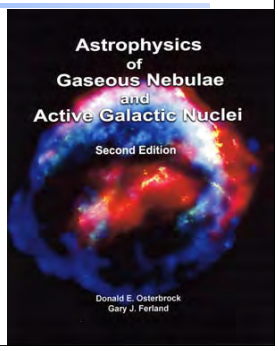
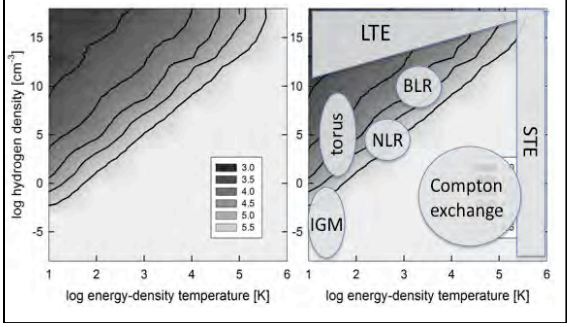
Ab initio spectral simulations

- Detailed microphysics
- Energetic radiation & particles interact with gas
- Ejected electrons heats, excite & ionize gas
- Ionization drives chemistry
- Kinetic temperature, ionization, full spectrum, predicted



The $n_H - T_u$ plane



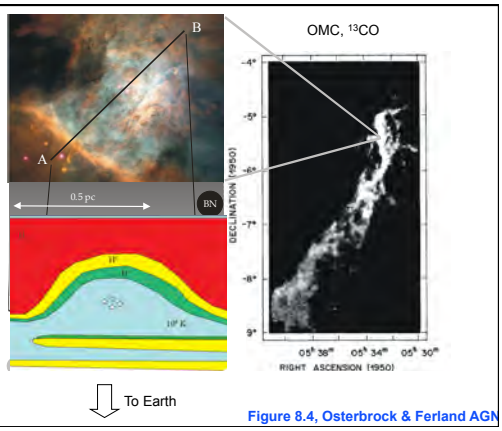
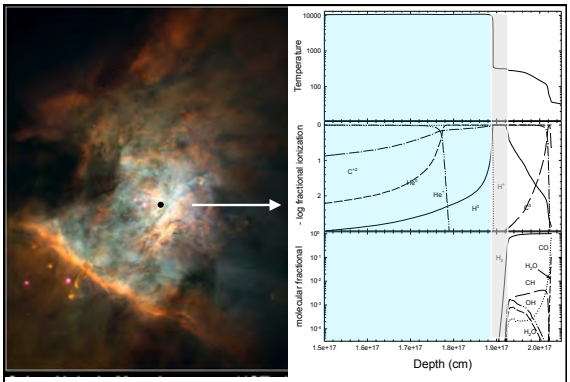
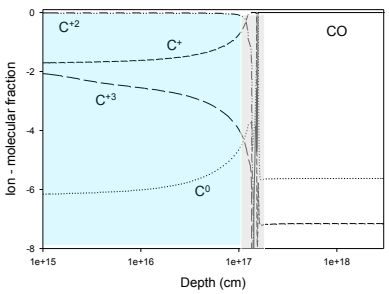


Figure 8.4, Osterbrock & Ferland AGN

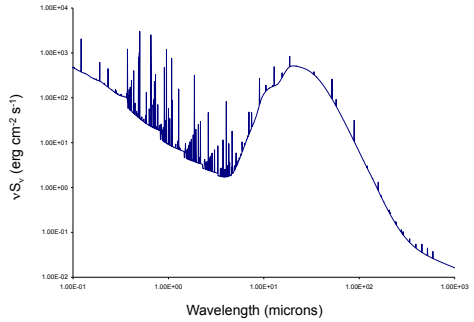


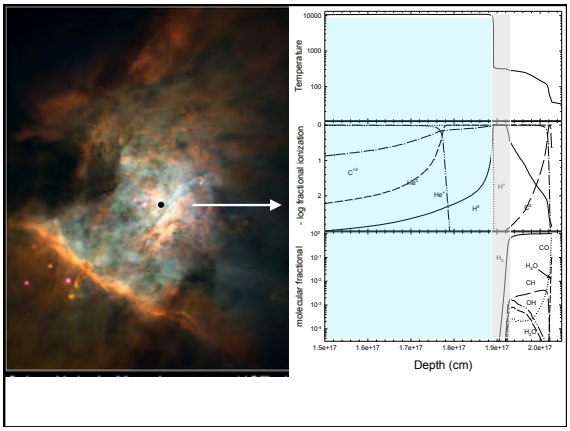
Ferland, G.J., 2003, ARA&A, 41, 517

Carbon ionization along ray

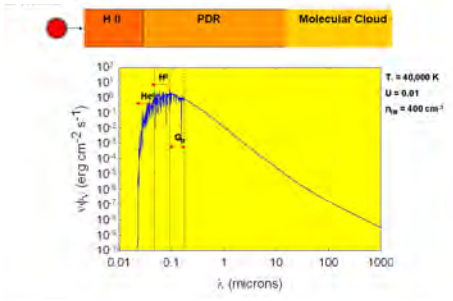


Spectrum at half-H_2 point



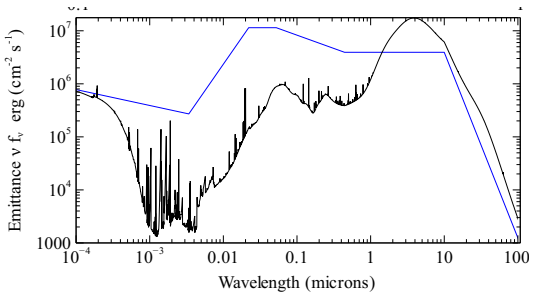


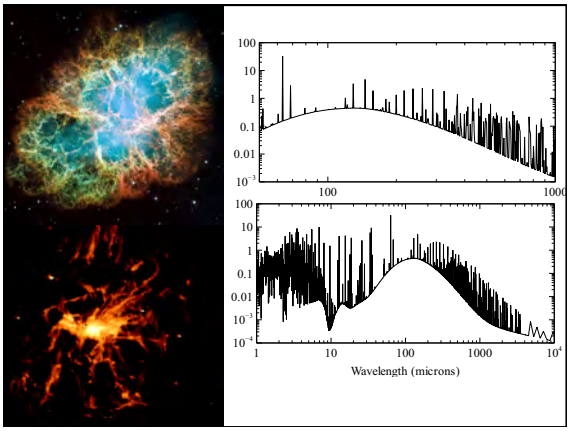
A holistic approach – the entire cloud



Abel et al ApJS 161, 65 astro-ph 0506514

AGN spectrum





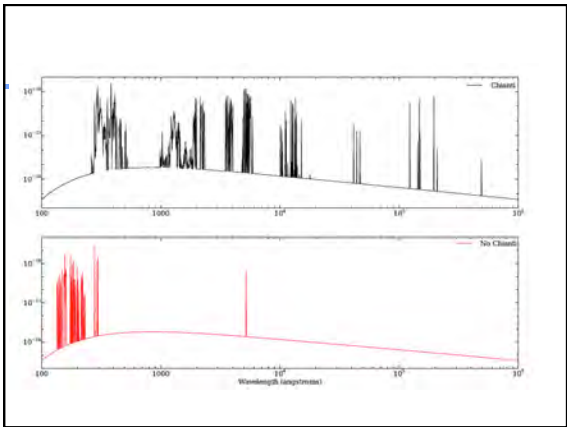
Databases used by Cloudy

- **Databases used within Cloudy**
  - Fe II with ~10^3 levels, H_2 with ~10^5 levels
  - Lamda molecular data base Schoeier+05
  - Chemistry UMIST
  - Chianti ionic data base Dere+09
  - Badnell RR & DR
  - Verner photoionization database with extensions
  - Kingdon charge transfer database with extensions
  - Ames PAH opacity database in progress

Our approach

- **Many databases are needed**
- **Use exactly the downloaded ascii files**
- **So that updates will be trivial**

- **This seldom works**



Properties of a good database

- **DRY – Don't Repeat Yourself**
- **Robustly machine readable**
  - Not fixed format, use field delimiters
- **Data provenance easily traced**
- **Data verified upon readin**
- **Data easily updated**
  - Computers are cheap and do exactly what we tell them to
  - People are expensive and make mistakes
  - Data should from the published paper