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E1 oscillator strengths and transition rates among levels of Cl I

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ABSTRACT

We present oscillator strengths and transition rates of E1 transitions between the fine-structure levels belonging to the configurations $3s^23p^5$, $3s3p^6$, and $3s^23p^4 nl$, where $nl = 4s, 5s, 6s, 4p, 5p, 3d, 4d$. The calculations have used extensive configuration interaction (CI) wavefunctions, with the associated Hamiltonian matrix adjusted to ensure that the eigenenergies agree with experimental energy level data ('fine tuning'). There are consequential small changes in the CI mixing coefficients from their *ab initio* values and these corrected coefficients are used in the calculation of the transition data. The method of optimization of the orbital radial functions (expressed in terms of Slater-type orbitals) is described and the radial function parameters are also presented. We show some comparisons between our work and those of earlier calculations and demonstrate how the inclusion of relativistic effects (which we achieve through the use of the Breit–Pauli approximation) can result in a substantial redistribution of the oscillator strength from the *LS* calculation. We also demonstrate that the fine-tuning process can make, particularly for intercombination lines, a substantial improvement in the agreement between theoretical and experimental oscillator strengths.

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1. Introduction

It is somewhat surprising that radiative data for an element as relatively light as neutral chlorine should be rather sparse in the literature. The NIST database [1] mostly quotes transition data from the early work of Lawrence [2] and Hofmann [3] or the even earlier work of Foster [4]. These are all experimental values. More recent work has tended to focus on a limited range of transitions. For example, Schwab and Andersen [5] were concerned with ²D–²P^o transitions, Hansen [6] focused on the interaction between 3s3p⁶ and 3s²3p⁴3d states, Biémont et al. [7] studied resonance transitions in Cl I, and a number of papers were concerned with astrophysical applications of certain transitions (for example, Refs. [8–10]). There have been a few more extensive calculations of Cl I transitions. Huang et al. [11] used the MCDF method to calculate transitions between the 31 lowest levels. More recently, Lavín et al. [12] used the RQDO method to establish results for transitions between the levels of 3p⁵ and 3p⁴4s or 3p⁴3d, and between [3p⁴]4s and 4p, 4p and 5s, and between 4f and 5g, while Berrington and Nagazaki [13] used the R-matrix code to study transitions between states up to *n* = 5. Perhaps the most thorough, systematic calculations were undertaken by Froese Fischer et al. [14] using the MCDHF method and by the present authors [15], with our results superseding our earlier work (Ojha and Hibbert [16]) and another calculation by Singh et al. [17], also undertaken with our code, CIV3 [18,19].

Some of our results, and details of the method of calculation we used, were published in our earlier paper [15], and were then used to address specific issues [20,21]. In the present paper, we give the full set of our results, comprising all electric dipole (E1) transitions between levels of the configurations 3s²3p⁵, 3s3p⁶, and 3s²3p⁴*nl*, (*nl* = 4s, 5s, 6s, 4p, 5p, 3d, 4d).

2. Method of calculation

The present calculation was undertaken using the CIV3 code [18,19], which expresses the configuration interaction (CI)

wavefunction in the intermediate coupling scheme as

$$\Psi(J) = \sum_{i=1}^M a_i \Phi_i(\alpha_i L_i S_i J). \quad (1)$$

In (1), Φ_i represents a configuration state function (CSF), constructed from a common set of one-electron orbitals of the form

$$\frac{1}{r} P_{nl}(r) Y_l^m(\theta, \phi) \chi_{m_s}(\sigma) \quad (2)$$

where Y is a spherical harmonic, χ is a spin function (often denoted by α or β for $m_s = \frac{1}{2}$ or $-\frac{1}{2}$, respectively) and the radial functions in (2) are expressed in analytic form as linear combinations of normalized Slater orbitals (STOs)

$$P_{nl}(r) = \sum_{j=1}^k c_{jnl} \eta_{jnl}(r) \quad (3)$$

and where the STOs take the form

$$\eta_{jnl}(r) = \left[\frac{(2\xi_{jnl})^{2l_{jnl}+1}}{(2l_{jnl})!} \right]^{1/2} r^{l_{jnl}} \exp(-\xi_{jnl} r). \quad (4)$$

Also in (1), α_i represents the angular momentum coupling scheme and other necessary labeling, and a_i is the corresponding component of the eigenvector, associated with this wavefunction, of the diagonalized Hamiltonian matrix whose typical element is $H_{ij} = \langle \Phi_i | H | \Phi_j \rangle$.

If the eigenvalues (expressed as E_i) of the Hamiltonian matrix are ordered to satisfy $E_1 < E_2 < E_3 < \dots$, then $E_i \geq E_i^{\text{exact}}$ is a consequence of the Hylleraas–Undheim theorem. These inequalities serve as a set of variational principles whereby the orbital function parameters can be optimized on one or more eigenenergies of the Hamiltonian matrix, and subject to the orthonormality conditions

$$\int_0^\infty P_{nl}(r) P_{n'l}(r) dr = \delta_{nn'}; \quad l < n' \leq n, \quad (5)$$

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