Electron impact excitation of Ne-like Ni XIX

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Abstract. In this paper we report atomic data, namely energy levels, radiative rates, lifetimes, collision strengths, and excitation rate coefficients, for transitions among 89 levels of the \((1s^2 2s^2 2p^6, 2s^2 2p^5 3\ell, 2s^2 2p^6 3\ell, 2s^2 2p^5 4\ell, \) and \(2s2p^6 4\ell\) configurations of Ni XIX. For the calculations of energy levels and radiative rates the GRASP code has been adopted, whereas for the calculations of collision strengths DARC is employed.

1. Introduction

Emission lines of Ni XIX have been observed in the spectrum of the solar corona, and are useful for plasma diagnostics. Additionally, nickel is an important impurity element in fusion reactors, and hence atomic data (namely energy levels, radiative rates, collision strengths, excitation rates, etc.) are required in order to estimate the power loss from the walls of the reactors. Furthermore, Ne-like ions are also very useful in lasing plasmas. Since there is a paucity of experimental data for most of the above named parameters, theoretical results are desirable. Therefore in this work, we report our results for transitions among 89 levels of the \((1s^2 2s^2 2p^6, 2s^2 2p^5 3\ell, 2s^2 2p^6 3\ell, 2s^2 2p^5 4\ell, \) and \(2s2p^6 4\ell\) configurations. Earlier calculations have been performed by Zhang and Sampson [1], Hibbert et al. [2], Mohan et al [3], and Singh and Mohan [4]. Zhang and Sampson, who adopted the Coulomb-Born-exchange method, reported results for energy levels, radiative rates (\(A\)-values) and collision strengths (\(\Omega\)) among 89 levels of the \((1s^2 2s^2 2p^6, 2s^2 2p^5 3\ell, 2s^2 2p^6 3\ell, 2s^2 2p^5 4\ell, \) and \(2s2p^6 4\ell\) configurations. However, they did not resolve resonances, and reported values of \(\Omega\) only at a few energies above thresholds. Since the contribution of resonances is often significant, even at the high temperatures at which data are required for Ni XIX, there is an urgent need to include their contribution. Additionally, they calculated values of \(\Omega\) for the resonance transitions only, whereas data are required for all transitions. Therefore, in this work we are attempting to make a significant improvement over their work.

Hibbert et al [2] reported results only for energy levels and \(A\)-values for transitions among the lowest 37 levels of Ni XIX. They adopted the CIV3 code [5] and performed semi-relativistic calculations, but reported \(A\)-values for the electric dipole (E1) transitions alone, whereas in plasma modelling corresponding results for other types of transitions, namely magnetic dipole (M1), electric quadrupole (E2), and magnetic quadrupole (M2), are also required. Therefore, there is a need to extend the calculations to higher excited levels, apart from calculating \(A\)-values for all types of transitions. Additionally, and more importantly, their energy levels, particularly for the levels of the \(2s2p^6 3\ell\) configurations, are underestimated by up to \(\sim 1.6\) Ryd (2%) with
those of Zhang and Sampson [1] or the experimental values of NIST. Therefore, it has become essential to resolve this large discrepancy.

Adopting the CIV3 wavefunctions of Hibbert et al [2], Mohan et al [3] have reported results for collision strengths (Ω) and effective collision strengths (Υ), but for LS transitions among the lowest 27 levels, i.e. 15 states of the (1s²) 2s²2p⁶ and 2s²2p⁵3ℓ configurations. They adopted the R-matrix code [6] and included the contribution of resonances to calculate values of Υ up to a temperature of 10⁷ K. Similarly, in a more recent paper Singh and Mohan [4] reported values of Ω for fine-structure transitions among the lowest 5 levels of the 2s²2p⁶ and 2s²2p⁵3s configurations. However, their values of Ω for fine-structure transitions show erratic variation with energy as already discussed and demonstrated by Aggarwal and Keenan [7]. Therefore, in this paper we focus on the LS transitions among the 15 states mentioned above.

2. Calculations
For the calculations of energy levels and A-values, we have adopted the GRASP [8] code, and for the computations of Ω the Dirac Atomic R-matrix Code (DARC: [9]). Thus our calculations are fully relativistic in the jj coupling scheme. The R-matrix radius has been adopted to be 3.64 au, and 25 continuum orbitals have been included for each channel angular momentum for the expansion of the wavefunction. This allows us to compute values of Ω up to an energy of 250 Ryd. The maximum number of channels for a partial wave is 401, and the corresponding size of the Hamiltonian matrix is 10086. In order to obtain convergence of Ω for all transitions and at all energies, we have included all partial waves with angular momentum J ≤ 39.5, although a higher range would have been preferable for the convergence of allowed transitions. However, to account for the inclusion of higher neglected partial waves, we have included a top-up, based on the Coulomb-Bethe approximation for allowed transitions, and geometric series for forbidden ones. Additionally, resonances are resolved in a fine energy mesh in order to account for their contribution, and the values of excitation rate coefficients have been calculated over a wide temperature range up to 10⁷ K.

3. Results and conclusions
Our results for all 89 energy levels among the 2s²2p⁶, 2s²2p⁵3ℓ, 2s2p⁶3ℓ, 2s²2p⁵4ℓ and 2s2p⁶4ℓ configurations have already been presented and discussed in detail by Aggarwal and Keenan [10]. To determine the energy levels, the contribution of the n = 5 configurations was found to be negligible. Furthermore, the lowest 27 energy levels of Hibbert et al [2] were observed to be equally accurate, in comparison to ours or the experimental ones, but their energy levels for the 2s2p⁶3ℓ configurations (28-37) differ from our calculations or the compilations of NIST by up to 1.5 Ryd or equivalently ≤ 2% - see Table 2 of Aggarwal and Keenan [10]. Similarly, the inclusion of Breit and QED corrections lowered the energies by ∼ 0.11 Ryd, and our energy levels were assessed to be accurate to better than 1%.

Our results for radiative rates (A-values), oscillator strengths (f-values), and line strengths (S-values) for all E1, E2, M1 and M2 transitions have also been reported and compared (Aggarwal and Keenan [10]) with the earlier available work. Based on the comparison made between the length and velocity forms of the oscillator strengths, as well as among a variety of calculations with differing amount of CI included, we assessed the accuracy of our radiative rates to be better than 20% for all strong transitions. However, for weaker transitions the A- or f-values are less accurate. The values of lifetimes (τ) for all excited levels were also presented, but comparison with the corresponding available results has been possible for only a few levels (lowest 27), for which there were no discrepancies. Furthermore, as shown in Table 5 of [10], the A-values of Hibbert et al [2] are in complete agreement with those of us, but for transitions involving levels up to 27 (2s²2p⁵3d 1P₀) only. For transitions involving higher levels of the 2s2p⁶3ℓ configurations, differences between the two sets of A-values are up to a factor of two.
As stated earlier, Mohan et al. [3] have reported results for \( \Omega \) as well as \( \Upsilon \) for transitions among the 15 states of the \( 2s^22p^6 \) and \( 2s^22p^53\ell \) configurations. Their results are the latest available in the literature, and also cover all possible transitions among the 15 states. Since they have adopted the configuration interaction (CI) wavefunctions in the \( R \)-matrix approach, have resolved resonances in thresholds region, and have taken care to ensure the convergence of \( \Omega \) values by adopting a wider range of partial waves, their reported results should be the most reliable available today. However, we find that for a majority of transitions, such as: 2 - 6, 7, 8, 3 - 6, 7, 8, and 5 - 6, 7, 8 (see [3] for transition indices) their reported values of \( \Upsilon \) demonstrate no relationship with the corresponding values of \( \Omega \). For example, for the 2-8 (\( 2p^53s \ 3P^o - 2p^53p \ 1P \)) transition, their values of \( \Omega \) are between 5.1 and 6.8 in the entire energy range of 80 \( \leq E \) \( \leq \) 140 Ryd, but the corresponding values of \( \Upsilon \) vary between 0.04 and 0.006 in the entire temperature range of 5.4 \( \leq \log T_e \) (K) \( \leq \) 7.0, i.e. the \( \Omega \) values behave as for an allowed transition whereas the \( \Upsilon \) values show a completely opposite trend of a forbidden transition. Therefore, their results for \( \Upsilon \) values cannot be adopted in a plasma modelling or diagnostic work. We now focus our attention to assess if their values of \( \Omega \) are correct.

In Fig. 1 we compare our values of \( \Omega \) with their results for two transitions, namely 1-15 (\( 2p^6 \ 1S - 2p^53d \ 1P^o \)) and 3-6 (\( 2p^53s \ 1P^o - 2p^53p \ 1D \)). Both of these are allowed transitions, and the \( f \)-values between the two independent calculations are comparable, as shown in Table 5 of [10]. To be specific, the GRASP and CIV3 \( f \)-values for the 1-15 transition are 2.46 and 2.30, respectively, and for the 3-6 transition are 8.68 \( \times 10^{-4} \) and 8.33 \( \times 10^{-4} \), respectively. Therefore, the values of \( \Omega \) should also be comparable for these (and many other similar) transitions, but they are not. Particularly noticeable are the differences for the 1-15 transition, for which the \( \Omega \) values of Mohan et al. [3] not only differ in magnitude, but also in behaviour, from ours as well as of Zhang and Sampson [1]. Since this is a strong allowed transition, the values of \( \Omega \) should increase with energy, as shown in our work, and should not decrease as shown by Mohan et al.

![Figure 1](image-url)  
**Figure 1.** Comparison of collision strengths from the present work (continuous lines) and of Mohan et al. [3] (broken lines) for the 1-15 (\( 2p^6 \ 1S - 2p^53d \ 1P^o \): circles) and 3-6 (\( 2p^53s \ 1P^o - 2p^53p \ 1D \): stars) allowed transitions of Ni XIX. Results of Zhang and Sampson [1] are shown as squares for the 1-15 transition.

In Fig. 2, we show similar results for three forbidden transitions, namely 1-4 (\( 2p^6 \ 1S - 2p^53p \ 3S \)), 1-6 (\( 2p^6 \ 1S - 2p^53p \ 1D \)) and 1-12 (\( 2p^6 \ 1S - 2p^53d \ 1F^o \)). For all of these (and many other)
transitions, there is complete agreement between our results and those of Zhang and Sampson
[1], but corresponding results of Mohan et al [3] not only differ in magnitude, by up to two
orders of magnitude in many cases, but also in behaviour. For forbidden transitions, the values
of Ω decrease with increasing energy, as shown in our work or that of Zhang and Sampson,
and not increase as shown by Mohan et al. Therefore, it is unfortunate that the earlier results
of Mohan et al are neither reliable for Ω nor for Υ. Apart from removing the anomalies in
their work, we are not only extending the range of levels (transitions), but are also making an
overall improvement by extending the energy range from 140 to 250 Ryd, so that the values
of Υ can be more accurately determined up to the temperature of $10^7$ K. Our complete set of
results, for both collision strengths and excitation rates, for all possible 3916 transitions among
89 fine-structure levels of Ni XIX will soon be reported in a separate paper.

Figure 2. Collision strengths from the present work (continuous lines) and of Mohan et al [3]
(broken lines) for the 1-4 (2p$^6$ 1S - 2p$^5$3p 3S: circles), 1-6 (2p$^6$ 1S - 2p$^5$3p 1D: stars) and 1-12
(2p$^6$ 1S - 2p$^5$3d 1Fo: squares) forbidden transitions of Ni XIX. Results of Zhang and Sampson
[1] are shown as triangles (1-4), diamonds (1-6) and crosses (1-12).

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