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Structural and collisional data for Mg III and Al IV

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Abstract

We present in this work energy levels, oscillator strengths, radiative decay rates and fine structure collision strengths for the Mg III and Al IV ions. The 11 configurations: $(1s^2)$ $2s^22p^6$, $2s^22p^53l$, $2s2p^63l$, $2s^22p^54l$ ($l \leqslant n-1$, where n is the principal quantum number), yielding the lowest 75 levels are used. The collisional data for these two ions are missing in the literature, especially the database CHIANTI, this is the principal motivation behind the present work. Calculations have been performed using the AUTOSTRUCTURE code. AUTOSTRUCTURE treats the scattering problem in the distorted wave approach. Fine structure collision strengths are calculated for a range of electron energies from 10 Ry to 240 Ry. The atomic structure data are compared to available experimental and theoretical results.

Keywords: Plasma diagnostics; X-ray spectra; Atomic structure; Impact excitation by electrons; Line broadening

1. Introduction

Neon-like ions have a high abundance over a wide range of electron temperatures and densities because of their closed-shell configuration ground state. Due to its various applications in astrophysics, plasma physics and spectroscopy, they have been the subject of investigation for many years. The ions of this sequence play an important role in the diagnostics of a wide variety of laboratory and astrophysical plasmas. For example, the energies and transition rates are used for the determination of radiative opacities of stellar envelopes, the Opacity Project (Seaton, 1987), for spectral diagnostics of solar, stellar and laboratory plasmas, for plasma modeling and for laser research, particularly in the soft X-ray region (Lee et al., 1987; Elton and X-Ray, 1990; Matthews, 1985; Feldman et al., 1984). They are used to study transport and confinement of high-Z impurity ions in tokamaks. Furthermore, oscillator strengths are important for the study of laboratory and solar spectra (Borges et al., 2004). Mg III and Al IV are two ions belonging to the neon-like sequence.

The Mg III spectrum was extensively studied by Andersson and Johannesson (1971). Later, an experimental work on this spectrum was published by Lundström (1973). An extensive level classification and wavelengths have been compiled by Kaufman and Martin (1991a). Hibbert et al. (1993) have calculated configuration-interaction wave functions in intermediate coupling for the states $2s^22p^6$, $2s^22p^53l$ ($l = 0, 1, 2$), and $2s^22p^63l$ ($l = 0, 1, 2$) of neon-like ions Ne I through Kr XXVII, incorporating variationally optimized orbitals and a modified Breit–Pauli Hamiltonian into the code CIV3. They have presented the percentage LS compositions of the LSJ levels, together with their energies, oscillator strengths, and probabilities of transition between them. Lifetimes of $2s^22p^53l$ levels have been also presented. More recently and using the multi-configuration Hartree–Fock (MCHF) method with relativistic effects, Fischer (2004) have obtained energy levels and transitions probabilities for transitions between computed levels for the Be-like ($4 \leqslant Z \leqslant 12$) to Ne-like ($10 \leqslant Z \leqslant 24$) sequences including the Mg III and Al IV ions (Z is the nuclear charge). A recent experimental study of Mg III was

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published (Brown et al., 2009). Further analyzes of the Mg III spectra have been performed and about 60 unobserved levels have been predicted (Liang et al., 2010) using the multichannel quantum defect theory (MQDT). The most recent results are those of Beiersdorfer et al. (2011), where the radiative decay rates of the $(2s^2 2p^5_{1/2} 3s_{1/2})_{J=0}$ level in neon-like ions have been calculated for nuclear charges ranging from $Z = 10$ to $Z = 110$.

In Artru and Kaufman (1975), a total of 225 new lines of Al IV have been observed in the wavelength range of 400–4700 Å, leading to the determination of all of the levels of the $2p^5 4p$, 4d, 4f, 5s, 5f, and 5g configurations. Martin and Zalubas (1979) have published energy levels for the atom and all positive ions of aluminum, where the authors have critically compiled their data using the published material on measurements and analyzes of the optical spectra. An extensive level classification and wavelengths for Al IV have been compiled by Kaufman and Martin (1991b). A more recent compilation of atomic transition probabilities for about 5000 lines of aluminium in all its ionization stages (except the hydrogenic one) has been published by Kelleher and Podobedova (2008).

To our best knowledge, there are no distorted wave fine structure collision strengths for the Mg III and Al IV ions to compare with. Although the number of published papers dedicated to the atomic structure of Mg III and Al IV is important, the only published electron scattering calculations are those of Ganas and Green (1980) and Liang and Badnell (2010). In Ganas and Green (1980), integrated cross sections for incident electron energies ranging from threshold to 5 keV were calculated for the 2p–3s resonance transition along the neon-like sequence. The authors in Ganas and Green (1980) used an analytic atomic independent particle model potential adjusted to experimental energy levels to generate wave functions for the ground and excited states of the considered ions. The obtained wave functions are used in conjunction with the Born approximation and the *LS*-coupling scheme to obtain generalized oscillator strengths, which are used to calculate integrated cross sections. The method of deriving generalized oscillator strengths and the formula used to obtain cross sections may be found in Ganas (1998). In Liang and Badnell (2010), electron impact excitation data were calculated for Ne-like ions from Na II to Kr XXVII using the intermediate-coupling frame transformation R-matrix approach, and the results of effective collision strengths were presented.

The principal motivation behind the present work is the missed collisional data for the two ions Mg III and Al IV in many databases. These data can be useful for many astrophysical investigations. Besides the importance of the structural and collisional data of multicharged ions in astrophysical and laboratory plasmas investigation, collision strengths have another importance which is related to another field of investigation: the comparison of these data with experimental or/and other theoretical results can be a powerful tool to check our line broadening calculations (Elabidi et al., 2008, 2009, 2011; Elabidi and Sahal-Bréchot, 2011; Elabidi, 2012). Indeed, our line broadening method is ab initio, this means that all the parameters required for the line broadening calculations such as radiative atomic data (energy levels, oscillator strengths...) and collisional data (collision strengths or cross sections, scattering matrices...) are evaluated during the calculation and not taken from other data sources. Consequently, the accuracy of our broadening parameters is strongly related to the accuracy of the atomic and collisional ones. This represents an other motivation and interest of the present work.

The aim of this paper is to provide fine structure collision strengths for Mg III and Al IV transitions in the distorted wave approximation. The atomic structure has been calculated for the 75 levels arising from the eleven configurations $(1s^2)\ 2s^2 2p^6$, $2s^2 2p^5 3l$, $2s 2p^6 3l$, $2s^2 2p^5 4l$ ($l \leqslant n-1$). Collision strengths have been computed for transitions from the ground and the four first excited levels to all the levels. The incoming electron energies used in our calculations are between 10 Ry and 240 Ry. Discussions and investigations of convergence of collision strengths with energy and with total angular momentum J^T are also given. Only the atomic structure data are compared to available experimental and theoretical results.

2. Atomic structure and electron-ion scattering

The atomic structure has been calculated using the AUTOSTRUCTURE (AS) code (Badnell, 1986, 1997) by constructing target wavefunctions using radial wavefunctions calculated in a scaled Thomas–Fermi–Dirac–Amaldi statistical model potential using the Breit–Pauli intermediate coupling (Bethe and Slapeter, 1957). The radial scaling parameters λ_{nl} (depending on n and l) are determined by minimizing the sum of the energies of all the target terms, computed in *LS* coupling, i.e. neglecting all relativistic effects. In this code, besides the one-body and the two-body fine structure interactions, the two-body non-fine structure operators of the Breit–Pauli Hamiltonian, namely contact spin-spin, two-body Darwin and orbit-orbit are incorporated. More details of how these interactions are incorporated are reported in Badnell (1997).

Recently, the Breit–Pauli Distorted Wave (BPDW) approach for electron impact excitation of atomic ions has been implemented in the AS code (Badnell, 1528-1535), which we use for the scattering problem in the present paper. We note that the distorted wave approximation (DW) is adequate for moderately and highly charged ions and the agreement between the DW and more sophisticated methods (close coupling for example) is good. Collision strengths are calculated at the same set of final scattered energies for all transitions: zero gives all threshold transitions, for example. For large l values, a 'top up' for dipole transitions makes use of the sum rule of Burgess (1974). For higher multipoles, a geometric series in energy in combination with the degenerate energy limit (Burgess et al., 1970) is used to take into account of large l contributions to collision strengths.