NUMERICAL SIMULATIONS OF INFRARED EMITTING REGIONS

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ABSTRACT

This paper centers on the development of Cloudy, a large-scale code designed to compute the spectrum of gas in photo-ionization or collisional balance. Such plasma is far from equilibrium, and its conditions are set by the balance of a host of micro-physical processes. The development of Cloudy is a three-pronged effort requiring advances in the underlying atomic data base, the numerical and computational methods used in the simulation, culminating in the application to astronomical problems. These three steps are strongly interwoven.
A complete simulation involves many hundreds of stages of ionization, many thousands of levels, with populations determined by a vast sea of atomic/molecular processes, many with accurate cross sections and rate coefficients only now becoming available. The scope of the calculations and the numerical techniques they use can be improved as computers grow ever faster, since previous calculations were naturally limited by the available hardware.
In recent years, Cloudy has undergone a major upgrade in the atomic data. A large part of this effort was concentrated on improving the photo-ionization cross sections. This work is not complete however, and this paper will give a detailed discussion of the remaining problems and our future plans for improving the atomic database. First of all we will discuss our plans for further improvement of the photo-ionization cross section database. Next we will discuss the need for more accurate recombination rates. In particular we will discuss the problems surrounding the calculation of accurate dielectronic recombination rates. For these, accurate energies of auto-ionizing levels will have to be measured in laboratory experiments, so a lot of work still needs to be done in this field. Furthermore we discuss the completeness of the line list included in Cloudy and the results of the Opacity Project and the Iron Project, which are important new sources for transition probabilities and collision strengths. Based on new SWS measurements of the [Ne V] lines of NGC 6302, we show that the suggestion of Oliva et al. (1996), that these new collision strengths would be too high for Ne V, is not correct.

Key words: Quantitative Spectroscopy — Photo-Ionization — Atomic Data – NGC 6302

1. INTRODUCTION

The majority of the quantitative information we have about the Universe comes from analysis and interpretation of spectra. This in turn rests on a foundation of basic atomic and molecular data. Astronomical plasmas are seldom in equilibrium, so often these basic data are combined with spectral synthesis codes to interpret observations. By such simulations, the potential of the new generation of astronomy satellites with high sensitivity and spectral resolution from infrared (ISO) through optical and UV (HST, HUT, EUVE) to X-ray (ASCA, AXAF) can be fully realized.
Deducing reliable abundances and luminosities of galactic and extra-galactic emission line objects is the central theme of the development of Cloudy. Emission lines are produced by warm ($\sim 10^4$ K) gas with moderate to low density ($n \leq 10^{12}$ cm^{-3}). Such gas is far from equilibrium, and its physical conditions cannot be known from analytical theory. Rather, the observed spectrum is the result of a host of micro-physical processes which must be simulated numerically.
The ionization, level populations, and electron temperature are determined self-consistently by solving the equations of statistical and thermal equilibrium. Lines and continua can be optically thick and their transport must be treated in detail. Predictions of the intensities of thousands of lines and the column densities of all constituents result from the specification of only the incident continuum, gas density, and its composition. By their nature, such calculations involve enormous quantities of atomic/molecular data describing a host of micro-physical processes, and the codes involved are at the forefront of modern computational astrophysics. Although the task is difficult, the rewards are great, since numerical simulations make it possible to interpret the spectrum of non-equilibrium gas on a physical basis. Cloudy has been developed as an aid to this interpretation, much as an observer might build a spectrometer.
These and the coming years will witness first light of a large number of new observational facilities over the whole range of the electro-magnetic spectrum, and we will be in a position to obtain spectra of faint objects with unprecedented precision. The basic atomic data base is growing in both precision and size, and high-end workstations have the power of yesterday's supercomputers — large scale numerical simulations

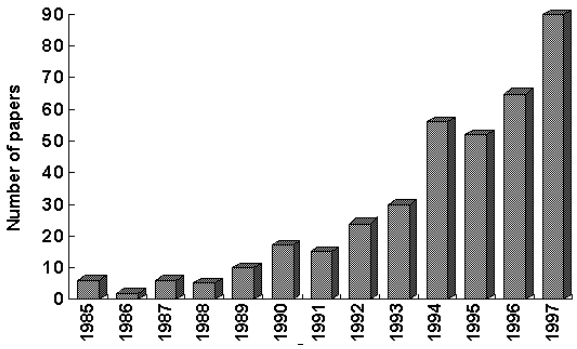

Figure 1. Refereed papers acknowledging Cloudy.

and spectral synthesis can now be done with unprecedented precision and facility. Cloudy is openly available, and other astronomers use it to publish roughly 70 refereed papers per year. It is a general spectroscopic tool whose development has an impact in many branches of astronomy.

1.1. Web Access and Community Use

Cloudy's source (about 110,000 lines of FORTRAN) and its documentation *Hazy, a Brief Introduction to Cloudy* (UK Physics Internal Report, 461 pages), are freely available on the World Wide Web through the Cloudy home page[1]. This page also contains a link to the group preprints. The atomic data used in Cloudy has also been made available separately on the *Atomic Data for Astrophysics* (ADfA) Web page[2] especially to serve the needs of spectral synthesis codes and astrophysical quantitative spectroscopy.

Cloudy is widely used by others in their analysis and theory of spectroscopic observations. Fig. 1 shows the number of refereed papers acknowledging the use of Cloudy through 1997. At least 240 papers have been published in 1993–1996.

2. DEVELOPMENT OF CLOUDY

2.1. Cloudy's Stability

A major use of spectral synthesis calculations is to deduce the conditions and abundances in the matter producing a spectrum. There is always a question of uniqueness since there may be more than one way to get any particular result, and we must work backwards to deduce the question (properties of the object) from the answer (the spectrum). Examining predictions over the very broadest possible range of physical parameters is vital to really understand what a spectrum is telling us. Today we usually use the code to generate very large grids, involving thousands of complete simulations, to generate contour or 3-D plots like that shown in Fig. 2.

[1] http://www.pa.uky.edu/~gary/cloudy
[2] http://www.pa.uky.edu/~verner/atom.html

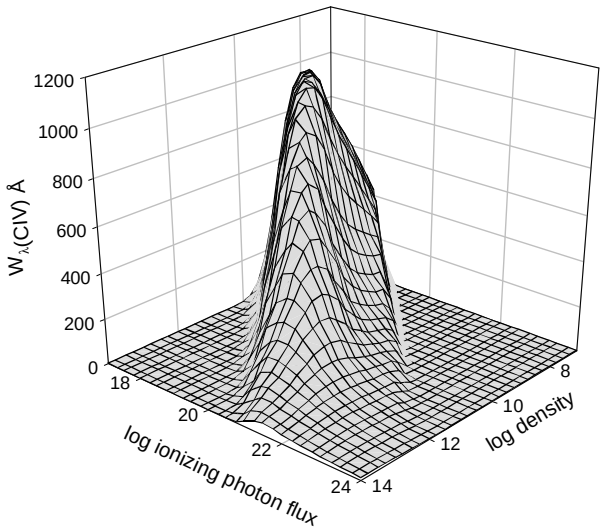

Figure 2. The C IV *λ1549 equivalent width for a wide range of densities and flux of photons.*

This is an example, based on Baldwin et al. (1995), showing that one of the strongest quasar emission lines is most efficiently produced over a very narrow range of conditions. The peak visibility occurs for the parameters long ago deduced as "standard" quasar conditions. We argued that this is just a selection effect.

A *major* effort has gone into making it possible to generate such large grids on a routine basis. Issues include the following:

The code must have enough intelligence to autonomously converge for models with very different conditions, without user intervention. This goal has largely been realized. All of the predictions shown here are the result of fully autonomous calculations with no outside intervention.

The code must respond appropriately, no matter what conditions it is asked to compute. It goes to the Compton, molecular, ISM, and LTE limits. The temperature limits are $2.8\ \mathrm{K} < T < 10^9$ K, and density limit $N \leq 10^{12}$ cm^{-3} because of the approximate treatment of line transfer, and since most ions are treated as two-level systems. The code will identify conditions which are inappropriate for its use.

The code must examine its results and predictions to confirm that the simulation is valid. It simply is not possible to go over the many tens of megabytes of results generated in large grids, after the fact, to confirm that all went well. As the code is developed, potential problems are identified and logic written to check for this in future calculations.

The code *will probably* converge a simulation with no problems, and it *will certainly* identify any problems at the end of the calculation. These are essential core features — vital if very large grids are to be computed reliably. Each simulation ends with a summary of all remarkable or surprising features, an analysis of any convergence problems, and checks

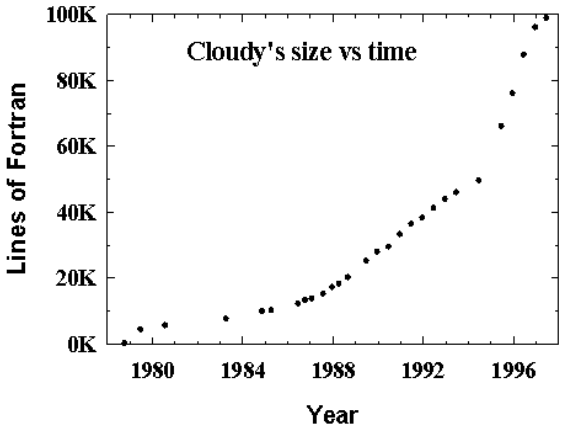

Figure 3. Cloudy's size as a function of time. This shows only the number of executable lines of FORTRAN. *The total distributed source now constitutes ∼110,000 lines of code.*

that the range of validity was not exceeded. One specific example of these internal checks is that the code now tracks timescales for all heating-cooling and ionization-recombination reactions. At the end of the calculation the code will identify the longest timescale. A warning is produced if the time-steady assumption is not valid.

2.2. Completeness of the Simulations

The code includes $\sim 10^4$ resonance lines from the 495 possible stages of ionization of the lightest 30 elements — an extension that required several steps. The charge transfer data base was expanded to complete the needed reactions between hydrogen and the first four ions, and fit all reactions with a common approximation (Kingdon & Ferland 1996). Radiative recombination rate coefficients were derived for recombination from all closed shells, where this process should dominate (Verner & Ferland 1996). Analytical fits to Opacity Project (OP) and other recent photo-ionization cross sections were produced (Verner et al. 1996a). Finally, rescaled OP oscillator strengths were used to compile a complete set of data for 5971 resonance lines (Verner et al. 1996b).

Many other improvements are summarized in Ferland et al. (1996). Fig. 3 shows a partial indicator of the scope of this activity, the number of lines of executable FORTRAN, as a function of time. The growth of the code in the past few years has been explosive, thanks to modern workstations.

2.3. Reliability in the Face of Complexity

This is the central difficulty in any large simulation since analytical answers are seldom known. Predictions are affected by the numerical approximations and atomic data used, as well as the presence of bugs which are certainly present in any large program. The best way to verify results is to compare completely independent calculations. We organized a workshop in 1994 to bring together researchers who have developed nebular codes. The result was the set of benchmarks published in the STScI Osterbrock-Seaton commemoration (Ferland et al. 1995). These benchmarks provide reference points to aid validation of any plasma code. We also make a continuous comparison of Cloudy with another independently written photo-ionization code, LineSpec (Verner & Yakovlev 1990).

3. FUTURE DEVELOPMENT OF CLOUDY

The long-term goal is for the ionization and thermal equilibria of all species and the radiative transfer of continua and lines to be exact for all conditions. By this standard, the code is well over half-way complete.

3.1. The Underlying Atomic Data Base

A major effort has gone into Verner's *Atomic Data for Astrophysics* (ADfA) database. The results of any fully non-equilibrium calculation are no better than the underlying atomic data. New data appear throughout the physics and chemistry literature; maintaining the data base is a major ongoing effort, but one that does not directly result in publications. The ADfA contains basic atomic data required for calculation of the ionization state of astrophysical plasmas and for quantitative spectroscopy. The home page had more than 6,000 visits and more than 12,000 data files were retrieved during October 1995 – October 1997. The contents of ADfA are driven by Cloudy's needs, which are defined by the spectroscopic problems. Because of this, and the public access we provide to our data, it has broad application to anyone working in quantitative spectroscopy.

3.2. Photo-Ionization Cross Sections

We have placed a great deal of effort into deriving accurate fits to the best photo-ionization cross sections, the corresponding radiative recombination coefficients, and incorporating them into Cloudy. We have created a complete set of analytic fits to the non-relativistic photo-ionization cross sections for the ground states of atoms and all ions of 18 elements, H through Si, and S, Ar, Ca, Fe (Verner et al. 1996). Near the ionization thresholds, these fits are based on the Opacity Project (OP; Seaton et al. 1992) theoretical cross sections, interpolated and smoothed over resonances. The OP data were not intended for energies well above the threshold. For these energies and for all inner-shell photo-ionizations we used calculated Hartree-Dirac-Slater photo-ionization cross sections (Verner et al. 1993, Verner & Yakovlev 1995). For the elements P, Cl, K, Sc through Mn, and Co through Zn, the Hartree-Dirac-Slater calculations were used over the entire energy range. The fit parameters and a FORTRAN

subroutine (PHFIT), which implements these fits are available now through ADfA.

The effort to improve these data is continuing, with the eventual goal of a complete photo-ionization cross section database, for all energies, of all atoms and ions of the first thirty elements. We plan the following developments:

- For some elements, accurate experimental data on the ground-state photo-ionization cross sections are only now becoming available. We are replacing the fits to the smoothed OP data by the fits to experimental data for such species.
- We shall replace the current fits by fits to more accurate theoretical cross sections (compared to the OP data) as soon as these new data become publicly available.
- Some photo-ionization cross sections include strong and wide resonances which cannot be smoothed, and energy positions of these resonances are accurately known by experiment. We are extending the treatment of such resonances in our fits.
- We are improving our current photo-ionization fits for the outer shells of non-OP elements up to zinc ($Z = 30$) by use of isoelectronic interpolation of the fits for the OP elements.
- Our current fits reproduce theoretical non-relativistic high-energy asymptotes which cannot be applied for energies above 50 keV. We plan to produce a set of fits for relativistic photo-ionization cross sections based on available X-ray experimental data (see, e.g., Veigele 1973) using an analytical formula with the correct relativistic high-energy asymptote.
- We are creating fits for excited shell photo-ionization cross sections of atoms and ions based on the OP data near thresholds, and on new Hartree-Dirac-Fock calculations far from threshold. These data are needed for dense environments, and for accurate radiative recombination rate coefficients.

3.3. Recombination Processes

A photo-ionization database is of restricted value unless it is matched with a self-consistent set of recombination coefficients. The predicted ionization balance would violate the approach to thermodynamic equilibrium were this not the case. The generation of self-consistent recombination involves three sets of physical processes — radiative, low-temperature dielectronic, and high-temperature dielectronic recombination. The computational challenges posed by each are discussed in turn. Although the challenges are great the rewards are far greater. We can reasonably expect, in the next five years, to be able to obtain the correct ionization balance for all ions of the lightest thirty elements, for all temperatures.

3.3.1. Radiative Recombination Rates

We have calculated radiative recombination rates for all H-like, He-like, Li-like and Na-like ions of elements from H through Zn, and fitted them with convenient analytical formulae (Verner & Ferland 1996). Using the proposed new fits to the excited shell photo-ionization cross sections data described above, we shall complete the calculations of radiative recombination rates for ions of all isoelectronic sequences of all elements up to zinc (Z=30), and fit them by analytical formulae. These rates will be sufficient for problems where the gas kinetic temperature is much, much less than the ionization potential of the species (this is the case, for instance, in the warm phase of the ISM). Higher temperatures will require the extensions described next.

3.3.2. Low-Temperature Dielectronic Recombination

Nussbaumer & Storey (1984, 1986, 1987) calculated the rates of low-temperature dielectronic recombination (LTDR) for first ions of C, N, O, Ne, Mg, Al, and Si using available experimental data on auto-ionization level energies. Nahar (1995) calculated for some ions total recombination rates, including LTDR, by use of a more sophisticated method which took into account the shapes of auto-ionization resonances. However, Nahar used theoretical OP positions of resonances which are less accurate than experimental ones, and the rate coefficients depend exponentially on this energy. For LTDR, errors in energy positions of resonances may be crucial, and the overall accuracy of the more complicated method by Nahar for the LTDR rates can give worse accuracy than a simpler method by Nussbaumer & Storey. We plan to calculate LTDR rates by the Nussbaumer & Storey's method using new experimental data on auto-ionization level energies. For species which do not have experimental data on auto-ionization levels, we will improve the OP theoretical energies by use of isoelectronic interpolation based on available experimental data. Preliminary study shows that such interpolations are reasonable, since the OP theoretical energies have systematic shifts in comparison with available experimental data. Finally, we plan to supplement our database with data compiled from the literature, and fit them by convenient analytical formulae. This extension to the recombination data base will provide nearly all the rate coefficients needed for a gas in photo-ionization equilibrium, where the gas kinetic temperature is less than the ionization potential of the dominant ionic species. This may apply, for instance, to the warm absorber, or the Fe Kα emission regions, of AGN.

3.3.3. High-Temperature Dielectronic Recombination

Most of the present collisional and photo-ionization codes, including Cloudy, use analytical fits for high-temperature dielectronic recombination (HTDR) rates based on calculations made in the low-density limit approximation (Aldrovandi & Pequignot 1973; Shull & Van Steenberg 1982; Arnaud & Rothenflug

1985; Arnaud & Raymond 1992). Application of these fits to the clouds of typical AGN emitting regions, with densities $10^{11} - 10^{13}$ cm^{-3}, is not entirely valid (Davidson 1975), although all photo-ionization codes now use either the low-density limit, or the Davidson approximation. We plan to use Summers (1979) data on the HTDR density dependence to create a set of two-parameter (temperature–density) analytical fits to the rates of HTDR.

3.4. The Line Data Base

We have compiled accurate wavelengths, energy levels, and atomic transition probabilities for the permitted resonance lines of all ionization states of astrophysically important elements (Verner et al. 1996b), and these data are in Cloudy. Thus, the resonance line list is fairly complete. However, the set of forbidden and intercombination lines is not complete, especially for high ionization transitions of 3rd row and higher elements. Using a compilation of experimental energy levels, we have calculated accurate wavelengths for a complete list of allowed, intercombination and forbidden transitions for nearly all ions and elements included in Cloudy. This list has been made publicly available on the World Wide Web[3,4] (van Hoof & Verner, this issue). We will compile atomic transition probabilities and collision strengths for these lines from the literature and from available atomic databases, including the Opacity Project database TOPbase (Cunto et al. 1993), the Iron Project (IP; Hummer et al. 1993) and the very recent database CHIANTI (Dere et al. 1997). We will discuss these data in more detail below.

3.4.1. Transition Probabilities

The Opacity Project is a valuable source of transition probabilities for the permitted multiplets of astrophysically important elements. However, the OP data cannot be directly used for astrophysical spectroscopy. Firstly, the OP gives only multiplet-averaged oscillator strengths. Secondly, the OP multiplets have only theoretical wavelengths. Therefore, the OP data must be adjusted to be used for spectroscopy. Recently, we used the OP data for compilations of atomic data for resonance absorption lines (Verner et al. 1994; Verner et al. 1996b). For LS-coupling permitted multiplets, we recalculated the multiplet-averaged gf-values to f-values of individual lines. Then, we used up-to-date compilation of experimental energy levels to assign accurate experimental wavelengths to the obtained lines. And finally, we improved the recalculated OP f-values by use of the experimental energies. A comparison of these improved f-values for lines of Fe ions with the best data from an evaluated compilation by Fuhr et al. (1988) shows that for the lines which can be classified as LS-type allowed lines, the improved OP f-values are fairly accurate. We plan to use the proposed procedure subsequently to adjust the OP f-values also for strong non-resonant LS-coupling permitted lines, and supplement the list of lines by data for intercombination and forbidden lines compiled from literature sources.

[3] http://www.pa.uky.edu/~peter/opt_list/linelist.html
[4] http://www.pa.uky.edu/~peter/line_list/linelist.html

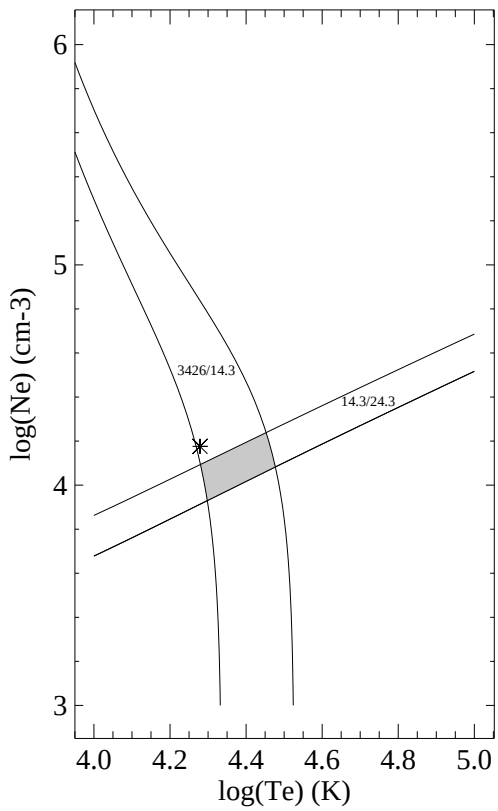

Figure 4. The diagnostic diagram derived from the [Ne V] lines in NGC 6302, using the new SWS measurements. The shaded area indicates the possible range of values derived in this work, the asterisk indicates the preferred values from Oliva et al. (1996). We conclude there is no significant discrepancy between the two.

3.4.2. Collision Strengths

The majority of the $\sim 10^4$ heavy element lines now use collision strengths from $\overline{g}$-approximations (Gaetz & Salpeter 1983; Mewe 1972). These can be computed on the fly for any line, but should only be used for transitions with no quantal calculations. The Iron Project is producing large numbers of collision strengths which must be fitted and incorporated, if this remarkable data set is to be exploited. All the collision strengths will be averaged over Maxwellian electron distributions, checked for asymptotic behavior by use of the Burgess & Tully (1992) method. We will fit the IP data with a procedure drawing on our previous work on photo-ionization cross sections (Verner et al. 1996a). We will develop a generalized scheme to represent the full temperature dependence in terms of analytical fits, with coefficients that can be stored along with other line information.

The inclusion of resonances in the calculation of collision strengths, as was done in the IP data, can lead to much higher values than were previously published. Recently these new values have been questioned by

Oliva et al. (1996; OPR hereafter) In their paper they analyze the [Ne V] lines of the planetary nebula NGC 6302. Based on this analysis they suggest that the collision strengths derived for Ne V by Lennon & Burke (1991, 1994) are approximately a factor of 2.5 too high. For this paper we have redone their analysis, using the new ISO-SWS data available for the [Ne V] 14.3 μm and 24.3 μm lines (Pottasch & Beintema, this issue). For the [Ne V] λ3426 line we adopted the value used by OPR. We used the collision strengths from Lennon & Burke (1994) and the transition probabilities from Baluja (1985). The results are shown in Fig. 4. The two lines shown for each of the ratios indicate the 1σ-error margins for these ratios. These error margins were calculated assuming an uncertainty of 0.1 dex in $c(\mathrm{H}\beta)$ (taken from OPR), a combined 30 % uncertainty in the absolute flux calibration of the SWS spectrum and the UV flux measurement, and a 10 % uncertainty in the relative flux ratio of the two infrared lines. The shaded area indicates the range of likely values for T_e and n_e. The asterisk marks the preferred values of OPR $T_\mathrm{e} = 19\,000$ K and $n_\mathrm{e} = 15\,000$ cm^{-3}. From our analysis we find $T_\mathrm{e} = 24\,000 \pm 5000$ K and $n_\mathrm{e} = 12\,600 \pm 2300$ cm^{-3}. One can see that the preferred values of OPR are only marginally outside the range of values we find. Therefore we argue that the discrepancy between the density from the [Ne V] and other lines found by OPR, mainly stems from the inaccuracy of the LRS measurement of the [Ne V] 14.3 μm line. Based on the NGC 6302 data there is *no reason* to assume that there are any problems with the collision strengths for Ne V calculated by Lennon & Burke (1994).

4. ACKNOWLEDGMENTS

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