PROTON COLLISIONAL EXCITATION IN THE
GROUND CONFIGURATION OF Fe$^{+12}$, II

DONALD A. LANDMAN

Institute for Astronomy, University of Hawaii, Honolulu, H.I. 96822, U.S.A.

(Received 19 February, 1973)

Abstract. Improved values of the proton impact excitation cross sections at coronal energies for all the Fe$^{+12}$ ground configuration ($3s^23p^2$) transitions are presented. These were obtained by direct computer integration of the Schroedinger equation (with the states expressed in intermediate coupling) resulting from the semi-classical Coulomb excitation theory formulation of the process. Comparison is made with previous results. The associated rate constants at coronal temperatures are given and compared with the corresponding electron impact excitation rate constants. Some cross-section values for the Fe$^{+12}$ $3s^23p \, ^2P_{1/2} \rightarrow ^2P_{3/2}$ excitation are also presented.

1. Introduction

In a previous paper (Landman, 1973) we calculated values of the proton impact excitation cross sections and rate constants at coronal temperatures for all transitions between Fe$^{+12}$ ground configuration ($3s^23p^2$) levels. The calculations were based on an adaptation of semi-classical nuclear Coulomb excitation theory as outlined by Seaton (1964). Earlier considerations of proton excitation in Fe$^{+12}$ (Masnou-Seeuws and McCarroll, 1972; De Boer et al., 1972; Chevalier and Lambert, 1969; Bahcall and Wolf, 1968) were limited to transitions between the $^3P$ ground term levels, the latter being treated as purely LS coupled. The purpose of our work is to extend the analysis to include the entire ground configuration in intermediate coupling so as to enable more accurate interpretations of observed forbidden line intensity ratios via more complete excitation equilibrium calculations.

In our previous paper we used first-order time dependent perturbation theory in the region where $\Sigma_f P_{if} \leq \frac{1}{2}$ ($P_{if}$ is the excitation probability from state $i$ to state $f$), and an approximation procedure when $\Sigma_f P_{if} > \frac{1}{2}$ which essentially distributed $P_{if}$ according to the statistical weights of the final levels. The resulting calculations led to the conclusion that under coronal conditions collisional excitation of the Fe$^{+12}$ $3s^23p^2$ levels by protons is comparable for each transition to direct electron excitation. We therefore considered it worthwhile to redo the calculations in a more exact way by solving the Schroedinger equation for the problem exactly for those combinations of proton energies and impact parameters for which the proton does not penetrate the ion, and using a correspondingly more informed approximation procedure when it does.

2. Theory and Computations

The theory of Coulomb excitation has been completely described elsewhere (Alder and Winther, 1966; Biedenharn and Brussaard, 1965) and need not be further discussed here.

Solar Physics 31 (1973) 81–89. All Rights Reserved
Copyright © 1973 by D. Reidel Publishing Company, Dordrecht-Holland
For the present calculations we used, with several minor adaptations to accommodate ionic rather than nuclear excitation, the multiple Coulomb excitation computer program of Winther and de Boer (1965). This program, together with extensive discussions and documentation, is reprinted with corrections in Alder and Winther.

For a given proton energy and scattering angle, the program calculates the excitation probabilities and differential excitation cross sections for quadrupole excitation of each level, the excitation amplitudes being evaluated by direct numerical integration of the coupled differential equations for the time dependent amplitudes. The calculations are completely 'symmetrized', and detailed balance for the two processes

\[ (2J_N + 1) v_N^2 \, d\sigma (N \rightarrow M) = (2J_M + 1) v_M^2 \, d\sigma (M \rightarrow N) \]

is automatically satisfied.

As input to the program, one must supply the reduced matrix elements

\[ M_{rs}^{(2)} = (-1)^J - J' \cdot M_{sr}^{(2)} = e \left( \frac{5}{4\pi} \right)^{1/2} \langle \alpha_s J_s || \sum_k r^2 C^{(2)} (\theta_k, \phi_k) || \alpha_r J_r \rangle, \]

where \( e \) is the magnitude of the electron charge, \( C^{(2)}_m = (4\pi/5)^{1/2} Y_{2m} \), \( J \) - the total angular momentum - and \( \alpha \) label the states, and the sum is over the electrons. To calculate these quantities for the \( \text{Fe}^{+12} \) ground configuration levels, we made use of the work of Krueger and Czyzak (1965). From their intermediate coupling parameters, we derived the wave functions presented, together with the other level dependent parameters used, in Table I. These wave functions, combined with Krueger and Czyzak's

\begin{table}[h]
\centering
\begin{tabular}{lccc}
\hline
\text{Level} & \text{Energy (eV)} & \text{Wave function} \\
\hline
\text{3}P_0 & 0 & 0.9806 \, |3P_{0m}\rangle + 0.1959 \, |1S_{0m}\rangle \\
\text{3}P_1 & 1.153 & \text{\text{\textit{a}}} \\
\text{3}P_2 & 2.301 & 0.9544 \, |3P_{2m}\rangle - 0.2985 \, |1D_{2m}\rangle \\
\text{1}D_3 & 5.959 & 0.9544 \, |1D_{3m}\rangle + 0.2985 \, |3P_{3m}\rangle \\
\text{1}S_0 & 10.845 & 0.9086 \, |1S_{0m}\rangle - 0.1959 \, |3P_{0m}\rangle \\
\hline
\end{tabular}
\caption{\text{Fe}^{+12}, 3s^23p^5 configuration parameters and wave functions}
\end{table}

Intermediate coupling parameters (in cm\(^{-1}\)):: \( \zeta_p = 11887, \eta = 5.00, E (3P) = 15246, E (1D) = 45439, E (1S) = 84414. \)

\( \text{\textit{a}} \) Krueger and Czyzak (1965).

Hartree-Fock values for \( \langle r^2 \rangle \) enabled us to derive the \( M_{rs}^{(2)} \) matrix by means of the relation

\[ \langle p^2 S'L'J' \| \sum_k r^2 C^{(2)} (\theta_k, \phi_k) \| p^2 S'LJ \rangle = -2\delta (S', S) (-1)^{L'+J'} \times \]

\[ \times [(2J + 1)(2J' + 1)(2L + 1)(2L' + 1)]^{1/2} \left\{ \begin{array}{c} L' \ J' \ S \\ J \ L \ 2 \end{array} \right\} \left\{ \begin{array}{c} 1 \ L' \ 1 \\ L \ 1 \ 2 \end{array} \right\} \times \]

\[ \times \sqrt{\frac{8}{3}} \langle r^2 \rangle_{S'L',SL}. \]

The results are given in Table II.