

Photoionization of atomic fluorine

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Synopsis We use R -matrix method to study the near threshold (17.5eV-20eV) photoionization of neutral fluorine atom and obtain total photoionization cross sections in 3P to 1D range. The theoretical calculation results fit the experimental results better after we consider core-valence electron correlation.

Photoionization cross sections of atoms or ions are widely used in calculations of plasma opacity in both astrophysics and radiation transport of thermal plasma. As for fluorine atom, people first observed abundant autoionization resonance structures in experiments. Then the high-quality experimental data inspired people to study photoionization of atomic fluorine theoretically. Most recently Saha employed MCHF method for detailed investigation of the autoionization resonances between 3P and 1D thresholds.

In the present study, we aim to use the nonrelativistic close-coupling R -matrix [1] approach with consideration of core-valence interaction to calculate the photoionization cross sections from 3P to 1D threshold of fluorine. And comparison is made with the experimental results. Eleven single electron orbits ($1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d, 4f, 5g$) are included to form the configuration interaction wave function of the positive fluorine using CIV3 program. To discuss the effects of core-valence electron correlation, we chose three different cases of electron excitation, which are listed in Table 1. Case A stands for the situation that all the electrons on $1s$ and $2s$ shells are kept frozen and only two electrons can be excited from $2p$ shell; case B that only one electron on $2s$ shell can be excited; case C that two electrons on $2s$ shell can be both excited.

Table 1. Target energy and ionization energy.

State	A	B	C	MCHF	Expt.
3P	0.0	0.0	0.0	0.0	0.0
1D	2.652	2.624	2.612	2.710	2.588
1S	6.361	7.248	5.649	5.560	5.569
$^2P^o$	17.51	16.62	17.27	17.25	17.44

Comparing these three different cases, it is clear that the energy levels fit the experimental results

much better after considering the core-valence electron correlation effects.

Between the energy range from 17.5eV to 20eV, fluorine atom is mainly ionized into F^+ (3P) state according to Table 1. In Fig. 1, the total cross sections of 3P state are displayed in both length and velocity gauges, compared with MCHF results and experimental results.

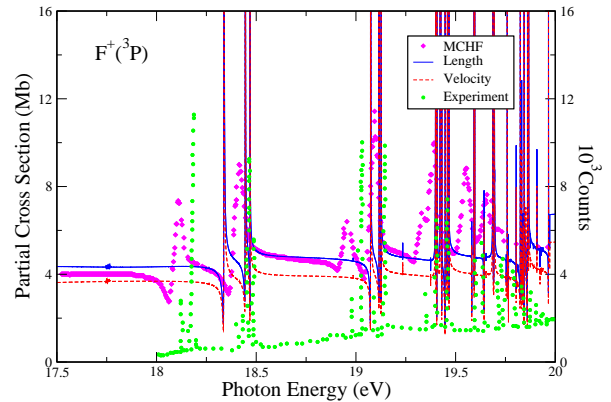


Figure 1. Total photoionization cross sections of fluorine between the 3P and 1D thresholds. MCHF calculations of Saha: violet diamond. Experimental data of Caldwell *et al.*: green dot.

Smaller step length is applied in RMATRIX1 [1] program as well as the consideration of configuration interaction. So that we distinguish the resonance states that are overlapped together in MCHF calculation results. It is shown that our theoretical result has a good agreement with the experiment, with more and sharper autoionization resonance peaks.

References

- [1] Keith A. Berrington *et al.* 1995 *COMPUT. PHYS. COMMUN.* **092** 000290

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