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Contents lists available at ScienceDirect

Atomic Data and Nuclear Data Tables

journal homepage: www.elsevier.com/locate/adt

Energy levels, radiative rates and electron impact excitation rates for transitions in Si III

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ARTICLE INFO

Article history:
Received 11 November 2016
Accepted 11 November 2016
Available online xxxx

Keywords:
Mg-like Si III
Energy levels
Radiative rates
Lifetimes
Collision strengths
Effective collision strengths

ABSTRACT

Energy levels and radiative rates (*A*-values) for four types of transitions (E1, E2, M1, and M2) are reported for an astrophysically important Mg-like ion Si III, whose emission lines have been observed in a variety of plasmas. For the calculations, well-known and widely-used GRASP code has been adopted, and results are listed for transitions among the 141 levels of the $3\ell3\ell'$ and $3\ell4\ell$ configurations. Experimental energies are available for only the lowest 58 levels but there is no major discrepancy with theoretical results. Similarly, the *A*-values and lifetimes show a satisfactory agreement with other available results, particularly for strong E1 transitions. Collision strengths are also calculated, with the DARC code, and listed for resonance transitions over a wide energy range, up to 30 Ryd. No similar results are available in the literature for comparisons. However, comparisons are made with the more important parameter, effective collision strength (Υ), for which recent *R*-matrix results are available for a wide range of transitions, and over a large range of temperatures. To determine Υ, resonances have been resolved in a narrow energy mesh, although these are not observed to be as important as for other ions. Unfortunately, large discrepancies in Υ values are noted for about half the transitions. The differences increase with increasing temperature and worsen as the upper level *J* increases. In most cases the earlier results are overestimated, by up to (almost) two orders of magnitude, and this conclusion is consistent with the one observed earlier for Be-like ions.

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http://dx.doi.org/10.1016/j.adt.2016.11.001
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Please cite this article in press as: K.M. Aggarwal, Energy levels, radiative rates and electron impact excitation rates for transitions in Si III, Atomic Data and Nuclear Data Tables (2016), http://dx.doi.org/10.1016/j.adt.2016.11.001

Contents

1. Introduction

Emission lines of many Mg-like ions have been observed in a variety of astrophysical plasmas, such as solar, early and late-type stars and planetary nebulae—see for example, work [1] and references therein. Lines from several of these ions (such as Ca IX, Ti XI and Fe XV) are also prominent in fusion plasmas. However, to interpret observations and to model these plasmas atomic data are required for several parameters, including energy levels, radiative rates (A-values) and effective collision strengths (Υ). Generally, energy levels for these ions are fairly well known, and the compilation of assessed experimental data is freely available from the NIST (National Institute of Standards and Technology) website http://www.nist.gov/pml/data/asd.cfm. However, corresponding informations for A- and Υ values are not available from measurements, but over the past few decades several workers have reported theoretical results for many of the Mg-like ions—see for example the data stored in the CHIANTI database at http://www.chiantidatabase.org/ or references in paper [2]. Most of these data, particularly for Υ, are limited to a few levels/transitions, and therefore require extension. More importantly, for some ions (such as P IV, Cl VI and K VIII) no collisional data are available.

Realizing the importance of atomic data for Mg-like ions, recently authors of [2] have reported calculations for a wide range of ions, up to $Z = 36$. They have considered a large number of levels (283 belonging to the $3\ell3\ell'$, $3\ell4\ell$ and $3\ell5\ell$ configurations) and have reported a consistent set of results for energy levels, A-values and Υ. For the determination of atomic structure they have adopted the *AutoStructure* (AS) code [3], and for the collisional calculations the R-matrix code [4]. Furthermore, they have resolved resonances in thresholds region and therefore, their data should be the best available to date.

The R-matrix code [4], adopted by authors of [2], basically calculates collision strengths (Ω) in LS coupling (Russell–Saunders or spin–orbit coupling), and in order to calculate Ω (and Υ) for *fine-structure* transitions, they utilized their *intermediate coupling frame transformation* (ICFT) method [5]. Unfortunately, in the recent literature questions have been raised about the reliability of their approach. For example, we have demonstrated [6,7] that the implementation of such an approach leads to a significant overestimation (of orders of magnitude) of Υ values over a wide range of temperatures for a large number of transitions in Be-like ions. Similar overestimations have also been noted for transitions in Al-like Fe XIV [8] and Ar-like Fe IX [9].

However, in a series of papers [10–12] the overestimation of Υ results with the ICFT methodology has been justified on the basis of the larger calculations performed by the group authors. For example, we included only 98 levels of the $2\ell2\ell'$, $2\ell3\ell'$ and $2\ell4\ell'$ configurations for most Be-like ions [6,13–15], and only 166 for C III [7], the additional 68 levels belonging to the $2\ell5\ell'$ configurations, well short of 238 considered by [16]. However, in a recent paper [17] we considered exactly the same 238 levels for N IV and arrived at the same conclusion that the ICFT results for Υ are indeed overestimated, by up to four orders of magnitude for over 40 per cent of the transitions. Moreover, the overestimation of Υ results is over the whole range of temperatures. Therefore, it has become necessary to test the (in)accuracy of the Υ results of [2] for Mg-like ions.

We also note here that large discrepancies in the ICFT calculations of [18] for transitions in Mg-like Fe XV were observed earlier [19]—see also Section 5 and Table E for transitions in Si III. The error in the code was later rectified by [20]. Moreover, in certain circumstances the ICFT approach does lead to the overestimation in the Υ values, as discussed by [21] for transitions in O III, and also explained by [10]. Nevertheless, in this paper we consider the results for Si III, which is not only an important Mg-like ion but its atomic data have recently been 'benchmarked' by [22].

Lines of Si III have been extensively analyzed by many workers—see for example, [1] and [22] and references therein. Of particular interest is the 120.7 nm emission line arising from the $1s^2\ ^1S_0$–$3s3p\ ^1P^o_1$ transition, which has been extensively observed in both solar and stellar plasmas—see for example, [23]. The early close-coupling calculations for Υ using the R-matrix method were undertaken by [24]. They considered only 12 lowest lying LS states of the $3s^2$, 3s3p, 3s3d, $3p^2$, 3s4s and 3s4p configurations, and reported results for Υ over the 5×10^3–2.5×10^5 K temperature range, sufficient for analysis of observations because the temperature of maximum abundance in ionization equilibrium for Si III is only ~50 000 K [25]. However, an error was later detected in their work and was rectified by [1], whose collisional data have mostly been utilized for observational analysis—see for example [26], and are also stored in the CHIANTI database. Nevertheless, their data remain for limited transitions among 20 fine-structure levels of the above listed 12 states, and hence are not fully sufficient for observational analysis because some of the strong lines of Si III are associated with higher excited levels, such as $3s4f\ ^1F^o_3$ [22].

A much larger calculation involving 45 fine-structure levels belonging to 25 LS terms ($n \le 4$) of four Mg-like ions, including Si III, was later performed by [18], but they reported results for Υ for only 15 transitions from the ground $3s^2\ ^1S_0$ to higher excited levels—see their table 3. However, their Υ results for all transitions are now available on the website: http://www.open.adas.ac.uk. Nevertheless, since their similar results for Fe XV were clearly demonstrated to be inaccurate [19], as already stated, we will focus our comparisons with the most recent and relevant results of [2], discussed earlier.

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