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COMPUTER CODES

Emissivity: A Program for Atomic Transition Calculations†

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Abstract. In this article we report the release of a new program for calculating emissivity and other physical parameters in atomic transition processes. The program, which can be downloaded with its documentation and a sample of input and output files from `www.scienceware.net/id1.html`, passed various rigorous tests and was used alongside R-matrix and Autostructure codes to generate theoretical data and analyze observational data. It is particularly useful for investigating atomic transition lines in astronomical context as the program is capable of generating a huge amount of theoretical data and comparing it to observational line list. A number of atomic transition algorithms and analytical techniques are implemented within the program and can be very useful in various situations. The program can be described as fast and efficient. Moreover, it requires modest computational resources.

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Key words: Atomic transition, recombination, autoionization, emissivity, computer code, thermodynamic equilibrium, decay routes, Saha population.

1 Introduction

The importance of atomic transition calculations cannot be overestimated as many scientific and technological applications rely upon them. For example they are extremely vital for astrophysical investigation and astronomical modeling. In laboratory-based studies,

†The computer program associated with this paper is available at the journal's homepage with the link `www.global-sci.com/code/v7-1118-c101.cpp`. It can be freely downloaded.

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they can be used to probe the conditions of laser induced plasmas and provide essential information required for analyzing fusion conditions. An important physical parameter in atomic transition processes is emissivity which is a measure of the power radiated by an emitting object. Various physical parameters and indicators associated with emissivity are usually computed during emissivity calculations.

There are two main methods for performing emissivity calculations. The first is by the use of a well-structured atomic database built for this purpose such as CHIANTI [1]. The other is by performing *ab initio* calculations by solving capture-decay equations based on user-prepared raw atomic data. Although the first method is more convenient, it cannot replace the other. One reason is the limitation of databases and the nature of their contents. These limitations include availability of particular data, quality of data, method of production, type of atomic target in atomic scattering calculations, coupling scheme under which the data was produced, and so on. In this article we present a computer code 'Emissivity' that performs emissivity calculations based on the second method. Despite the name 'Emissivity' which is attached to the program for historical reasons, the program can perform other atomic transition calculations, as well as emissivity, and hence it is useful in several situations where atomic database tools are of limited use.

2 Theoretical background

In a thermodynamic equilibrium situation an excited atomic state is populated by recombination and radiative cascade from higher states, and depopulated by autoionization and radiative decay to lower states. Many recombination lines arise from radiative decay and subsequent cascade of strongly autoionizing resonance states near the ionization limit. These lines are dominated by low temperature dielectronic recombination which is a two step process that involves the capture of a colliding continuum electron by an ion to form a doubly excited state. These excited autoionizing atomic systems give rise to resonances in the photoionization cross sections. The populations of such resonance states are determined by the balance between autoionization and radiative decay. When autoionization dominates, the populations are then given by the Saha equation for thermodynamic equilibrium

$$N_{X_{(n-1)+}} = N_e N_{X_{n+}} \frac{g_{X_{(n-1)+}}}{2g_{X_{n+}}} \left(\frac{h^2}{2\pi m_e kT_e} \right)^{3/2} e^{-\Delta E_t / kT_e}, \tag{2.1}$$

where ΔE_t is the energy of the recombined electron in the $X_{(n-1)+}$ state relative to the ionization threshold, and the other symbols have their usual meaning as given in Nomenclature Section 6.

The Saha equation, which describes the ratio of different stages of ionization, is based on the assumption of Local Thermodynamic Equilibrium (LTE) in a gas where collision dominates other physical processes. Consequently, the local velocity and energy distributions of particles are given by the Maxwell and Boltzmann distributions respectively