1. X-rays from a Hot Plasma

EMISSION LINES FROM HOT ASTROPHYSICAL PLASMAS

John C. Raymond

Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, USA

ABSTRACT. The spectral lines which dominate the X-ray emission of hot, optically thin astrophysical plasmas reflect the elemental abundances, temperature distribution, and other physical parameters of the emitting gas. The accuracy and level of detail with which these parameters can be inferred are limited by the measurement uncertainties and uncertainties in atomic rates used to compute the model spectrum. This paper discusses the relative importance and the likely uncertainties in the various atomic rates and the likely uncertainties in the overall ionization balance and spectral line emissivities predicted by the computer codes currently used to fit X-ray spectral data.

1. INTRODUCTION

High resolution X-ray spectroscopy gives us access to the huge amount of information contained in X-ray spectral lines. The *Einstein* and EXOSAT satellites have provided a taste of detailed spectroscopy of cosmic plasmas, and the next generation of X-ray satellites should give us spectra comparable to those obtained from solar flares. The interpretation of spectral lines from cosmic plasmas, which so far has been limited mostly by the spectral resolution or statistical quality of the data, may then be limited by the accuracy of theoretical models of the X-ray emission. The accuracy of our inferences about the elemental composition, the density, and the temperature structure of the emitting plasma is no better than the accuracy of the atomic rates and other assumptions which go into the model.

Here we'll concentrate on the atomic rates and their reliability. To keep the discussion simple, the temperature of the emitting gas is assumed constant as a function of time. Density effects are ignored and diffusion due to steep temperature and density gradients is taken to be negligible. The electron velocity distribution is taken to be Maxwellian, and electric and magnetic fields are assumed to be weak. We'll also assume that photoionization is insignificant and that line and continuum optical depths are small. The limits of validity of these assumptions and some of the consequences of their violation are discussed in Raymond (1988).

The following sections discuss the processes which determine the ionization state of the plasma and the intensities of the spectral lines. Comparisons are then made between various spectral calculations and between a model computation and the X-ray spectrum of a solar flare.

2. IONIZATION BALANCE

Under the above assumptions, the ionization state of each element in the plasma is determined by a set of equations

$$0 = \frac{1}{n_e}\frac{dn_i}{dt} = q_{i-1}n_{i-1} - (q_i+\alpha_i)n_i + \alpha_{i+1}n_{i+1} \tag{1}$$

for each ion of the element, where q_i is the ionization rate coefficient from ion *i* and α_i is the recombination rate coefficient from ion *i*.

The accuracy of the available ionization and recombination rate coefficients varies widely. Ionization cross sections have been measured for a number of low and moderate ions by crossed beam experiments to 10 - 20% accuracy (e.g. Gregory *et al.* 1987). For many ions, cross sections computed in the Distorted Wave approximation are likely to be good to 20 - 30% (Younger 1981), but these are not yet available for all the astrophysically important ions. Auger ionization following innershell excitation makes an important contribution for some iso-electronic sequences. The best compilation of ionization rates is given by Arnaud and Rothenflug (1985). At fairly high densities, such as solar flares, corrections due to the population of metastable levels may increase the ionization rates somewhat.

The recombination coefficient is made up of radiative recombination and dielectronic recombination. The former,

$$A^{+j} + e^- \rightarrow A^{+j-1} + h\nu \tag{2}$$

is the inverse process of photoionization, so the detailed balance relation is used with the photoionization cross section to compute the rate, and the rate is just as accurate as the photoionization cross sections. For hydrogenic ions, the rates are accurate to a few percent. For more complex ions, the recombination to excited levels is computed by scaling hydrogenic rates, and the rate of recombination to the ground state is computed from the ground state photoionization cross section (e.g. Reilman and Manson 1979). Overall, radiative recombination the rates are generally good to around 30%. Radiative recombination rates to ions of the Li-like and Na-like sequences, which are quite a lot like hydrogenic ions, are probably more accurate. Radiative recombination rates for low ionization states of iron and nickel, which have very complicated structures, are worse. More accurate photoionization cross sections for both ground and excited levels should be available before long as a result of the Opacity Project (see Pradhan 1987).

In the dielectronic recombination process, an electron encounters an ion and excites it, but finds itself with negative energy, so that it is bound in some high *nl* state of the recombined ion. For example, a Li-like ion has a ground 2s level and excited 2p level. The process

$$2s + \varepsilon l \rightarrow 2pnl \tag{3}$$

has a very large cross section at energies ε just below the threshold for 2s - 2p excitation. The ion in the 2p*nl* state can either autoionize (reversing the process which formed it) or emit a photon, usually a 2s - 2p photon, to reach the bound, highly excited 2s*nl* state of the Be-like ion. The contributions of a large number of *nl* levels must be summed to find the total dielectronic recombination rate. Burgess (1965) fit the dielectronic recombination rates of many ions to a simple formula which is still widely used. It is probably good to its advertised accuracy of about 30% in the cases for which it was intended; elements up to calcium, and temperatures near the peak of the ionic abundance in coronal equilibrium. The Burgess formula requires modification at lower temperatures (Nussbaumer and Storey 1983), at high densities (Summers 1974), in strong electromagnetic fields (Müller *et al.* 1987), and in cases in which the doubly excited level can autoionize to levels other than the ground state (Jacobs *et al.* 1978). At present there is no no compliation of dielectronic recombination rates which adequately includes all these effects. Even sophisticated calculations of dielectronic recombination in complex ions can disagree by factors of two, and the only measurements of dielectronic recombination rates are dominated by field effects. Hahn (1985) reviews the theory, and recent calculations for some ions are given by Roszman (1987), Smith *et al.* (1985), and McLaughlin and Hahn (1984). Figure 1 compares several computed dielectronic recombination rates for the Li-like ion Fe XXIV. All the calculations agree at low temperatures, where recombination by way of 2s - 2p dominates, but they disagree badly at high temperatures, where excitation to the $n = 3$ levels becomes important. Unfortunately, the Fe XXIV emission lines are formed in the high temperature regime.

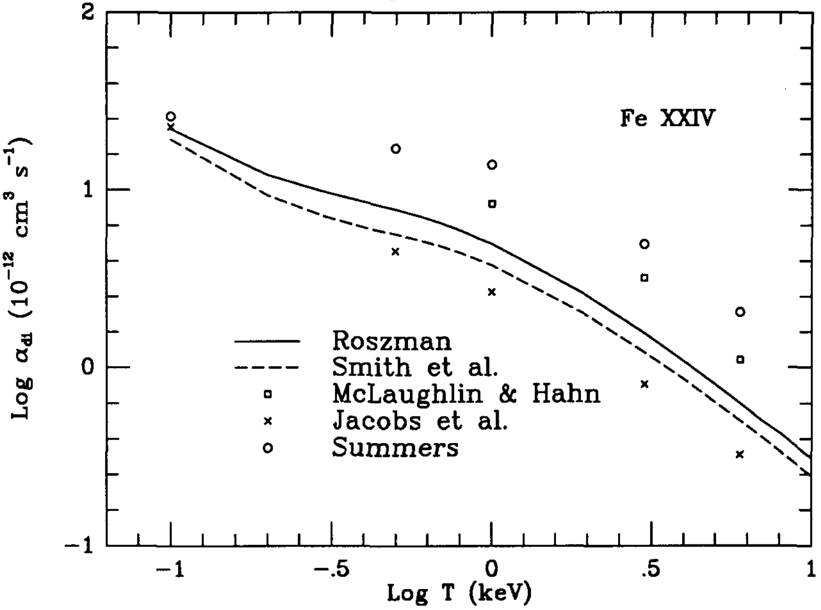

Figure 1. Dielectronic recombination of Fe XXIV.

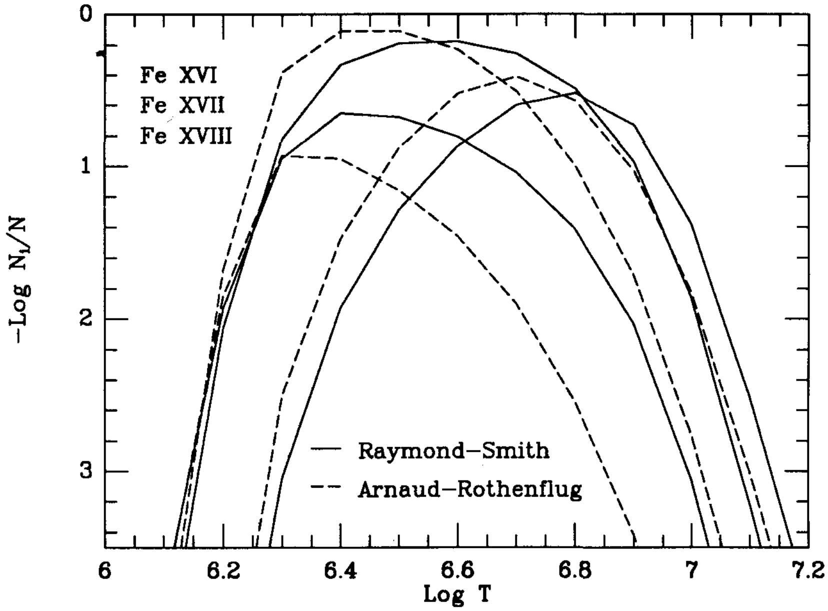

Figure 2. Concentrations of Fe XVI, Fe XVII and Fe XVIII.

Putting all the ionization and recombination rates together, we arrive at a computed ionization balance by solving the set of equations (1) for each element. Figure 2 compares the ionization balances computed for a few ions of iron by Arnaud and Rothenflug (1985) and the current version of the Raymond and Smith (1977) X-ray emission code. The ionic abundance curves in the different calculations look quite similar, but the peak temperatures are shifted by around 0.1 in log T. Figure 2 also shows an example of a more extreme difference. The Fe XVI abundance, which is controlled by dielectronic recombination of the complicated Ne-like ion Fe XVII, differs by more than a factor of two even at its peak.

3. RADIATION

The continuum emission includes bremsstrahlung, which has been computed to a few percent accuracy up to temperatures around 10^8 K, where relativistic corrections and electron-electron bremsstrahlung begin to be significant. The radiative recombination continuum is computed along with the radiative recombination rates, and is equally accurate. Radiative recombination continua of H- and He-like ions are generally by far the most important, and accurate cross sections are available. The two-photon continua of H- and He-like ions (arising from the metastable 2s and 1s2s ^{1}S levels respectively) make significant contributions to the X-ray continuum, and reliable cross sections for the excitation rates to these levels are available.

At temperatures below about 10^7 K, and in some energy bands at higher temperatures, the X-ray radiation is largely due to bound-bound transitions of the more abundant elements, especially O, Si, and Fe. The emissivity in a given line depends on the elemental abundance, the ionization balance and the excitation rate of the line. The reliability of the excitation rates varies widely. For excitations to $n = 2$ states of H- and He-like ions, extensive theoretical calculations in Close-Coupling and Distorted Wave methods are available, and for these simple ions the excitation rates are probably good to 10-20%. Thus the O VII and O VIII, Si XIII and Si XIV, or the Fe 6.7 keV features are not only the strongest lines in most X-ray spectra, they are also the most reliably interpreted. Higher lying levels of these ions, as well as most of the more complex ions, have not been as extensively treated. Distorted Wave cross sections are available for most of the $n = 2$ to $n = 3$ lines of Fe XVII through Fe XXIV which dominate the 1 keV complex of lines, but neither cascades nor resonances in the excitation cross sections, which significantly enhance some of the lines of Fe XVII (Smith *et al.* 1985) have been included for most of the ions. Some indication of trouble with the theoretical excitation cross sections comes from studies of the relative intensities of the $n = 2$ to $n = 3$ lines of Li- and Be-like ions in laboratory and a solar flare plasmas, in which most relative line intensities agree to the expected 20% level, but a few lines discrepant by a factor of two (Huang *et al.* 1988; Mackenzie *et al.* 1985).

A correction which must be included for some lines is the contribution of dielectronic recombination satellites. The decay of the doubly excited level in the dielectronic recombination process produces a photon near the wavelength of the resonance transition. Satellites to lines of He- and Ne-like ions tend to be most important, and the satellite contributions are largest for highly charged ions. The satellites are strongest relative to direct excitation of the resonance lines at low temperatures, so the cool side of the temperature range of an He- or Ne-like ion gives the largest satellite contribution. The satellite lines to the He-like resonance lines have been extensively studied for their diagnostic uses, and their predicted intensities are probably good to 20% (see review by Bely-Dubau 1988).

Another correction is the contribution of recombination to emission line intensities, following radiative recombination to excited levels or during the cascade of the recombining electron following dielectronic recombination. These terms are not generally included except for H- and He-like ions, where they increase the intensities of some lines by 20 - 30% in collisional ionization equilibrium (Mewe and Schrijver 1978). In a rapidly cooling plasma, or in a photoionized gas such as the accretion disk corona of an X-ray binary, this contribution can be much larger.

4. COMPARISON AMONG THEORIES

Several computer codes put together ionization balance calculations with excitation rates to predict X-ray emission spectra as a function of temperature for use in interpreting X-ray observations (Mewe, Gronenschild, and van den Oord 1985; Raymond and Smith, updated version of 1977 code; Gaetz and Salpeter 1983; Hamilton and Sarazin 1984; Shull 1981; Landini *et al.* 1985). Doschek and Cowan (1985) give a line emissivity list for the 10 - 200 Å range based on observed solar X-ray spectra rather than theoretical calculations. Comparison of these calculations gives some idea of their accuracy. Figure 3 shows the emissivity of the O VII λ21.6

line from several of these models. The uncertainties in both the ionization balance and the excitation rate for this line are fairly small, and the four calculations give quite similar results. The Fe XVII line at λ15.01 is shown in Figure 4. Here the

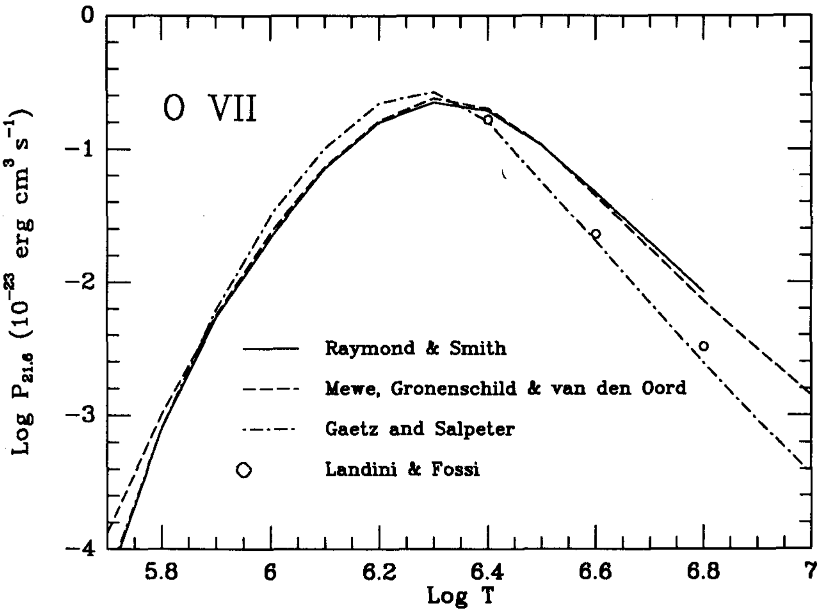

Figure 3. The O VII resonance line predicted by different models.

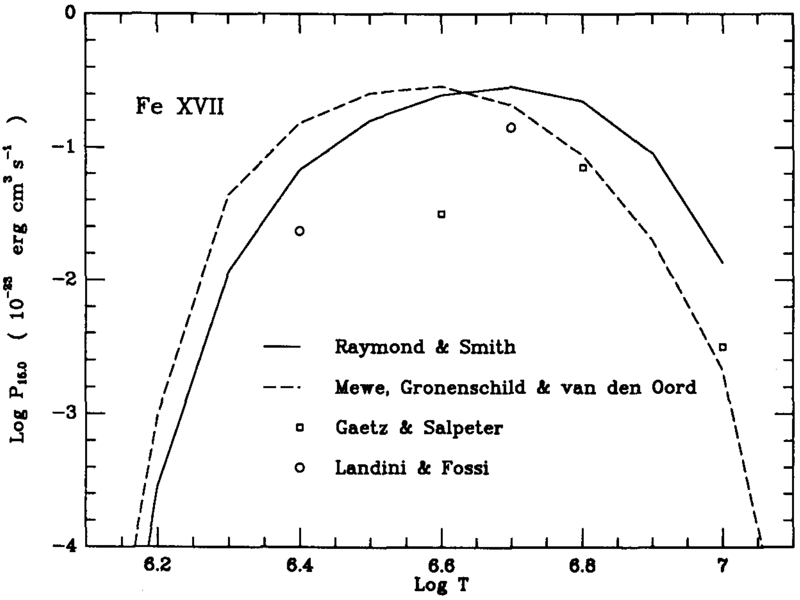

Figure 4. The Fe XVII resonance line.

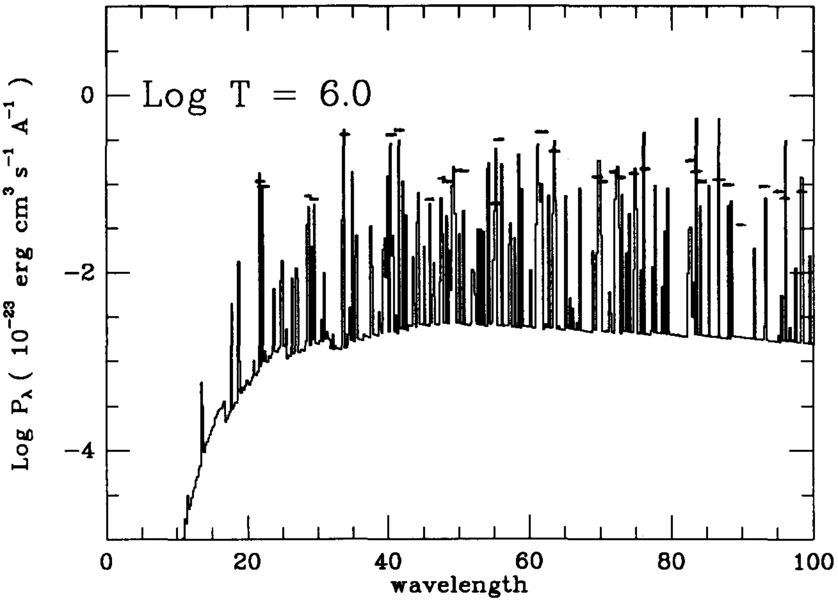

Figure 5. Comparison of X-ray emission codes.

disagreement among the calculations is much worse, mostly due to differing ionization balances used, though the excitation rates also differ somewhat.

Figure 5 shows the overall spectrum emitted by 10^6 K gas with solar abundances and 0.2 Å resolution as computed with the current version of the Raymond and Smith (1977) code. The emissivities of the strong lines given by Mewe, Gronenschild and van den Oord (1985) are indicated by the horizontal bars. It can be seen that the lines of H- and He-line C, N, and O agree quite well, as expected from the reliable rate coefficients for these simple ions. Many of the longer wavelength lines disagree by a factor of two, however. Much of this is due to differing ionization balance calculations, so that a line which peaks at log T = 6.0 in one model may peak at log T = 6.1 in the other. In general, low resolution spectra fit with different thermal X-ray emission models yield the same temperature, but somewhat different emission measures (Schmitt *et al.* 1985). With higher resolution data, the inferred plasma parameters will depend on the particular lines used. For the usual case in which a fairly broad range of temperatures is present, the shift in ionization balance of about 0.1 in log T among the various calcualtions will probably lead to a similar difference in inferred temperatures.

5. COMPARISON WITH OBSERVATIONS

Testing the models against observed spectra is obviously necessary. It is obviously necessary to have many more independent line intensities than model parameters. Only solar X-ray spectra provide adequate spectral resolution, statistical quality and wavelength coverage.

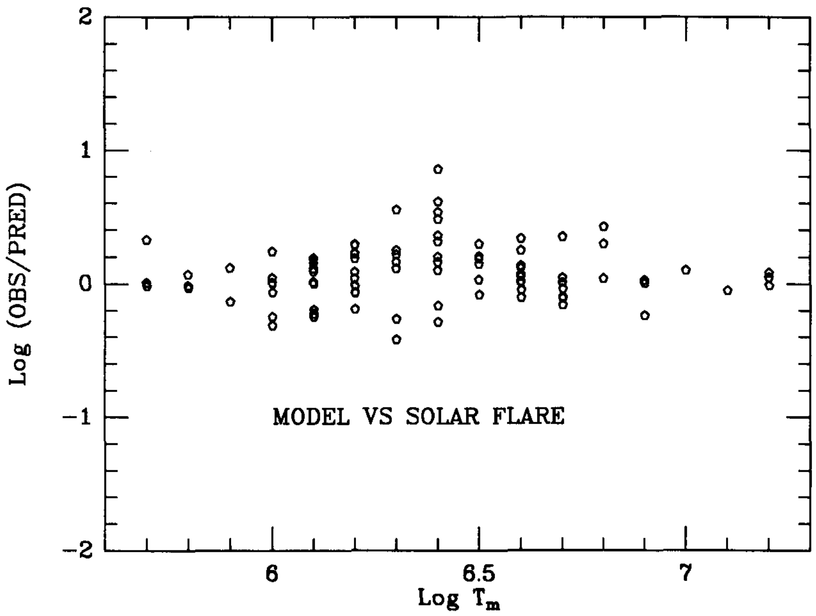

Figure 6. Comparison of model with solar flare observations.

A composite solar flare spectrum can be constructed by joining the 8-22 Å spectrum obtained with the SOLEX experiment on the P78-1 satellite (McKenzie *et al.* 1980) to the 15-100 Å flare spectrum obtained during a rocket flight (Acton *et al.* 1985) by scaling to the same O VII λ21.6 intensity. Some error results from this merging, but the long wavelength range contains mostly low temperature lines, while the short wavelength lines are formed at high temperatures. One then chooses a distribution of emission measure with temperature to match the intensities of some of the "most reliable" lines and iterates to improve the overall fit. The electron density is chosen to match the relative intensities of the O VII lines. Standard abundances were assumed, except that Mg was increased by a factor of 1.6, and Ca and Ni were doubled. Figure 6 shows a plot of the ratio of observed intensity to the intensity predicted by the model for 95 lines. The average absolute value of the log of the ratio of observed to predicted intensities is 0.17, indicating a factor of 1.5 typical error, with the worst line being stronger than predicted by a factor of 5. Based on the uncertainties quoted in the observational papers, it is likely that half the error is observational and half in the model. Further tweaking of the model parameters and further work on deconvolving line blends could reduce the discrepancy somewhat. It is not clear whether the remaining errors come from inadequate atomic physics or from a breakdown in some assumption such as ionization equilibrium or Maxwellian velocity distribution. Better model calculations, starting with improved collisional excitation rates for the complex ions, will be needed for the interpretation of AXAF and XMM X-ray spectra.

REFERENCES

Acton, L.W., Bruner, M.E., Brown, W.A., Fawcett, B.C., Schweizer, W., and Speer, R.J. 1985, *Ap. J.*, **291**, 865.

Arnaud, M., and Rothenflug, R. 1985, *Astr. Ap. Suppl.*, **60**, 425.

Bely-Dubau, F. 1988, in *Hot Thin Plasmas in Astrophysics*, Ed. R. Pallavicini (Kluwer: Dordrecht), p. 21.

Burgess, A. 1965, *Ap. J.*, **141**, 1588.

Doschek, G.A., and Cowan, R.D. 1985, *Ap. J. Suppl.*, **56**, 67.

Gaetz, T.E., and Salpeter, E.E. 1983, *Ap. J. Suppl.*, **52**, 55.

Gregory, D.C., Wang, L.J., Meyer, F.W., and Rinn, K. 1987, *Phys. Rev. A*, **35**, 3256.

Hahn, Y. 1985, *Adv. Atomic and Mol. Phys.*, **21**, 123.

Hamilton, A.J.S., and Sarazin, C.L. 1984, *Ap. J.*, **284**, 601.

Huang, L.K., Lippmann, S., Stratton, B.C., Moos, H.W., and Finkenthal, M. 1988, *Phys. Rev. A.*, **37**, 3927.

Jacobs, V.L., Davis, J., Kepple, P.C., and Blaha, M. 1977, *Ap. J.*, **211**, 605.

Landini, M., Monsigniori Fossi, B.C., Paresce, F., and Stern, R.A. 1985, *Ap. J.*, **289**, 709.

McKenzie, D.L., Landecker, P.B., Broussard, R.M., Rugge, H.R., Young, R.M., Feldman, U., and Doschek, G.A. 1980, *Ap. J.*, **241**, 409.

McKenzie, D.L., Landecker, P.B., Feldman, U., and Doschek, G.A. 1985, *Ap. J.*, **289**, 849.

McLaughlin, D.J., and Hahn, Y. 1984, *Phys. Rev. A.*, **29**, 712.

Mewe, R., and Schrijver, J. 1978, *Astr. Ap.*, **65**, 99.

Mewe, R., Gronenschild, E.H.B.M., and van den Oord, G.H.J. 1985, *Astr. Ap. Suppl.*, **62**, 197.

Müller, A., Belic, D.S., DePaola, B.D., Djuric, N., Dunn, G.H., Mueller, D.W., and Timmer, C. 1987, *Phys. Rev. A*, **36**, 599.

Nussbaumer, H., and Storey, P.J. 1983, *Astr. Ap.*, **126**, 75.

Pradhan, A.K. 1987, *Physica Scripta*, **35**, 840.

Raymond, J.C. 1988, in *Hot Thin Plasmas in Astrophysics*, R. Pallavicini, ed. (Dordrecht: Kluwer), p. 3.

Raymond, J.C., and Smith, B.W. 1977, *Ap. J., Suppl.*, **35**, 419.

Reilman, R.F., and Manson, S.T. 1979, *Ap. J. Suppl.*, **40**, 815.

Roszman, L.J. 1987, *Phys. Rev. A.*, **35**, 3368.

Schmitt, J.H.M.M., Harnden, F.R., Peres, G., Rosner, R., and Serio, S. 1985, *Ap. J.*, **288**, 751.

Shull, M.J. 1981, *Ap. J., Suppl.*, **46**, 27.

Smith, B.W., Raymond, J.C., Mann, J.B., Jr., and Cowan, R.D. 1985, *Ap. J.*, **298**, 898.

Summers, H.P. 1974, *Culham Laboratory Internal Memo* IM-367, Culham Laboratory, Ditton Park, Slough, England.

Younger, S.E. 1981, *JQSRT*, **26**, 329.

DISCUSSION-J. Raymond

S. Kahn: At what density are dielectronic recombination rates affected, say from Fe XVII?

J. Raymond: A highly charged ion with no δ n=0 transitions to the ground state is only affected at extremely high densities: around 10^{20} cm^{-3} for Fe XVII.

Y. Gnedin: You made comparison of predictions and observations mainly for solar flares. What is a situation with supernova remnants?

J. Raymond: Supernova remnants have more model parameters – abundances and non-equilibrium ionization – as well as fewer observed lines. One can choose the best fit model, but not really test the model beyond that.

J. Schmitt: You performed a comparison of line emission [ratios] between the Raymond & Smith and Mewe & Gronenschild code at Log T = 6.0. Could you comment on what this comparison looks like at Log T = 7.0 especially longward of 50Å ?

J. Raymond: The shift of around 0.1 in Log T should occur there, as well as at lower temperatures. Mewe & Gronenschild treat some multiplets as individual lines which Raymond & Smith lump together.

Dickel: Individual lines can be off a lot, but if you have many lines of one or more atoms and ions, how well can you get the temperature and density?

J. Raymond: Many atoms and ions still leave the problem of the uncertainty of $\sim$ 0.1 in Log T of the ionization balance calculations. Temperature sensitive line ratios of individual ions give a check on this. In the case of Fe XVII, though a similar scatter among several ratios is seen.

J. Canizares: In anticipation of the future X-ray spectroscopy missions, it would be very useful to have "empirically corrected" emission measures for some of the stronger lines that tend to be used for plasma diagnostics (for example the Fe XVII lines). In other words, it would be useful for observers to know which lines you have the most confidence in.

J. Raymond: The Doschek and Cowan line list determined from solar spectra is the thing to use.

H. Gursky: Can you comment on the effect of the physics of plasmas on the calculations you present?

J. Raymond: The major plasma effect to worry about is a non-Maxwellian electron distribution, since the only astrophysical plasma we can measure, the solar wind, shows non-Maxwellian tails. If such a tail is present at energies like 10kT, it can drastically affect the ionization.