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Energy levels and radiative rates for transitions in Cr-like Kr XIII, Tc XX and Xe XXXI

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ABSTRACT

Energy levels, radiative transition probabilities, Landé *g*-factors, and radiative lifetimes are reported for 144 levels of the $3p^6 3d^6$ and $3p^5 3d^7$ configurations of the Cr-like ions Kr XIII, Tc XX and Xe XXXI. Since to our knowledge no prior data for energy levels or *A*-values, experimental or theoretical, are available in the literature for these ions, calculations have been performed with three independent atomic structure codes, namely GRASP, FAC and a code implementing the QR approach, with increasing configuration interaction (CI) basis with each code. This is to establish the accuracy of the calculated results so that data can be confidently applied in the modeling of plasmas. Our recommended data are determined within the QR approach, because not only has the largest CI basis been included in this calculation, the reliability has already been established in our earlier work for other Cr-like ions, for which some experimental and theoretical data were available for comparison. Results for radiative rates (*A*-values) and transition wavelengths (λ) are listed for all strong E1, E2 and M1 transitions among the 144 levels of each ion.

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Contents

1. Introduction

Atomic data (including energy levels and radiative rates, A-values) are required for the spectral diagnostics and modeling of a variety of plasmas. Generally, ions with $Z \leq 28$ are more important for studies of astrophysical plasmas, whereas those with higher Z may have applications in fusion and laser-produced plasmas. The necessary atomic data for ions with low Z are mostly available in the literature (see for example, the CHIANTI database [1,2] at http://www.chiantidatabase.org and the atomic and molecular database Stout [3]), as many workers have performed calculations adopting a variety of methods and codes due to their astrophysical relevance. However, there is a paucity of similar data for ions with higher Z, although the demand for their data has significantly increased with the development of the ITER project. Among many elements for which data are required for the modeling of fusion plasmas are Krypton [4] and Xenon [5]. Therefore, in this paper we report results for energy levels and A-values for two Cr-like ions, namely Kr XIII ($Z = 36$) and Xe XXXI ($Z = 54$). Since these ions differ in Z by 18, we have also calculated data for Tc XX ($Z = 43$), which will be useful in drawing some important conclusions.

The first measurements of Kr spectra were made by Chen et al. [6], in the 3700–6000 Å wavelength range, via electron beam ion trap (EBIT) experiments. Lines of Kr ions are useful for the development of fusion plasma diagnostics, and [6] were successful in measuring these for several ions, including Kr XIII (5151±11.5 Å). Similarly, Qi et al. [7] measured lines of several Kr ions (Kr VIII to Kr XIV) in laser plasmas. Finally, Zakharov [8] has emphasized the importance of Kr ions, because lines of several ionization stages (Kr VII to Kr XXIII) are a possible source of X-ray emission in the water window waveband. However, in spite of the importance of Kr ions, no atomic data are available in the literature, particularly for Kr XIII. The situation for Xe XXXI is no better, although Wyart et al. [9] identified several lines of Xe ions (including Xe XXXI) in tokamak spectra. Similarly, Nagels et al. [10] and Shlyaptsev et al. [11] have measured lines of Xe XXXI (as well as other ions) from laser plasmas. Theoretical and experimental wavelength corresponding to the 3d–3p transition of the Xe XXXI ion was reported in [12]. However, to our knowledge, no lines of Tc XX have been measured to date.

Calculations of atomic data for Cr-like ions are comparatively more difficult, as was recently experienced by us [13,14] for four ions, namely Co IV, Ni V, Cu VI, and Zn VII. This is because the inclusion of very large CI is required to achieve a reasonably satisfactory agreement between the theoretical and experimental energy levels. For example, we included over 10^9 configuration state functions (CSFs) in our work within the quasi-relativistic (QR) approach [15], because calculations with other atomic structure codes, such as GRASP (general-purpose relativistic atomic structure package [16]) and FAC (the flexible atomic code [17]), could not produce accurate energy levels, even with the inclusion of up to 76 138 CSFs. However, a major advantage for the ions with $27 \leq Z \leq 30$ was that measurements of energy are available for many levels, particularly those of the $3d^6$ ground configuration.

As may be seen from the results in [13,14,18], our QR approach produces level energies close to the experimental data for ions with an open $3d^N$ shell, even for the ionization stages lower than those considered in the present work. In the absence of any atomic data, theoretical or experimental, for the ions under consideration here, our task has become more difficult. However, after gaining experience for other Cr-like ions [13,14,18], we are confident of our calculations using the QR approach. Nevertheless, as in earlier papers we have also performed calculations with GRASP and FAC, because the ions studied here (Kr XIII, Tc XX and Xe XXXI) are comparatively heavier. Therefore, the importance of CI effects is expected to be less compared to relativistic effects.

2. Level structure of excited configurations

Initially, we have undertaken preliminary calculations of the energy level spectra for the Kr XIII, Tc XX and Xe XXXI ions within a relatively small CI basis in the QR approach. This was an important step before a proper high-accuracy calculation, allowing us to

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