Atomic Data: Energy Levels, Transition Rates, and Collision Strengths; An Example of Mg VIII

A. K. Bhatia
Goddard Space Flight Center, Greenbelt Maryland 20771

A number of satellites have been launched to observe radiation from various astrophysical sources. Line radiation is emitted when the levels in ions/atoms excited by electron or proton impact decay to lower levels by photon emission. From this radiation, the physical parameters, such as electron temperature and density of astrophysical plasmas, can be inferred. Electron impact excitation is, in general, more important than proton impact excitation except for fine structure levels in the ground levels. A number of methods have been used for calculating excitation cross sections: most commonly used are distorted wave (DW) approximation and the R-matrix approach. In DW approximation, channel coupling and resonances are neglected, and therefore the method is considerably simpler than the R-matrix approach. Rate coefficients and collision strengths, averaged over a Maxwellian distribution, are accurate to nearly 20% in DW approximation and 10% in R-matrix approach. A comparison of collision strengths in Ca XIII calculated in these two approximations is given in Ref. [1]. Proton excitation rate coefficients are calculated by semi-classical approximation [2]. With a number of collaborators, I have carried out DW calculations for a number of ions. In addition to excitation cross sections, energy levels, oscillator strengths, and transition rates are required. A number of papers have been published on atomic data for various ions. Cumulative indexes of *Atomic Data And Nuclear Data Tables*, **64**, 321 (1996) alone list 15 publications. Recent publications [3,4] are on Fe XV. The atomic data in Ref. [3] have been used to investigate the rocket spectrum of a solar flare in the 10 - 100 Å range and to identify the strong line at 69.65 Å. The atomic data in Ref. [4] have been used to calculate intensity ratios in the EUV range and compare with those observed by SERTS in an active region of sun. The calculated results should also be useful in analyzing observations from SOHO.

The atomic data are required not only to study intensities of emitted lines but also to study elemental abundances and opacity. Atomic data have also been used to study the Bowen fluorescence mechanism (e.g. in O III [5] and N III [6]). The atomic data are also of importance in planetary atmospheric studies, laser physics, and for diagnostics of Tokomak plasmas.

To calculate the atomic data, a set of programs developed at University College has been used extensively: the Superstructure and DW programs. In the Superstructure program, configuration interaction can be taken into account, and the radial functions are calculated in a modified Thomas-Fermi potential. Spin-orbit interactions, which give fine structure splitting, and relativistic corrections are treated as a perturbation to the nonrelativistic Hamiltonian. It is important to choose target configurations carefully in order to obtain accurate energy levels, oscillator strengths, and transition rates. The same radial functions are used in the DW calculation to calculate the excitation cross sections.

As an example, our most recent calculation is on the Mg VIII ion carried out in collaboration with Dr. R. J. Thomas [7]. EUV spectral lines of Mg VIII have been observed from the solar corona by Skylab, by SERTS, and more recently by SOHO. SERTS flights [8] were in 1989, 1991, and in 1993, and lines for which intensities were measured are 311.78, 313.74, 315.02, 317.01, 339.00, 430.44, and 436.73 Å. All these lines, with the exception of 430.44 and 436.73 Å, have been

measured by SOHO [9] flown in 1995. The figure in Ref. [7] shows a comparison of active region spectra taken by SERTS-89 and by CDS on SOHO.

Twenty levels are included by using the configurations $2s^2 2p$, $2s2p^2$, $2p^3$, $2s^2 3s$, $2s^2 3p$, and $2s^2 3d$ in the Superstructure program described by Eissner et al. [10]. Optimum Thomas-Fermi potential is obtained by minimizing the sum of term energies. The energy levels, oscillator strengths, and radiative rates have been calculated in intermediate coupling. These are given in Tables 1 and 2 of Ref. [7]. The potential obtained in the calculation of energy levels, oscillator strengths, and transition rates is used in the DW program described by Eissner and Seaton [11]. Reactance matrices are calculated in LS coupling and transformed to intermediate coupling by using term-coupling coefficients [12] obtained from the Superstructure program. It is not practical to include a very large number of incident partial waves. Therefore, contribution from higher incident partial waves to dipole-allowed collision strengths is included using Coulomb-Bethe approximation [13]. Collision strengths are calculated at five incident energies (15.0, 22.5, 30.0, 37.5, and 45 Ry), and they are given in Table 2 of Ref. [7].

The temperature of maximum abundance for this ion is $\log T_e = 5.9$ K. The rate coefficients are calculated at this temperature by averaging the collision strengths over a Maxwellian distribution. Level populations are calculated by the solving statistical equilibrium equations at a particular electron density, and intensity ratios are calculated using

$$I_{ij} = n_j \, A_{ji} \, \Delta E_{ij} \qquad \text{(energy units)}$$

where n_j is the fractional level population, A_{ji} is the transition rate, and ΔE_{ij} is the energy difference between the levels j and i.

A comparison with relative intensities observed by SERTS-89 in an active region is given in Table 1. The calculated intensity ratio I(313.74) / I(317.01) = 1.69 agrees reasonably well with the observed value 1.40. Inclusion of three more configurations, 2s3p3s, 2s2p3p, and 2s3p3d does not change the above calculated ratio appreciably. These lines originate from the same upper level, and therefore the ratio depends only on transition rates. This indicates that the calculated transition rates are reliable. The relative intensities of 436.73 and 430.44 Å remain in some disagreement with the calculated values. However, the intensity ratio I(436.73) / I(430.44) is found to be density sensitive, and at $\log N_e = 9.2$ (interpolated), its value is 1.68 which is the observed value from SERTS-89 (Thomas and Neupert). This density is comparable to the value of $\log N_e = 9.6$ derived by Brickhouse, Raymond, and Smith [14] from the same SERTS-89 spectrum, except using Fe IX line ratios formed at a similar temperature to those of Mg VIII.

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Table 1: Relative Intensities Observed by SERTS-89 compared to Calculated Values at Te=8x105K

Transition		λ(Å)	I_{obs}	I_{cal}				
				log(N_e)				
i	j			6	7	8	9	10[c]
1	10	311.778	0.313[a] ± 0.056	0.199	0.199	0.199	0.199	0.199
1	9	313.736	0.317 ± 0.049	1.380	1.062	0.540	0.395	0.378
2	10	315.024	1.000 ± 0.123	1.000	1.000	1.000	1.000	1.000
2	9	317.008	0.227 ± 0.052	0.816	0.628	0.319	0.233	0.223
1	8	335.230	---[b]	0.437	0.357	0.225	0.188	0.184
2	8	339.000	0.213 ± 0.033	0.627	0.511	0.322	0.269	0.263
1	6	430.445	0.159 ± 0.019	1.614	1.208	0.542	0.356	0.334
2	7	436.726	0.267 ± 0.032	0.108	0.255	0.498	0.566	0.574

[a] Blended with Ni XV, see Thomas & Neupert (1994)

[b] Masked by Fe XVI 335.40 Å

[c] Above log(N_e) = 10, ratios do not change

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