

Mutual neutralization in low-energy $H^+ + F^-$ collisionsJ. Zs. Mezei,^{1,2,3} J. B. Roos,³ K. Shilyaeva,^{4,3} N. Elander,³ and Å. Larson^{3,*}¹*Laboratoire Ondes et Milieux Complexes FRE-3102, CNRS and Université du Havre, BP 540, Le Havre, France*²*Institute of Nuclear Research, Bem ter 18/c, H-4026 Debrecen, Hungary*³*Department of Physics, Stockholm University, S-106 91 Stockholm, Sweden*⁴*Department of Physics, Gomel Fr. Scaryna State University, Sovetskaja Street 102, 246019 Gomel, Belarus*

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The cross section for mutual neutralization in collisions between H^+ and F^- ions at low energies ($E \leq 10$ eV) is calculated using a molecular close-coupling approach. Two different representations of the quasidiabatic potentials and couplings of HF are used. The effect of autoionization on the cross section is investigated. The coupled Schrödinger equation for the nuclear motion is solved using a numerical integration of the corresponding matrix Riccati equation and the cross section for mutual neutralization is computed from the asymptotic value of the logarithmic derivative of the radial wave function. The magnitude of the cross section for mutual neutralization in this reaction is small compared to other systems. This can be understood by the lack of avoided crossings at large internuclear distances. Resonant structures are found in the cross section and these are assigned with dominant angular momentum quantum number. The cross section for mutual neutralization in collisions of D^+ and F^- ions is also calculated.

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I. INTRODUCTION

In hydrogen and fluorine containing plasmas [1], mutual neutralization in collisions of H^+ and F^- ions can be an important source of charge removal. This reaction has as far as we know never been studied theoretically or experimentally. Here, we present a theoretical study of the reaction



at low collision energies.

We have previously studied dissociative recombination [2] and ion-pair formation [3] in electron recombination with HF^+ ions. A quasidiabatic representation of relevant potentials and couplings was then determined from the calculated adiabatic potentials [3]. The HF system is special in the sense that the ion-pair channel is the first asymptotic channel for the excited states of $^1\Sigma^+$ symmetry. The next channel is the $H(n=2) + F(^2P)$ that lies about 0.0267 eV above the ion-pair channel. Therefore, this system does not have any avoided crossings at very large distances that are found to be crucial for mutual neutralization in collisions of $H^+ + H^-$ [4], for example. As we here will show, the lack of these curve crossings will cause a cross section for mutual neutralization that is small in magnitude but has a rich structure originating from, what we think are, narrow resonances.

The outline of the paper is as follows. The calculation of relevant quasidiabatic potentials and couplings is summarized in Sec. II. Here states of $^1\Sigma^+$ symmetry up to the asymptotic limit $H(n=4) + F(^2P)$ are included. Two different models describing the relevant electronic states are presented. In the first model, only the electronic couplings among the excited states are included, while the second model also accounts for couplings to the ground state of HF. The method of solving the coupled Schrödinger equation for the nuclear motion and calculating reactive scattering cross sections is summarized

in Sec. III. Section IV presents and discusses the resulting cross sections for mutual neutralization. We have here also carried out calculations on mutual neutralization in $D^+ + F^-$ collisions. Unless otherwise stated atomic units are used in the paper.

II. POTENTIAL ENERGY CURVES AND COUPLINGS

The relevant potential energy curves of HF of $^1\Sigma^+$ symmetry have previously [2] been calculated *ab initio* using a multireference configuration interaction (MRCI) technique. In the first step of the calculation, the molecular orbitals are generated from a self-consistent-field calculation (SCF) using a contracted ($14s8p2d/11s7p2d$) basis set for H and a ($10s7p2d/6s5p2d$) triple zeta with polarization and additional functions to describe the negative ion for F. Then, in the second step, in order to obtain a more compact representation of the orbitals, natural orbitals are calculated. In this step, a configuration interaction (CI) calculation on the ground state of HF is carried out consisting of all singles and doubles, where the 1σ orbital is frozen and the active space contains four orbitals, namely, 2σ , 3σ , $1\pi_x$, and $1\pi_y$. The natural orbitals are then abstracted from this calculation. The final step consists of the MRCI calculation using the natural orbitals and a reference space consisting of 8 natural orbitals with the highest occupation numbers, the lowest σ orbital which is frozen, three σ , and four π orbitals, two π_x and two π_y orbitals. Single excitations from this set of reference configurations into the virtual orbitals are included. At each geometry, 25 roots are calculated. Using this technique the electronically bound adiabatic states of $^1\Sigma^+$ symmetry are computed.

The excited neutral states consist of both Rydberg states converging to the ground ionic core ($X^2\Pi$) as well as Rydberg states converging to excited ionic cores. In a quasidiabatic representation, these excited core Rydberg states might cross the ionic ground state potential and become resonant states. In order to calculate the resonant states embedded in the ionization continuum, electron scattering calculations are

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carried out using the complex Kohn variational method [5]. These calculations will provide us with both the energy positions and autoionization widths of the resonant states. To obtain consistency, it is crucial to have the same target (HF^+) electronic wave function in the scattering and structure calculations.

The nuclear dynamics is studied using a quasideiabatic representation of the electronic states. In our previous study on HF [3], we proposed a method to obtain not only the quasideiabatic potentials, but also the electronic couplings between the neutral states. In this method, a guess of the quasideiabatic potential curves is first obtained by tracking the states using the configuration interaction coefficients. The Rydberg states will have the same electron configuration as the ground state of the ion, i.e., $[(1\sigma)^2(2\sigma)^2(3\sigma)^2(1\pi)^3]$ plus an outer electron in a diffuse orbital. The resonant states are Rydberg states that converge to electronically excited ionic cores. These cores all have the (3σ) orbital singly excited. The quasideiabatic ion-pair state will be dominated by the electron configurations $(1\sigma)^2(2\sigma)^2(3\sigma)^1(4\sigma)^1(1\pi)^4$. By following the configurations of the resonant states, the quasideiabatic potential energy curves can be obtained. The diabatic (\mathbf{V}) and adiabatic (\mathbf{E}) potential matrices are related by the orthogonal transformation matrix \mathbf{T} according to [6]

$$\mathbf{V} = \mathbf{T}^{-1}\mathbf{E}\mathbf{T}. \quad (2)$$

The diabatic potential matrix has the diabatic potential curves on the diagonal and the electronic couplings as off-diagonal matrix elements. The adiabatic potential matrix is diagonal and its nonzero elements describe the adiabatic potential curves. It is here assumed [3] that the transformation matrix is given by a product of matrices describing successive 2×2 rotations of the adiabatic states:

$$\mathbf{T} = \mathbf{T}_1\mathbf{T}_2 \dots \mathbf{T}_n. \quad (3)$$

In the case of rotations among states 1 and 2, the matrix \mathbf{T}_i is given by

$$\mathbf{T}_i = \begin{pmatrix} \cos(\gamma_i) & -\sin(\gamma_i) & 0 & 0 & \dots \\ \sin(\gamma_i) & \cos(\gamma_i) & 0 & 0 & \dots \\ 0 & 0 & 1 & 0 & \dots \\ 0 & 0 & 0 & 1 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \quad (4)$$

The rotational angles γ_i are assumed to be smooth functions that go from 0 to $\pi/2$, describing diabatic and adiabatic states that coincide on both sides of the avoided crossings. Here, we use the analytical form

$$\gamma_i(R) = \frac{\pi}{4} \{1 + \tanh[\alpha_i(R - R_i)]\} \quad (5)$$

for the rotational angles. The total transformation matrix in Eq. (3) can be shown to be orthogonal [3]. After the diabatic potential matrix \mathbf{V} is set up we perform an optimization procedure, where the unknown parameters α_i and R_i of the rotational angles are determined in order to optimize the agreement between the diagonal elements of \mathbf{V} and the estimated diabatic potentials obtained by tracking the configurations as described above. When the parameters are optimized, also the electronic couplings are obtained as

the off-diagonal elements of the matrix \mathbf{V} . By construction [see Eq. (2)], the obtained quasideiabatic potentials have the adiabatic potentials as eigenvalues. However, we do not show that the coupling elements of the nuclear kinetic energy operator (nonadiabatic interactions) for the quasideiabatic states are identically zero. Therefore, the proposed method does not produce any strict diabatic states [7], but rather quasideiabatic potentials and couplings.

In our previous study on the HF system [3], two different models describing the set of the potential energy curves and couplings were proposed. In model I, the ion-pair state is supposed to interact only at small internuclear distances with the Rydberg states converging to the ground ionic core. Thus, there were no couplings included between the ground state of HF, $X^1\Sigma^+$, and the excited states of the same symmetry. In Fig. 1, the quasideiabatic potentials of $^1\Sigma^+$ symmetry for model I of HF are shown. The ion-pair state is the dashed (black) curve.

The electronic coupling elements are obtained as off-diagonal elements of the diabatic potential matrix. The largest coupling elements come from states that in the quasideiabatic representation cross each other. Some of the relevant couplings of the quasideiabatic potentials obtained in model I were displayed in Fig. 3 of Ref. [3].

There has been a debate in the literature on whether or not the ion-pair state is interacting with the ground state of HF [8,9]. At small distances, the ground state has an ion-pair character, while at larger distances it covalently goes to the lowest limit $\text{H}(n=1) + \text{F}(^2P)$. Hence, there is a large avoided crossing between the ground state of HF and the ion-pair state. Similar avoided crossings are possessed by the alkali halides such as LiF, LiCl, and NaI [10–12]. In model II of the quasideiabatic states, the curve crossing between the ion-pair state and the ground state of HF is included. As discussed in our previous study [3], the inclusion of the curve crossing between the ion-pair and the ground state of HF results in an

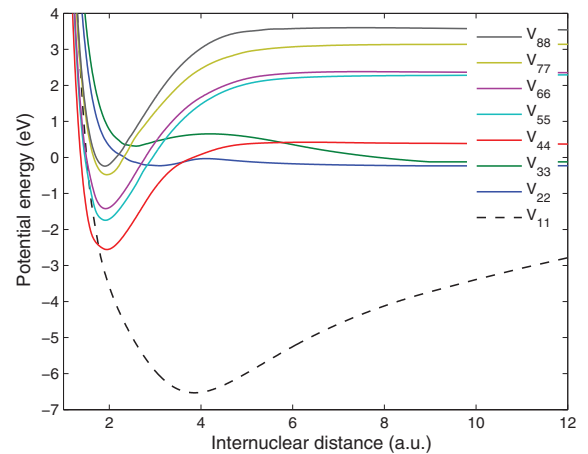


FIG. 1. (Color online) Model I: Quasideiabatic potential energy curves of $^1\Sigma^+$ symmetry of HF. The covalent potentials are shown as colored solid lines from the top to the bottom according their asymptotical limits, while the potential of the ion-pair state is displayed with the dashed (black) curve. The ground state of HF is not displayed in the figure. The energy scale is relative to the asymptotic limit of the ion-pair state.

electronic coupling between these states that is an order of magnitude larger than all other coupling elements (see Fig. 4 of [3]). The couplings between the higher excited states of model II remain very similar to those of model I.

In the study of dissociative recombination and ion-pair formation in electron recombination of HF⁺ the two models of the potentials have produced very similar cross sections. The inclusion of the couplings between the ion-pair and the ground states did not have any effect on the dynamics in the reactions.

It is well known that to correctly describe the translational motion of the electrons along with the nuclei, the so-called electron translational factors (ETFs) have to be incorporated [13]. By including the ETFs, nonvanishing asymptotic nonadiabatic interactions can be avoided [14]. However, the presently studied system is such that asymptotic couplings are not likely to have significant influence on the mutual neutralization reaction. Rather, the reaction is believed to be driven by the avoided crossings occurring at smaller ($R < 10a_0$) internuclear distances.

In Table I, the channels included in the present study are listed. The energy is relative to the asymptotic H⁺ + F⁻ ion-pair limit. The potential curves associated with each limit in model I and II are also given.

Since the spin-orbit coupling is not considered when the potential energy curves are calculated, the average values for the different J components for the atomic limits for F are used.

III. SCATTERING FORMALISM

In order to solve the coupled equations for the nuclear motion, a partial wave expansion is used for the nuclear wave functions:

$$\chi_i(\mathbf{R}) = \frac{1}{R} \sum_{l=0}^{\infty} A_l u_{i,l}(R) P_l(\cos \theta). \quad (6)$$

In the quasidiabatic representation of the potentials, we now obtain the coupled equations for the radial nuclear wave functions $u_{i,l}$ that takes the form

$$\left[-\frac{1}{2\mu} \frac{d^2}{dR^2} + \frac{l(l+1)}{2\mu R^2} \right] u_{i,l} + \sum_{j=1}^M \tilde{V}_{ij} u_{j,l} = E u_{i,l}, \quad (7)$$

where μ is the reduced mass of the molecular system and M is the number of coupled states included in the study. Here eight states are included in model I and nine states in model II.

Autoionization from the resonant states is included by letting the potential energy curves become complex valued

TABLE I. Channels included in the present study.

Atomic States	Model I	Model II	Energy (eV)
H($n=1$) + F(2P)		V_{11}	-10.1722
H ⁺ + F ⁻	V_{11}	V_{22}	0.0
H($n=2$) + F(2P)	V_{22}, V_{33}, V_{44}	V_{33}, V_{44}, V_{55}	0.0267
H($n=3$) + F(2P)	V_{55}, V_{66}	V_{66}, V_{77}	1.9153
H($n=4$) + F(2P)	V_{77}, V_{88}	V_{88}, V_{99}	2.5764

when they are above the ion potential and to have only real parts otherwise:

$$\tilde{V}_{ii}(R) = \begin{cases} V_{ii}(R) - i\frac{1}{2}\Gamma_i(R), & R < R_x, \\ V_{ii}(R), & R \geq R_x. \end{cases} \quad (8)$$

Here, Γ_i is the autoionization width of the electronically resonant state and R_x is the internuclear distance where the potential curves of the resonant state and ion cross. This is the so-called local (boomerang) model for including autoionization [15,16] and it is valid when the total energy of the system is high enough that autoionization into a complete set of vibrational eigenstates is possible. In the study of dissociative recombination of HF⁺ we confirmed the validity of this approximation for energies similar to those studied for the present reaction [2]. By making the inner part of the diagonal potential of the electronically resonant states complex as in Eq. (8), we obtain a non-Hermitian problem [17–20].

In order to numerically integrate the Schrödinger equation, we introduce the logarithmic derivative of the radial wave function

$$\mathbf{y}_l = \mathbf{u}'_l \mathbf{u}_l^{-1} \quad (9)$$

and the radial Schrödinger equation is transformed into a matrix Riccati equation

$$\mathbf{y}'_l + \mathbf{Q}_l + \mathbf{y}_l^2 = \mathbf{0}. \quad (10)$$

The physical boundary condition for the logarithmic derivative at origin becomes a diagonal matrix with infinite elements. Using a numerical procedure developed by Johnson [21–23], the matrix Riccati equation is integrated out to a region where the potentials have reached their asymptotic form. In the present study $R_f = 50a_0$ is used.

By combining the value of logarithmic derivative at R_f with the correct regular and irregular solutions of the asymptotic states, the reactance matrix can be calculated [4]. The elements of the scattering matrix [$S_{ij,l}(E)$] are obtained as a Cayley transformation between the open partitions of the reactance matrix. Finally the cross section for mutual neutralization can be computed from the scattering matrix elements

$$\sigma_{ij}(E) = \frac{\pi}{k_j^2} \sum_{l=0}^{\infty} (2l+1) |S_{ij,l} - \delta_{ij}|^2, \quad (11)$$

where k_j is the asymptotic wave number of the incoming channel given by

$$k_j = \sqrt{2\mu(E - E_j^{th})}. \quad (12)$$

E_j^{th} is the asymptotic energy of state j . It can be shown [18,20] that the formalism outlined above to calculate the cross section remains valid even when autoionization is added to the model.

Here, R_f is varied from $50a_0$ outward and the cross section was found not to change significantly. To determine the number of partial waves included in the summation [Eq. (11)], the same convergence criteria used in our previous study on H⁺ + H⁻ [4] is applied. To reach convergence, 25 of the partial waves at 1 meV and more than a hundred partial waves at 10 eV collision energies had to be included.

In the state-dependent cross sections for mutual neutralizations, resonant structures may occur. These resonant

structures can originate by so-called Feshbach resonances created when the bound states interact with states that are open for dissociation. Similar resonances are found in our previous study on ion-pair formation in electron recombination with HF^+ [3]. Alternatively, shape resonances are formed by the centrifugal barrier added to the diagonal elements of the potential matrix.

In order to understand and identify these resonances, we examine what partial waves contribute to the resonant structures by calculating the difference between the inelastic cross section and the contribution to this channel from a specific angular momentum:

$$\Delta\sigma_{ij,l}(E) = \sigma_{ij}(E) - \sigma_{ij,l}(E). \quad (13)$$

By comparing the difference cross sections with the total cross section, we can assign the angular momentum to a possible resonant structure.

IV. RESULTS AND DISCUSSION

A. Cross section for mutual neutralization

We start by solving the scattering equations for model I of the potentials, where eight states are included and no couplings to the ground state of HF. We investigate the role of the autoionization by turning on and off the complex term added to the potential curves of the resonant states. In Fig. 2 the total neutralization cross section in collisions between H^+ and F^- is displayed when autoionization is not included (black solid curve) and included (red dashed curve). The cross section shows a sharp threshold at 0.0267 eV, where the $\text{H}(n=2) + \text{F}(^2P)$ channel becomes energetically open. The cross section does not show the $1/E$ behavior at low collision energies that is typical for attractive Coulomb interaction [24]. Instead resonant structures dominate the cross section. These resonant structures are more pronounced when autoionization is not included. The inclusion of autoionization will reduce the cross section for mutual neutralization and smear out the resonant structures. Some resonant structures will still remain. The magnitude of the total neutralization

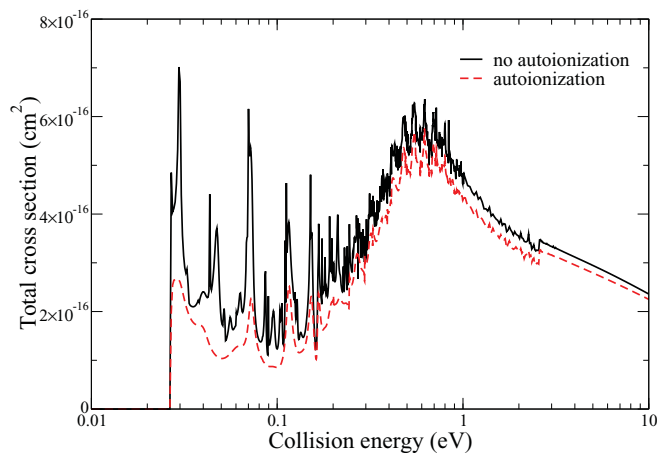


FIG. 2. (Color online) Total cross section for mutual neutralization in low-energy collisions of H^+ and F^- calculated using model I of the potentials and with and without including autoionization from electronic resonant states.

cross section around $E = 0.03$ eV is about 2.5×10^{-16} cm^2 . This should be compared with the total cross section for mutual neutralization of $\text{H}^+ + \text{H}^-$, which has a magnitude of about 2×10^{-13} cm^2 at the same energy. Furthermore, the low-energy cross section of the $\text{H}^+ + \text{H}^-$ reaction has a very smooth $1/E$ energy dependence. The H_2 system has avoided crossings at internuclear distances around $36a_0$. It is these avoided crossings at large internuclear distances that drives the reaction of mutual neutralization in $\text{H}^+ + \text{H}^-$ collisions at low energies. The HF system does not have these kinds of avoided crossings at large distances. This can be understood since the ion-pair limit is situated below the excited $\text{H}(n=2) + \text{F}(^2P)$ channel. The mutual neutralization reaction is instead driven by the avoided crossings with the Rydberg states occurring at small distances. This will explain the smaller magnitude and pronounced structures of the cross section for mutual neutralization in $\text{H}^+ + \text{F}^-$ collisions.

We then compute the state-dependent cross sections for the mutual neutralization reactions $\text{H}^+ + \text{F}^- \rightarrow \text{H}(n) + \text{F}(^2P)$, where $n = 1, 2, 3, 4$, using the two models of the potentials with and without inclusion of autoionization. As can be seen in Fig. 3, the two models produce very similar cross sections. The inclusion of the electronic couplings between the ion-pair and the ground states does not significantly influence the dynamics. The cross section for scattering into the ground-state fragments is much smaller than the cross section for scattering into the channel $\text{H}(n=2) + \text{F}(^2P)$. It can be concluded that the electronic couplings to the ground state do not have any significant impact on the state-dependent cross sections. Similar results were found in the study of dissociative recombination of HF^+ [3].

There is a sharp threshold in the $n=2$ cross section when this channel becomes energetically open. This cross section shows distinct structures indicating the presence of resonances. Both models of the potentials show similar structures even though they do not agree in positions and magnitudes. The cross sections for scattering into the $n=3$ and $n=4$ channels

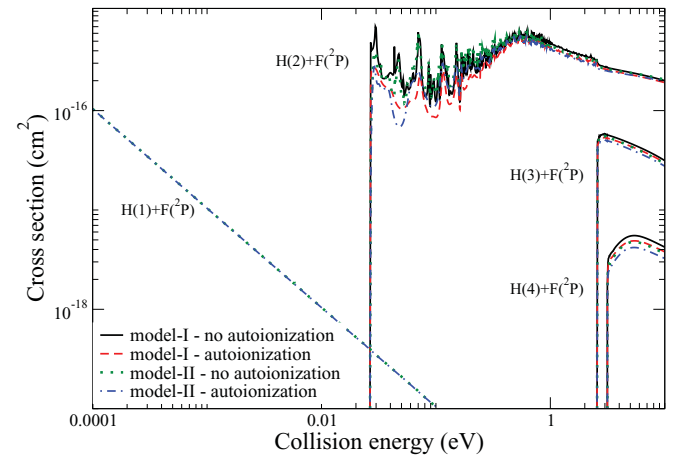


FIG. 3. (Color online) State-dependent cross sections for mutual neutralization at low-energy collisions of H^+ and F^- to form $\text{H}(n) + \text{F}(^2P)$, where $n = 1, 2, 3$ and 4 . The cross sections are calculated using the two different models of the diabatic electronic states with and without autoionization included.

show sharp onsets followed by smooth decays. No resonant structures are found in these state-dependent cross sections.

B. Resonant structures

In order to understand and identify the sharp oscillations found in the cross section of mutual neutralization, the contribution to the resonant structures from the partial wave l is examined by calculating the difference cross section defined in Eq. (13). We have here used model I of the diabatic states and performed the analysis without and with inclusion of autoionization. In Fig. 4 we show the identification of resonant structures originating from the $l = 13$ and $l = 21$ partial waves by displaying the total cross section (black solid and red dashed lines), the contribution from the specific partial wave (blue dotted line), and the difference cross section (green dotted-dashed line). The very narrow structures originating from the $l = 13$ partial wave are completely smeared out when autoionization is included. The $l = 21$ partial wave however will contribute to the cross section with a broader resonant structure that will be broadening by the inclusion of autoionization but it remains strong and well pronounced.

In Fig. 5, we label the structures in the $n = 2$ cross section in the region $0.02 \text{ eV} \leq E \leq 0.1 \text{ eV}$ with the angular momentum quantum number.

Some resonant structures originate almost exclusively from a single partial wave, while for other structures, several partial waves contribute.

A more detailed understanding of the resonant structures requires an analysis similar to the one used in the study of the $N^{3+} + H \rightarrow (NH)^{3+} \rightarrow N^{2+} + H^+$ reaction [25]. The underlying theory is based on that the S matrix is a meromorphic function that thus can be expanded in the residues of its complex poles, the resonance energies. The contribution of a particular resonance to a cross section is thus expressed as a residue term.

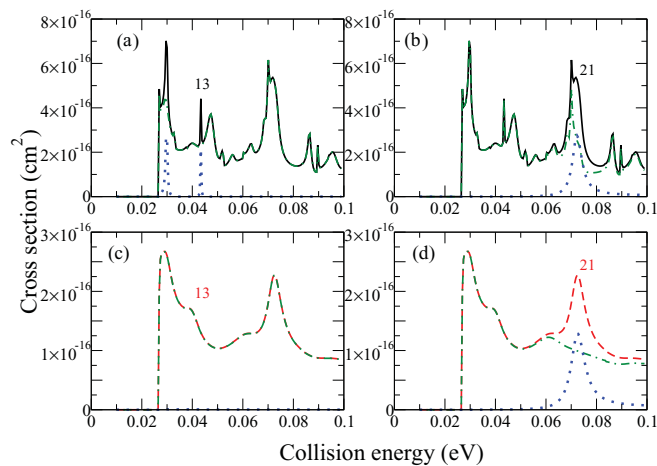


FIG. 4. (Color online) Identification of the contribution to the resonant structures from the $l = 13$ [in (a) and (c)] and $l = 21$ [in (b) and (d)] partial waves. Here model I is used for the diabatic potentials and the analysis is performed without [in (a) and (b)] and with [in (c) and (d)] inclusion of autoionization.

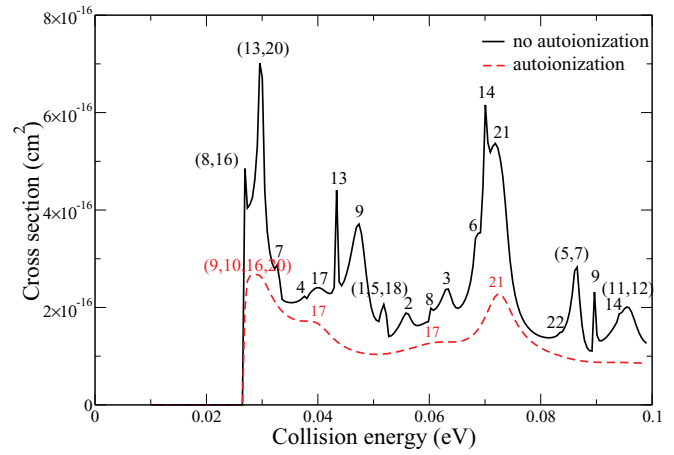


FIG. 5. (Color online) Labeling of the resonant structures with the angular momentum quantum number using the model I of the diabatic electronic states and without and with including autoionization.

C. Mutual neutralization in $D^+ + F^-$ collisions

By changing the reduced mass of the molecular system to the mass of DF, mutual neutralization in collisions of $D^+ + F^-$ is calculated. Due to the smaller mass difference between the colliding ions, the $D^+ + F^-$ mutual neutralization reaction might be easier to experimentally measure in an apparatus such as the double electrostatic storage device DESIREE [26], which currently is being under construction in Stockholm, Sweden. In Fig. 6, the total cross section for mutual neutralization in collisions between $D^+ + F^-$ (green dotted and blue dashed-dotted lines) is compared with the corresponding cross section in collisions between $H^+ + F^-$ (black solid and red dashed lines).

Model I of the potentials is applied when the cross section is calculated and the effect of the autoionization is investigated. The cross section for mutual neutralization in collisions between $D^+ + F^-$ shows the same sharp threshold effect at 0.0267 eV , where the $D(n = 2) + F(^2P)$ channel becomes energetically open. However, between this threshold and to an energy of about 0.3 eV , the cross section for $D^+ + F^-$

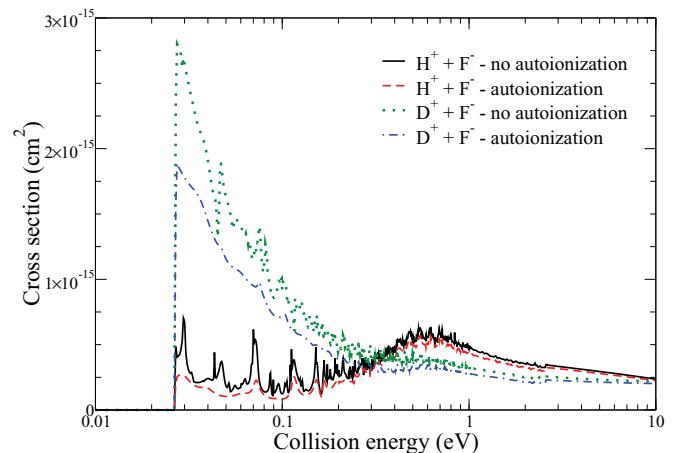


FIG. 6. (Color online) Total cross sections for mutual neutralization in collisions of $D^+ + F^-$ and $H^+ + F^-$ calculated using model I of the potentials and without and with including autoionization.

is considerably larger than the cross section for $H^+ + F^-$. The cross section shows a clearer $1/E$ energy dependence, but some structures can be seen. These structures are, however, less pronounced than the resonant structures found in the $H^+ + F^-$ cross section. A comparison with the analysis of the $N^{3+} + H \rightarrow (NH)^{3+} \rightarrow N^{2+} + H^+$ reaction studied in [25] may here be helpful in order to understand the difference between the $D^+ + F^-$ and the $H^+ + F^-$ mutual neutralization cross sections. It was there found that the resonant structures appeared in a narrow energy window centered around the rotational barrier maximum, close to the threshold of the incoming channel. Some resonances were just below this maximum and some just above. If we now compare the mutual neutralization of the two isotopic systems we note that the rotational and vibrational level structure in the heavier isotopologue is more dense due to the about twice as heavy reduced mass of DF compared to HF. Thus, there can be more resonances per energy unit within the energy window that produce resonant structures in the cross section. This implies that each of the partial wave cross sections would have more resonant structures per energy unit and when added together the total cross section will be larger at low energies. Furthermore, using classical arguments, the centrifugal barrier will prevent dissociation along the $H(n=2) + F(^2P)$ channel at low energies. This will cause a screening of the reaction. For the heavier isotopologue the offset of this screening is shifted toward lower energies.

V. CONCLUSIONS

The quasidiabatic potentials of HF have been calculated by combining multireference configuration interaction cal-

culations with electron scattering calculations. Two sets of models of the quasidiabatic potentials are tested. In model I, the ion-pair state is crossing the excited states of HF at small internuclear distances. In model II, the ion-pair state and the electronic ground state are allowed to cross. There are no curve crossings for this system occurring at large internuclear distances. Autoionization of the electronically resonant states is included using a local approximation. The first cross section for mutual neutralization in collisions between $H^+ + F^-$ is calculated by numerically integrating a matrix Riccati equation. The two models provide very similar cross sections. The cross section has a sharp threshold and is dominated by the formation of the $H(n=2) + F(^2P)$ fragments. The magnitude of the cross section is small compared to a system such as $H^+ + H^-$, which has curve crossings between ionic and covalent states occurring at large internuclear distances. Sharp oscillations are observed in the cross section for $H^+ + F^-$. The structures are broadening or smeared out when autoionization is added to the model. The resonant structures are assigned with angular momentum quantum numbers. The cross section for mutual neutralization in collisions of $D^+ + F^-$ is calculated and found to be significantly larger than that of its lighter isotopologue at low energies.

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