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Breit-Pauli Oscillator Strengths and Transition Probabilities for Transitions among the Fine-Structure Levels of Cl I

P Oliver,[1] A Hibbert[1]

[1] *Department of Applied Mathematics and Physics, Queen's University Belfast, Belfast, Northern Ireland*

poliver02@qub.ac.uk

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We are currently undertaking an extensive large-scale calculation to obtain the oscillator strengths and transition rates for all E1 transitions in Cl I between the fine-structure levels of the odd-parity configurations $3s^23p^5$, $3p^4(^1D)4p$, $3p^4(^3P)np(4 \leq n \leq 5)$ and the even-parity configurations $3s3p^6$, $3p^4(^3P,^1D,^1S)ns(4 \leq n \leq 5)$, $3p^4(^3P)6s$, $3p^4(^3P,^1D)3d$, $3p^4(^3P)4d$, within the *Breit-Pauli* approximation, using the method of interaction of configurations (CI) enveloped in the general atomic structure code CIV3 of Hibbert [1,2]. The CI wavefunctions have been constructed from a common orthogonal set of twenty-two one-electron functions (OEFs), which have been carefully selected to ensure that the *LS*-dependency of the orbitals and all important correlation effects have been accurately represented. Specifically, the 1s→3p orbitals were taken to be the *Hartree-Fock* functions [3] of the Cl I ground state; the 3d, 4s, 4p, 5s were optimised as real *spectroscopic* orbitals, while the remaining functions served as '*correcting*' and '*correlation*' orbitals. In the *LS*-coupling regime, the configuration state functions (CSFs) included in the atomic wavefunction expansions were obtained by performing single and double electron replacements for each symmetry from the available orbitals *nl* in the set of dominant configurations $3s^23p^5$, $3s3p^6$, $3p^4nl$. This ensures the inclusion of all *internal* and *semi-internal* correlation effects and the satisfactory convergence of *all-external* effects.

Results are compared with experimental and other available theoretical data. In the *LS*-coupling scheme our theoretical excitation energies are consistent with the experimental NIST [4] compiled values. We also observe excellent agreement in the dipole length and velocity forms of the calculated oscillator strengths (a measure of the uncertainty in the results), demonstrating a marked improvement over the corresponding results of Ojha [5]. We will present preliminary *ab initio* calculations of the oscillator strengths for transitions between the *LSJ*-coupled fine-structure levels within the Breit-Pauli approximation, which will be compared with the most recent work of Singh et al. (2006) [6].

[1] A. Hibbert, Comp. Phys. Commun. **9** (1975) 141
[2] R. Glass and A. Hibbert, Comp. Phys. Commun. **16** (1978) 19
[3] E. Clementi and C. Roetti, Atomic Data and Nuclear Data Tables **14** (1974) 177
[4] NIST, http://physics.nist.gov/cgi-bin/AtData/levels_form
[5] P. Ojha and A. Hibbert, Physcia Scripta **42** (1990) 424
[6] N. Singh, A.K.S. Jha and M. Mohan, Eur. Phys. J. D **38** (2006) 285