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Energy levels and radiative rates for transitions in Cr-like Co IV and Ni V

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ABSTRACT

We report calculations of energy levels and radiative rates (*A*-values) for transitions in Cr-like Co IV and Ni V. The quasi-relativistic Hartree–Fock (QRHF) code is adopted for calculating the data although GRASP (general-purpose relativistic atomic structure package) and flexible atomic code (FAC) have also been employed for comparison purposes. No radiative rates are available in the literature to compare with our results, but our calculated energies are in close agreement with those compiled by NIST for a majority of the levels. However, there are discrepancies for a few levels of up to 3%. The *A*-values are listed for all significantly contributing E1, E2 and M1 transitions, and the corresponding lifetimes reported, although unfortunately no previous theoretical or experimental results exist to compare with our data.

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Contents

1. Introduction

Iron group elements (Sc–Zn) are becoming increasingly important in the study of astrophysical plasmas, as many of their lines from different ionization stages are frequently observed. These lines provide a wealth of data on plasma characteristics, including temperature, density and chemical composition. Additionally, iron group elements are often impurities in fusion reactors, and to estimate the power loss from the impurities, atomic data (including energy levels and oscillator strengths or radiative decay rates) are required for many ions. The need for atomic data has become even greater with the developing ITER project. Since there is a paucity of measured parameters, one must depend on theoretical results. Therefore, over the last few years we have reported atomic parameters for many ions of the iron group elements — see for example [1–4] and references therein. Among Co ions, results have already been provided for Co XXVII [5], Co XXVI [6], Co XXV [4], Co XXII [7], Co XVI [8], and Co XI [9]. Similar data for several Ni ions have also been reported, i.e. Ni XI [10], Ni XIII – Ni XVI [11], Ni XVII [8], Ni XIX [2], Ni XXIII [7], Ni XXVI [4], Ni XXVII [6], and Ni XXVIII [5]. Here we focus our attention on Cr-like Co IV and Ni V.

Several emission lines of Co and Ni ions have been observed in astrophysical plasmas, as listed in the CHIANTI database at http://www.chiantidatabase.org. Similarly, many lines of these ions, below 2000 Å, are also listed in the compilation by Kelly [12]. However, we are not aware of any observed lines of Co IV but Raassen and Hansen [13] have identified forbidden lines of Ni V in Eta Carinae (η Car). Similarly, Preval et al. [14] have analysed many lines of Ni V in the near- and far-ultraviolet range (1150–3145 Å and 910–1185 Å) belonging to the 4s–4p transitions, from the high-resolution spectra from hydrogen-rich (DA) white-dwarf star G191-B2B, obtained from the Hubble Space Telescope Imaging Spectrograph (STIS), and determined photospheric abundance of many elements, including Ni. Furthermore, many emission lines of Co IV and Ni V are listed in the 200–475 Å wavelength range in the *Atomic Line List* (v2.04) of Peter van Hoof at http://www.pa.uky.edu/~peter/atomic/, because these are useful in the generation of synthetic spectra. Similarly, experimental data are available in the literature for Co IV and Ni V by Poppe et al. [15], who identified the multiplets of $3d^6\ ^5D–3d^5(^6S)4p\ ^5P^o$ lines from a laboratory spectrograph. Following these identifications, they calculated energies for several other levels of the ($3d^5$) 4s and 4p configurations, based on some analytical expressions. These energies were compiled by Sugar and Corliss [16] and are available on the website of NIST (National Institute of Standards and Technology) at http://www.nist.gov/pml/data/asd.cfm [17].

The situation with regard to theoretical results is similar. Energies for a few levels of the ($3d^5$) 4s and 4p configurations are available [18,19], from calculations based on *least square fitting* of Slater–Condon parameters, and are biased towards the known (observed or measured) results and iso-ionic, iso-electronic and iso-nuclear trends. A wider set of data for 136 terms of the $3d^6$, $3d^5$4s and $3d^5$4p configurations has been reported for Co IV by one of the current authors [20], calculated in *LS* coupling with the CIV3 code [21], which neglects two-body relativistic operators, although these are not very important for this moderately heavy ion. More importantly, limited CI (configuration interaction) with some configurations involving the 4s, 4p and 4d orbitals is included, and *A*-values are not reported. Similarly, Kingston et al. [22] calculated energies but for only a few *LS* states of Ni V. Therefore, the available data are not suitable for applications in plasma modelling, because results are required for *fine-structure* levels and their corresponding transitions. However, recently Ong et al. [23] have reported energies for 131 levels of Ni V. They adopted the methodology of *configuration interaction* and *many-body perturbation theory* (CI+MBPT) for their calculations and the energies obtained agree within 2% of the NIST compilation. However, their reported levels are only a subset of the NIST compilation and particularly *missing* are the lowest 34 levels of the $3d^6$ configuration. Additionally, they have not calculated the *A*-values. Therefore, there is scope for extending their calculations.

In this work we report atomic data for energy levels and *A*-values for transitions among the $3d^6$, $3d^5$4s and $3d^5$4p configurations of Co IV and Ni V. For the calculations, we first employed the fully relativistic GRASP (general-purpose relativistic atomic structure package) code originally developed by Grant et al. [24], but later revised by one of its authors (P.H. Norrington). The code is based on the *jj* coupling scheme, is referred to as GRASP0 and is available at the website http://web.am.qub.ac.uk/DARC/. Furthermore, it includes the major modifications made in other versions, such as GRASP92 [25] and GRASP2K [26,27]. Relativistic corrections arising from the Breit interaction and QED (quantum electrodynamics) effects (vacuum polarization and Lamb shift) are also included. Finally, we have used the option of *extended average level* (EAL), in which a weighted (proportional to the level statistical weight $2j + 1$) trace of the Hamiltonian matrix is minimized. This produces a compromise set of orbitals describing closely lying states with moderate accuracy. However, it soon became clear that the level of CI required for Cr-like ions is too large, and the desired calculations could not be performed with the GRASP code within a reasonable time frame (a few months). Since our aim is to calculate only energy levels and *A*-values, we hence