

Dielectronic Recombination in F^{6+} Above and Below the Ionization Threshold

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ABSTRACT: Relativistic perturbation theory calculations are carried out for dielectronic recombination cross sections involving 2 levels in the $F^{5+} (1s^2 2\bar{p}6\bar{p})$ sub-configuration, 2 levels in the $F^{5+} (1s^2 2p6\bar{p})$ sub-configuration, 2 levels in the $F^{5+} (1s^2 2\bar{p} 6p)$ sub-configuration, and 4 levels in the $F^{5+} (1s^2 2p 6p)$ sub-configuration. Nine of the $j_1 j_2 j$ levels are found to lie below the $F^{6+} (1s^2 2s)$ ionization threshold, with the $F^{5+} (1s^2 2p6p)$ $J=2$ level at -0.03 eV and the $F^{5+} (1s^2 2p6p)$ $J=3$ level at $+0.18$ eV.

1. INTRODUCTION

Resonance states just below the ionization threshold may contribute to dielectronic recombination in astrophysical and laboratory plasmas [1, 2, 3]. Proper inclusion of the below-threshold resonance states may make substantial changes in the thermally averaged rate coefficients.

Recently calculations have been made [4] for resonance states just below threshold which could emit light for the study of planetary nebulae and symbiotic star systems. For example, dielectronic recombination in $C^{2+} 1s^2 2s^2$ could lead to $C^+ 1s^2 2s 2p 3d$ resonance states which lead to interesting visible and ultraviolet spectral lines. In this paper we look at dielectronic recombination in $F^{6+} 1s^2 2s$ leading to $F^{5+} 1s^2 2p 6p$ resonance states which may also produce interesting spectral lines and has near threshold resonances that would enhance the recombination of F^{6+} in low temperature plasma environments.

The rest of the paper is structured as follows: in section 2 we review theory, in section 3 we present results, and in section 4 we give a brief summary. Unless otherwise stated, all quantities are given in atomic units.

2. THEORY

The dielectronic recombination cross section for an N electron ground level with statistical weight g_i combining into an $(N + 1)$ electron doubly excited level with statistical weight g_j is given by [5]:

$$\sigma_{i \rightarrow j} = \frac{\pi^2}{E_c \Delta E_c} \frac{g_j}{2g_i} A_\alpha(j \rightarrow i) B_j \quad (1)$$

where E_c is the energy of the continuum electron and ΔE_c is the bin width. The branching ratio for radiative stabilization is given by:

$$B_j = \frac{\sum_n A_r(j \rightarrow n)}{\sum_k A_a(j \rightarrow k) + \sum_n A_r(j \rightarrow n)} \quad (2)$$

where the radiative A_r and autoionization A_a rates are evaluated using lowest order perturbation theory. The summation over n is for radiative decay to non-autoionizing levels.

For radiative and autoionization rates, the energies and bound state wavefunctions are calculated using a multi-configuration Dirac-Fock atomic structure code [6]. The continuum state wavefunctions are calculated using a single-channel radial Dirac equation, where the Dirac local exchange distorting potential is constructed from Dirac-Fock bound radial orbitals. Dielectronic recombination is extended to states just below the ionization potential as outlined in [1].

3. RESULTS

Low-order relativistic calculations were carried out for the 16 levels of the F^{5+} even-parity sub-configurations:

$1s^2 2s^2$ ($J = 0$), $1s^2 2\bar{p}^2$ ($J = 0$), $1s^2 2\bar{p}2p$ ($J = 1, 2$), $1s^2 2p^2$ ($J = 0, 2$), $1s^2 2\bar{p} 6\bar{p}$ ($J = 0, 1$), $1s^2 2\bar{p} 6p$ ($J = 1, 2$), $1s^2 2p 6\bar{p}$ ($J = 1, 2$), and $1s^2 2p 6p$ ($J = 0, 1, 2, 3$). The last 10 levels are within 0.5 eV of the $F^{6+} 1s^2 2s$ ionization threshold.

Autoionization rates were determined for the decay of the 10 levels involving the $6\bar{p}$ and $6p$ subshells to the 7 levels of the even-parity sub-configuration: $1s^2 2sks$ ($J = 0, 1$), $1s^2 2sk\bar{d}$ ($J = 1, 2$), $1s^2 2skd$ ($J = 2, 3$), and $1s^2 2s k\bar{g}$ ($J = 3$). Energies and autoionization rates for the 10 levels near threshold are presented in Table 1. Near threshold we assume that the continuum electron energy is the absolute value of the actual energy. The autoionization rates presented in Table 1 are summed over the 7 continuum levels. For example the autoionization rate for $1s^2 2\bar{p}6\bar{p}$ ($J = 0$) level at -0.45 eV is 2.17×10^{12} Hz to $1s^2 2sks$ ($J = 1$), 7.94×10^{11} Hz to $1s^2 2sk\bar{d}$ ($J = 1$), and 0.00 Hz to the remaining 5 levels, resulting in the overall rate of 2.96×10^{12} Hz.

Table 1. Auger and Radiative Rates.

Sub-configuration	J value	Energy (eV)	Auger Rate (Hz)	Radiative Rate (Hz)
$1s^2 2\bar{p}6\bar{p}$	0	-0.45	2.96×10^{12}	4.79×10^9
$1s^2 2\bar{p}6\bar{p}$	1	-0.38	1.01×10^{13}	4.89×10^9
$1s^2 2p6\bar{p}$	1	-0.38	1.43×10^{12}	5.35×10^9
$1s^2 2p6\bar{p}$	2	-0.28	1.53×10^{12}	5.51×10^9
$1s^2 2\bar{p}6p$	1	-0.26	5.67×10^{13}	5.01×10^9
$1s^2 2\bar{p}6p$	2	-0.25	6.79×10^{12}	4.14×10^9
$1s^2 2p6p$	0	-0.17	3.41×10^{13}	4.60×10^9
$1s^2 2p6p$	1	-0.16	1.66×10^{11}	4.19×10^9
$1s^2 2p6p$	2	-0.03	1.57×10^{12}	3.03×10^9
$1s^2 2p6p$	3	+0.18	2.57×10^{14}	2.49×10^9

Radiative rates were determined for the decay of the 10 levels involving the $6\bar{p}$ and $6p$ subshells to the 4 levels of the odd-parity sub-configurations: $1s^2 2s 2\bar{p}$ ($J = 0, 1$) and $1s^2 2s 2p$ ($J = 1, 2$). The radiative rates for the 10 levels near threshold are also presented in Table 1. The radiative rates presented in Table 1 are summed over the 4 bound levels. For example the radiative rate for the $1s^2 2\bar{p} 6\bar{p}$ ($J = 0$) level at -0.45 eV is 1.08×10^9 Hz to $1s^2 2s 2\bar{p}$ ($J = 0$), 1.64×10^9 Hz to $1s^2 2s 2\bar{p}$ ($J = 1$), 5.51×10^6 Hz to $1s^2 2s 2p$ ($J = 1$), and 2.06×10^9 Hz to $1s^2 2s 2p$ ($J = 2$), resulting in an overall rate of 4.79×10^9 Hz.

Dielectronic recombination cross sections for F^{6+} using Eq.(1) are presented in Figure 1 using $\Delta E_c = 0.02$ eV. Convoluted dielectronic recombination cross sections for F^{6+} are presented in Figure 2 using a convolution energy of 0.02 eV. The presence of resonances just below the F^{5+} ionization potential indicates that these resonances should be included in total recombination rate coefficients.

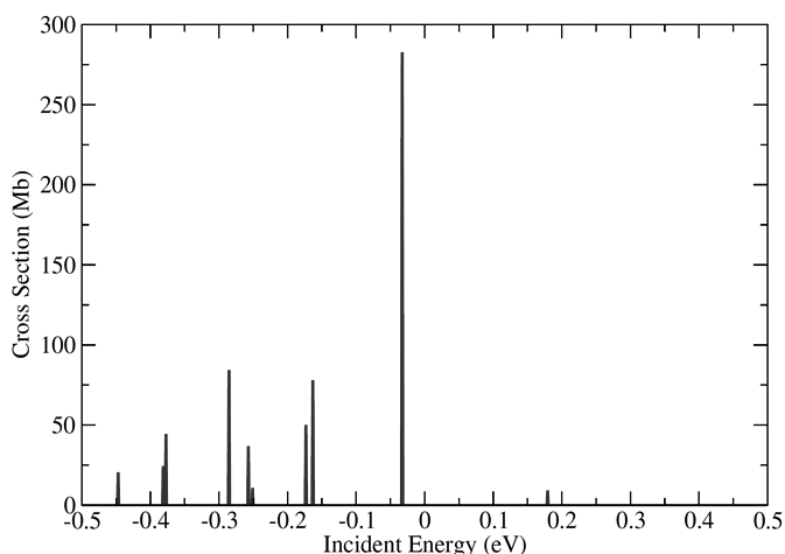


Figure 1. Dielectronic recombination cross sections for F^{6+} ($1.0 \text{ Mb} = 1 \times 10^{-18} \text{ cm}^2$).

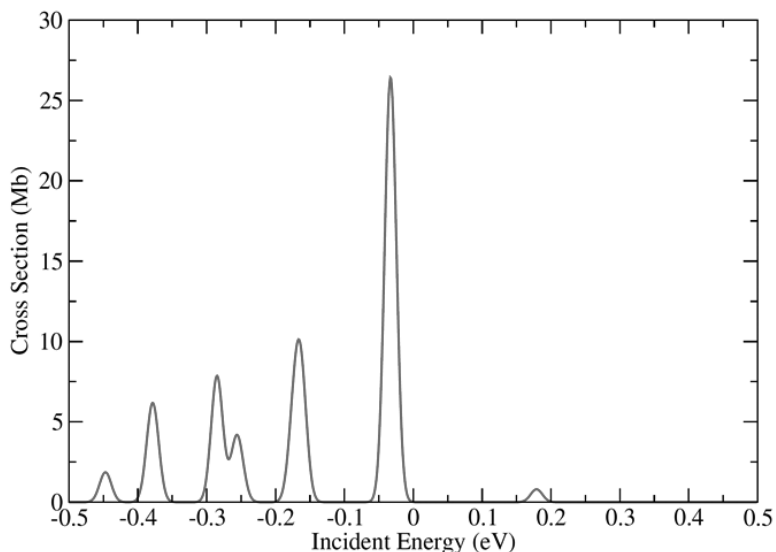


Figure 2. Convoluted dielectronic recombination cross sections for F^{6+} ($1.0 \text{ Mb} = 1 \times 10^{-18} \text{ cm}^2$).

4. SUMMARY

Low order relativistic perturbation theory has been applied to calculate the dielectronic recombination in F^{6+} above and below the ionization threshold. Resonances attributed to the $1s^2 2p6p$ configuration straddle the threshold, with a strong resonance feature at -0.03 eV. In the future we plan to examine additional atomic ion systems to map out their dielectronic recombination above and below the ionization threshold.

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