
COMMENTS

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Comment on "Suppressed electron capture in slow $O^+(^4S^o, ^2D^o, ^2P^o)$ -He collisions"

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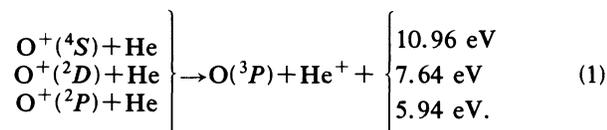
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Electron capture in collisions of O^+ ions with He atoms is studied on the basis of a molecular-orbital expansion approach. The cross section for electron capture by metastable $O^+(^2D, ^2P)$ ions is found to be larger by an order of magnitude than that for capture by ground-state $O^+(^4S)$ ions over the entire energy region studied. The energy dependencies of cross sections for electron capture by the ground and metastable ions are found to differ considerably below 2 keV. The present result, obtained by combining the cross section of 90% of the ground state and that of 10% of metastable states, reproduces reasonably well the experimental result of Kusakabe *et al.* [J. Phys. Soc. Jpn. **59**, 1987 (1990)], who reported using the mixture of the ground and metastable O^+ ions. The present finding clearly contradicts another experimental result of Wolfrum *et al.* [Phys. Rev. A **45**, R4218 (1992)], who reported no effect from the metastable states.

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I. INTRODUCTION

Recently, reports appeared at two experimental attempts by Kusakabe *et al.* [1] and Wolfrum, Schweinzer, and Winter [2] to study single-electron capture in collisions of O^+ ions with He atoms in the keV regime. The results have led to two conflicting conclusions: Kusakabe *et al.* [1] predicted larger cross sections when metastable ions were present, whereas Wolfrum, Schweinzer, and Winter [2] found no contribution from metastable ions. The processes they dealt with are the following with respective asymptotic energy defects:



In this study, we intend to shed more light on the col-

lision dynamics for the above processes on the basis of a molecular-orbital expansion method and to resolve the above disagreement.

II. THEORETICAL MODEL**A. Molecular states**

The electronic states of HeO^+ are described by the multireference single- and double-excitation configuration interaction (MRD-CI) method [3]. The helium-atom basis set is the same as in our previous study [4]. The oxygen-atom basis set is of a double-zeta polarization type $(9s5p1d)/[5s3p1d]$ with additional diffuse s , p , and d orbitals of exponents $\alpha_s=0.032$, and $\alpha_p=0.028$ and $\alpha_d=0.015$ for describing Rydberg excited states [5]. As a gauge of precision, we believe that the quality of the present molecular electronic states is equivalent to or better than that of the results of Augustin *et al.* [6], because the size of the present basis set and the CI's used are larger.

The present adiabatic potential curves are shown in Fig. 1. The ground $1^4\Sigma^-$ state couples directly only with electron-capture $2^4\Sigma^-$ and $4^1\Pi$ states, whereas the two metastable doublet states couple with each other in addi-

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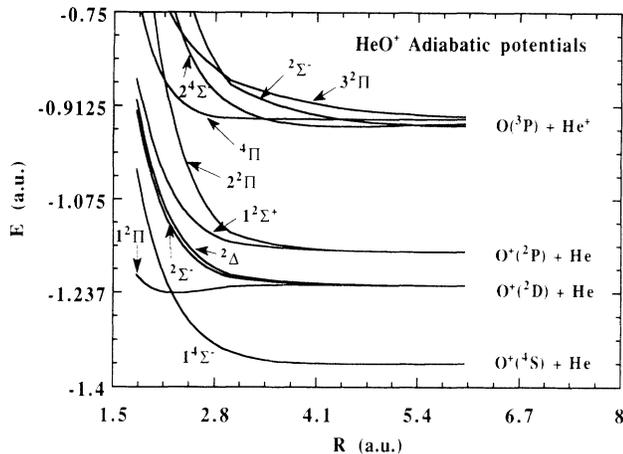


FIG. 1. Adiabatic potentials of the HeO^+ system. Energies are given relative to -76.0 a.u.

tion to the electron-capture doublet $2^2\Sigma^-$ and $3^2\Pi$ states. Particularly noteworthy is a sharp avoided crossing between $2^2\Pi[\text{O}^+(2P)+\text{He}]$ and $3^2\Pi[\text{O}(3P)+\text{He}^+]$, found at $R \cong 1.9$ a.u. This avoided crossing is expected to play a key role in electron capture from the metastable ion. All combinations of radial and rotational coupling matrix elements are also determined.

B. Collision dynamics

A semiclassical molecular-orbital expansion method was employed [7]. In this model, a total wave function was expanded as a product of an electronic wave function and an atomic-type electron translation factor. Substituting the total wave function into the time-dependent Schrödinger equation yields a set of first-order coupled equations. By solving the coupled equations numerically, we can readily obtain scattering amplitudes; the square of the amplitude gives the transition probability. Molecular states included in the dynamical calculations are the ten states shown in Fig. 1: $\text{O}^+(4S)+\text{He}; 1^4\Sigma^-, \text{O}^+(2D)+\text{He}; 2^2\Sigma^-, 1^2\Pi, 2^2\Delta, \text{O}^+(2P)+\text{He}; 2^2\Sigma^+, 2^2\Pi$ and $\text{O}(3P)+\text{He}^+; 2^4\Sigma^-, 4^2\Pi, 2^2\Sigma^-, 3^2\Pi$. Note that in keV collisions, a spin-changing process is not expected to be important. Accordingly, we neglect the process in the present study.

III. RESULTS

The present cross sections for electron capture by the ground $\text{O}^+(4S)$ state and metastable $\text{O}^+(2D, 2P)$ states are presented in Fig. 2. The cross sections clearly show that electron capture by the metastable $\text{O}^+(2D, 2P)$ states is more probable by an order of magnitude than that by the ground state. Electron capture by the metastable-state ions reaches a minimum at 1 keV and shows a slight increase as the energy decreases compared to the sharply decreasing trend in the ground-state ions. The dominant process in electron capture by metastable-state ions is the $2^2\Pi \rightarrow 3^2\Pi$ transition of $\text{O}^+(2P)$ ions, through strong radial coupling as speculated above, below 2 keV. This process is followed by the $1^2\Sigma^+ \rightarrow 3^2\Pi$ transition via the $2^2\Pi$ state through an angular coupling. Electron capture

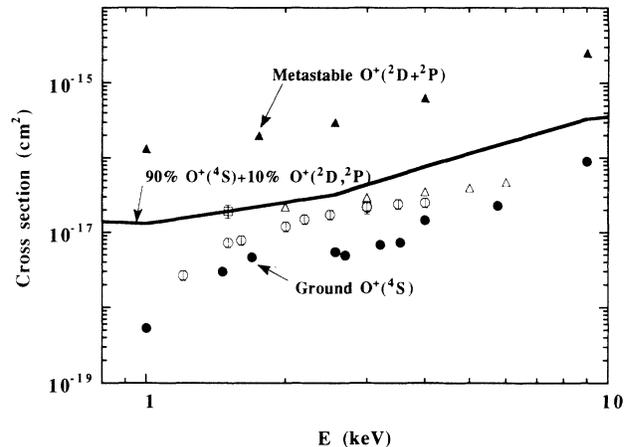


FIG. 2. Electron-capture cross sections. Theory (present): Solid circle; capture by a ground $\text{O}^+(4S)$ state. Solid triangle; capture by metastable $\text{O}^+(2D+2P)$ states. Experiment: Open circle; capture by a ground $\text{O}^+(4S)$ state, Kusakabe *et al.*, Ref. [1]. Open square; capture by mixed ground and metastable $\text{O}^+(4S, 2D, 2P)$ states, Ref. [1]. Open triangle; capture by mixed ground and metastable O^+ (or ground O^+ only; there is no difference), Ref. [2].

by the $\text{O}^+(2D)$ ions becomes important above 2–3 keV, with the $1^2\Pi$ state being the dominant channel via radial coupling with $3^2\Pi$.

Included in Fig. 2 are the experimental data of Kusakabe *et al.* [1] for electron capture by the ground and the mixture of the ground and metastable states, and also those of Wolfrum, Schweinzer, and Winter [2] for the ground state. (Wolfrum, Schweinzer, and Winter [2] reported no difference in the cross section even if the metastable states are included.) The present results for electron capture by the ground state agree reasonably well with those of Kusakabe *et al.*, both in magnitude and energy dependence. By combining 90% of the cross section of the ground $\text{O}^+(4S)$ state and 10% of that of the metastable $\text{O}^+(2D+2P)$ states, we obtain a good reproduction of the experimental data of Kusakabe *et al.* for the mixture case. Our [90% $\text{O}^+(4S)+10\%$ $\text{O}^+(2D, 2P)$] data also match well with the experimental data of Wolfrum, Schweinzer, and Winter, which are supposedly due to the sole contribution of ground $\text{O}^+(4S)$ ions. Our excitation and deexcitation cross sections for the process $\text{O}^+(2D)+\text{He} \leftrightarrow \text{O}^+(2P)+\text{He}$ are similar in magnitude over the entire energy range studied, with 1×10^{-16} cm^2 at 0.36 keV and 5×10^{-15} cm^2 at 10 keV. These cross sections are comparable in magnitude to those for electron capture by the metastable ions. Excitation (deexcitation) cross sections interfere with those for electron capture, resulting in the oscillation, but they will not mask electron capture.

Kusakabe *et al.* used a technique of electron impact ionization of the CO_2 molecule to generate O^+ ions. For the ground $\text{O}^+(4S)$ ions, 21- and 24.5-eV electron beams were introduced, while 150-eV electrons were used for a mixture of ground and metastable $\text{O}^+(2D, 2P)$ ions. However, the fraction of metastable-state ions is not known. Wolfrum, Schweinzer, and Winter, on the other hand,

used a similar technique on the H₂O molecule with 30-, 40-, and 130-eV electrons. They reported that in their 130-eV electron impact, the ions produced were 47% O⁺(⁴S), 40% O⁺(²D), and 13% O⁺(²P). In contrast, for 30-eV electron impact, only ground O⁺(⁴S) ions were produced (100%). As Hughes and Tiernan reported [8], the appearance potentials for O⁺(²D) and O⁺(²P) ions are 26.5 and 28.3 eV, respectively. Hence, a mixture of a small fraction of metastable O⁺ ions could well be expected when 30-eV electrons are used. Therefore, we suspect that in the work of Wolfrum, Schweinzer, and Winter metastable O⁺(²D, ²P) ions were actually present in all experiments. Similar values in the high-energy re-

gion above 2 keV in the experimental data of Wolfrum, Schweinzer, and Winter and Kusakabe *et al.* support our conclusion.

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