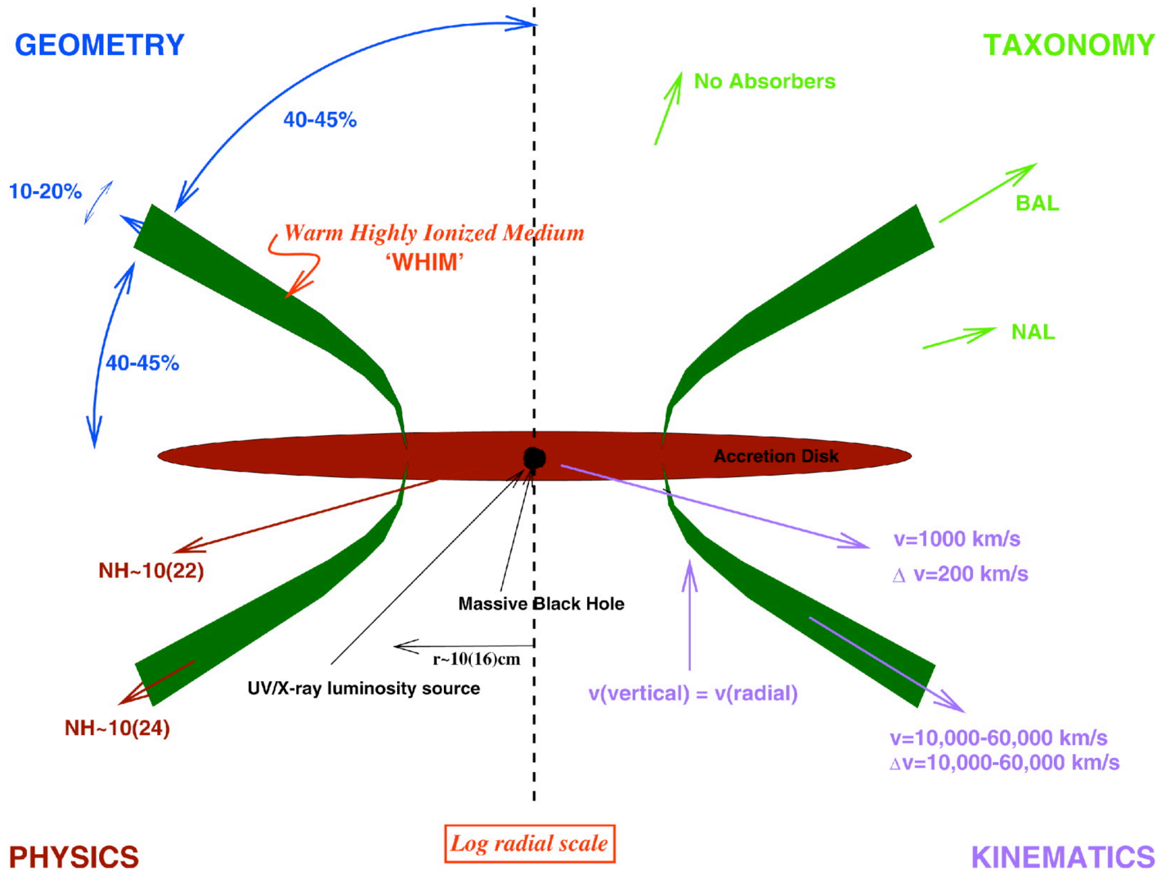


# New observations at high precision create demand for COMPLETE and accurate Lab Astro data sets

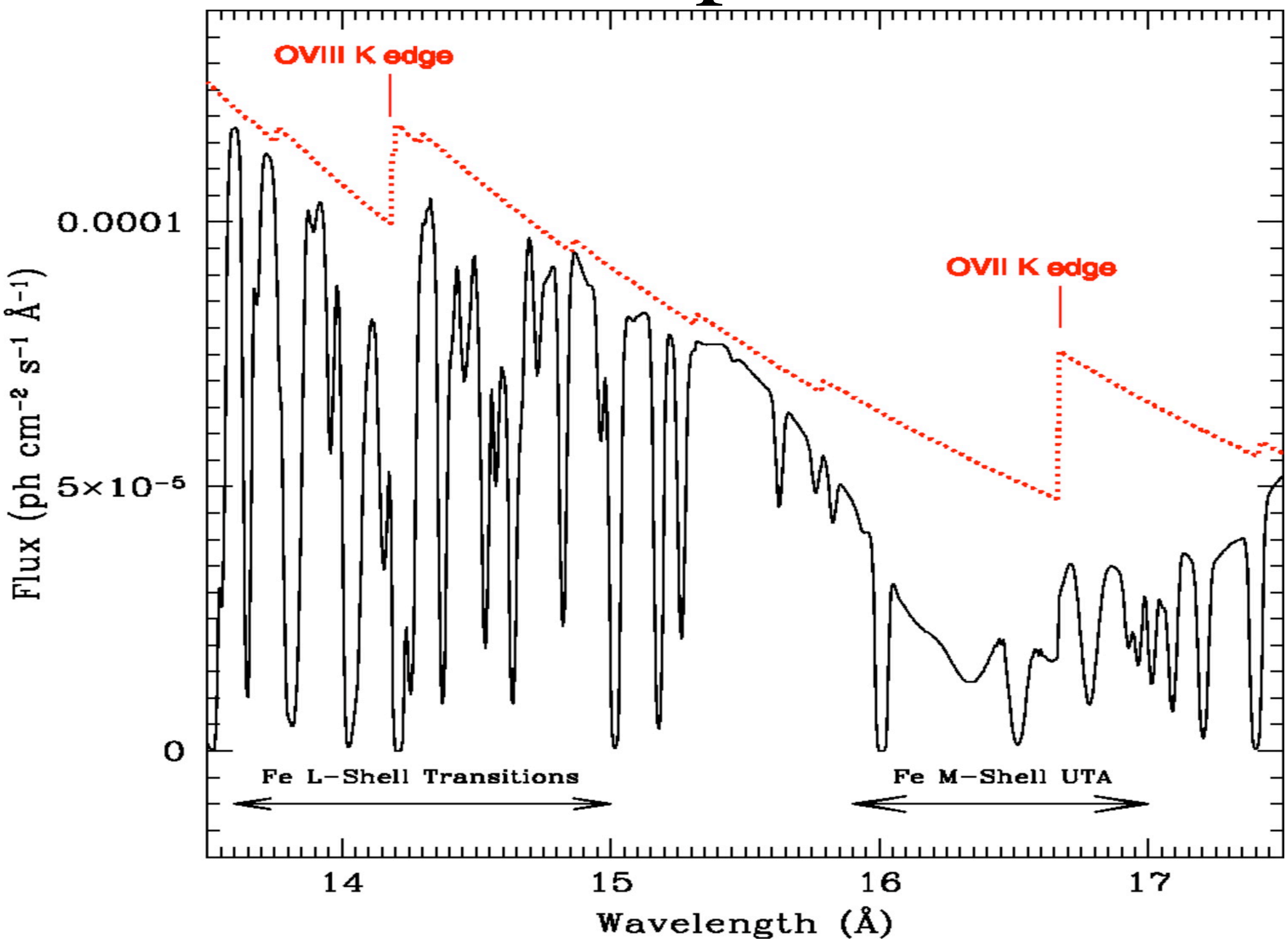
# Probing the Neighborhood of a Black Hole (Quasars/AGNs)

- Improved UV, X-ray spectra (STIS, FUSE, Chandra, XMM-Newton)
- Challenge to explain em./abs. features
- Spectral models essential to understand
  - The physical state of the gas
  - Its location and dynamics wrt central blackhole

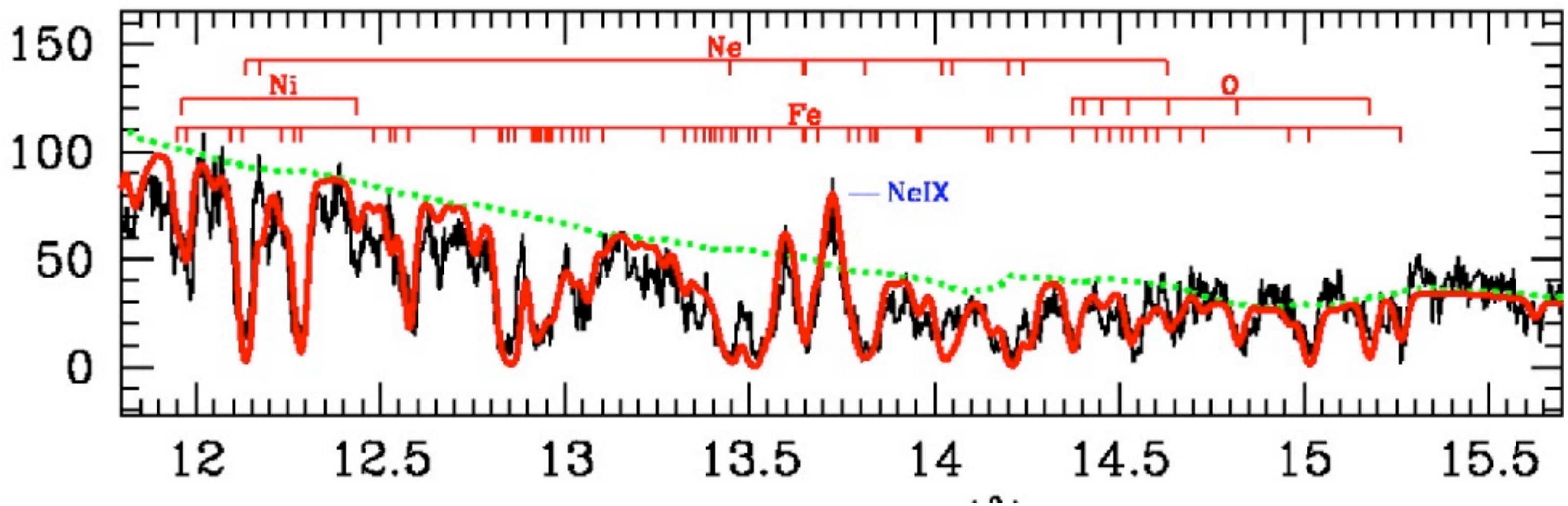
# Structure of a Quasar (M. Elvis, ApJ 545, 63 (2000))



# Models with Absorption Edges and with Absorption Lines



# Chandra HETGS spectrum of NGC 3783 (900 ks observation)




Krongold, et al., ApJ 597, 832 (2003)

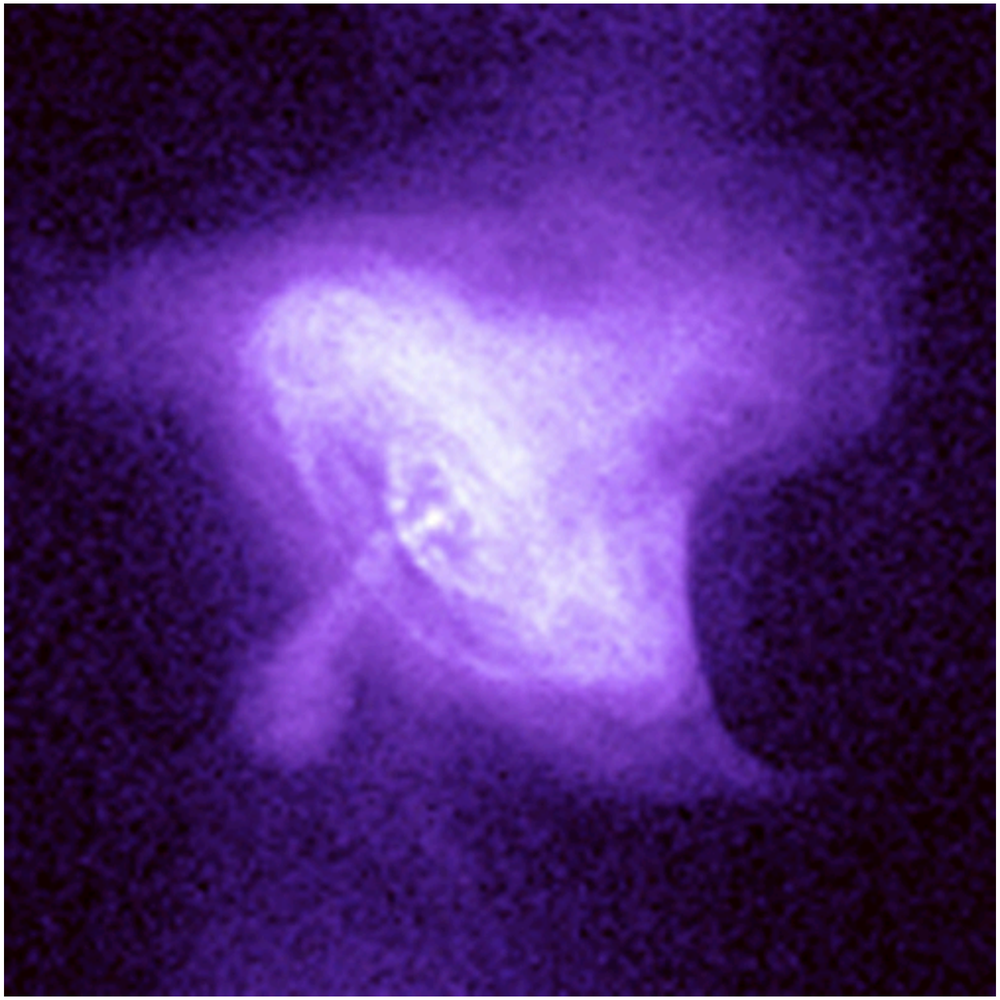
# Photo-ionized Plasma Models

- Need for MANY inner-shell absorption lines for species in a range of ionization states
- Improved spectral observations (lines) --> models (lines) --> can obtain velocities of the absorbing medium
- Conclusion:  spectra confirm that this gas is in the form of a wind

I T A M P

New experiments
New theoretical methods
available to provide data at much
higher accuracy than in the past

# Collisionally Ionized Plasmas: Models, Expts., Theory



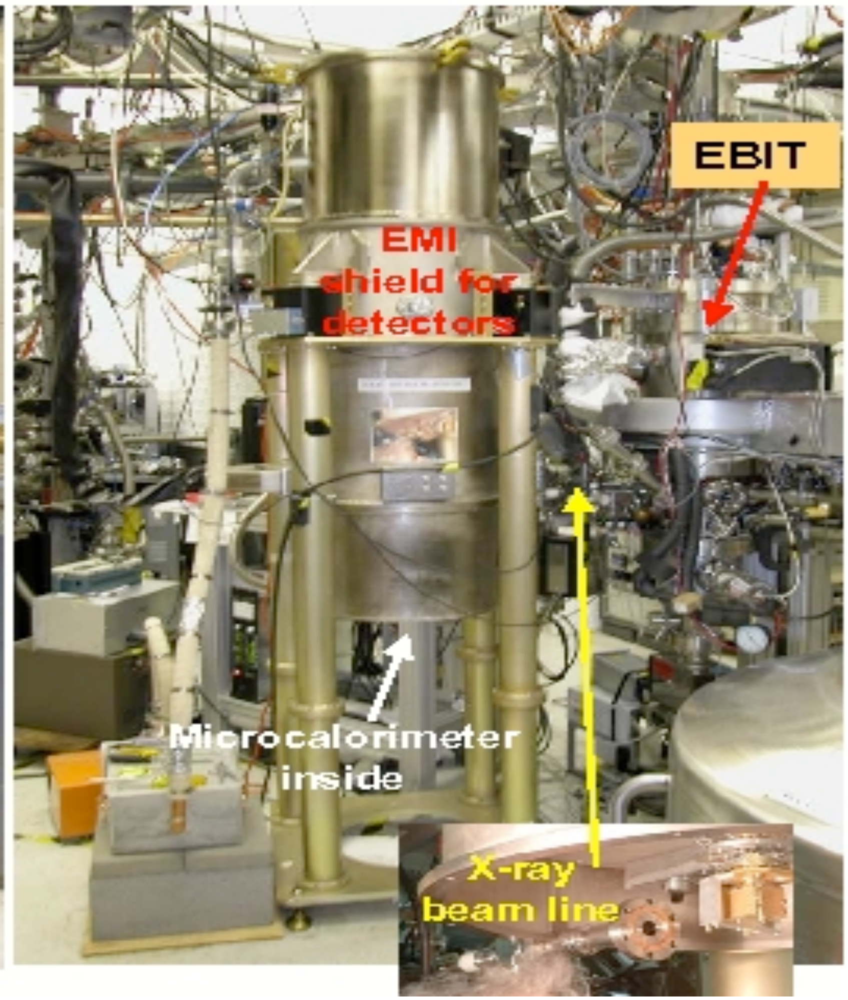
# Models Require:

- Detailed understanding of atomic collision processes over wide T range
- Huge amount of data:
  - Line identifications
  - Line strengths
  - Electron impact excitation cross sections
  - Dielectronic recombination cross sections
  - Radiative recombination cross sections
  - Ionization cross sections

# Models based on theoretical calculations

- Theory is able to explore a much broader range of the parameter space (temperatures, electron energies, densities, etc.) than expts.
- Theory data are more fundamental (cross sections) and do not include effects of laboratory plasma
- Important to have experimental measurements to benchmark the theory

# Electron Beam Ion Trap

# III. TSR DR Measurements

ITAMP

# Line intensity ratios can be powerful diagnostics of astrophysical plasmas --> determine T, electron density, ion abundances, opacity effects

# Fe XVII 3C/3D Line Ratio

**3C** $\lambda = 15.015 A \quad (2p^5 3d)^1 P_1^o \rightarrow (2p^6)^1 S_0$

Dipole allowed transition, strongest line in solar x-ray spectrum

**3D** $\lambda = 15.262 A \quad (2p^5 3d)^3 D_1^o \rightarrow (2p^6)^1 S_0$

Spin-forbidden intercomb. line

# Ni XIX 3C/3D Line Ratio

3C line (dipole-allowed, spin-allowed)

at 12.435 A

3D line (intercombination transition)

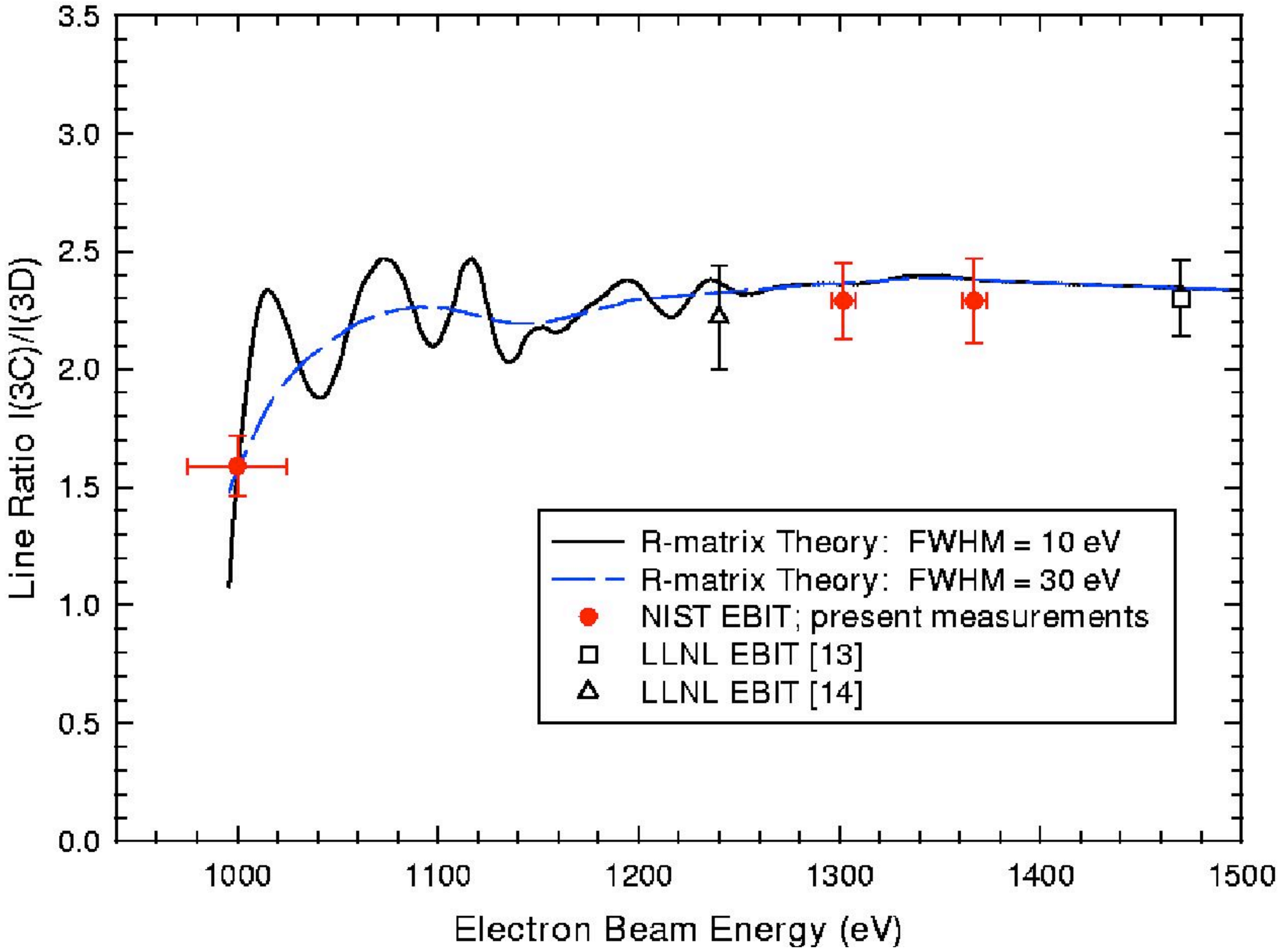
at 12.656 A

G.X. Chen et al., Phys.Rev.Lett. 97, 143201 (2006)

# 3C/3D Conclusions

- Benchmarks provided by the EBIT expts were extremely valuable
- Theory -- high accuracy (~ 5%) -- fully relativistic close-coupling calculation for the EIE of Ni XIX (incl. channel coupling effects/Rydberg series of resonances)
- For astrophysics, when Maxwellian average is needed, theory is highly desirable

# Ni XIX 3C/3D Line Ratio



# Improving the Interfaces

- Much can be lost
  - LabAstro “data” production -->
  - Databases -->
  - Incorporation in astrophysical models
- Very little support for databases
  - Development
  - Updating and maintaining
  - Critically evaluating data

I T A M P

# NASA Laboratory Astrophysics Workshop (Feb. 2006)

Held at UNLV, Las Vegas, NV

White paper developed by the Scientific Organizing Committee

http://www.physics.unlv.edu/labastro

# Sustainability of the Laboratory Astrophysics enterprise

- Funding for Laboratory Astrophysics in the U.S. is at an all-time low
  - Major paradigm shift (re atomic and molecular physics support at US govt. funding agencies)
  - Priorities for funding in the A&M Physics community do not align with astrophys. needs
  - Concerns regarding the maintenance of facilities
  - Concerns regarding training the next generation (students, postdocs)
  - Lack of faculty appointments in Lab. Astro.

# White Paper: General Findings

Necessity to develop and maintain complete (all ionization stages) and critically evaluated databases of atomic/molecular/solid state data

In many areas, theory and experiment are converging, so that the astrophysics is itself more secure

# General Findings (cont'd)

As observations are made at higher redshifts, phenomena associated with high energies are observed at long wavelengths!

Data requirements for advances in astrophysics from space missions are often the same as for gov't. sponsored research on plasmas & ground-based astronomy: Synergy possible

# Current and Future Needs

- Atoms and Ions in Astrophysics
  - Accurate and complete wavelengths
  - Oscillator strengths and transition probabilities
  - Rate coefficients for electron impact excitation and proton impact excitation
  - State-specific cross sections for dielectronic and radiative recombination
  - State-specific cross sections for charge exchange

# Current/Future Needs (cont'd)

- Molecular Astrophysics
  - High-resolution spectroscopic studies of hydrides, organic ions and radicals, biogenic compounds
  - Detailed understanding of chemical reactions and processes --> important reaction pathways, formation of new molecules
  - Collisional excitation cross sections
  - Quantum mechanical calculations

# ITAMP Current/Future Needs (cont'd)

- Dust and Ices in Astrophysics
  - Formation/destruction of interstellar grains
  - Physical properties of grains
  - Emission features of large aromatic molecules
  - Optical properties of candidate grain materials, including gas-phase molecules/nanoparticles/bulk
  - X-ray absorption by molecules and solids
  - UV spectroscopy of large organic and aromatic molecules needed for identification - IR not spec.

# General Recommendations

- Nat'l Research Council study of the need for/importance of Laboratory Astrophysics for the future of astronomical science
- Higher visibility for Lab Astro research within the astronomy community
- "Mission" support of Lab Astro
- Adequate funding for on-going database activities: compilation/critical evaluation

# With thanks to:

Jim Babb

Nancy Brickhouse

Guo-Xin Chen

Alex Dalgarno

Vasili Kharchenko