Measurements and Phase-Shift Analysis of the Differential Cross Sections for the Elastic Scattering in C^{2+} – He System at E_{cm} = 2.8 eV

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A study of elastic scattering often aims to derive information on the interaction potentials of a collision system. The observed structures in the cross sections such as rainbow scattering or glory scattering have often been used to evaluate interaction potentials.[1)] Measured cross sections also enable comparison with theoretical results based on the interaction potentials obtained by *ab initio* calculations. This procedure allows direct comparison between experiment and theory.

While intensive studies have been made for charge-transfer reactions involving multiply-charged ions, [2–3)] those for elastic scattering have been scarce. We have selected the C^{2+} – He system for the following reasons: (1) Since the electronic states of the C^{2+} ion in the ground state and the He atom are both $^1S_0$, the symmetry of the state of each molecule concerned with the collision is only $^1\Sigma^+$ at low energies. (2) The ionization potential of the C^+ ion, 24.38 eV, is lower than that of the target He atom: 24.59 eV. Therefore, the charge-transfer reaction is endothermic, and the cross section is very small at low energies.[2)] Hence, a single potential curve is safely assumed to control the scattering process. The present paper reports on the measured relative differential cross section (DCS) for the elastic scattering and the phase-shift analysis of the measured DCS based on the *ab initio* potentials.

The experimental method was reported previously.[4)] Briefly, the doubly charged ions were produced by an electron-beam ion-source (EBIS). The ^{13}CO gas was used as the source gas. Despite the report[2)] that about 3.5% of the doubly charged ions created by the EBIS are in the metastable state, the effect of the metastable ions was disregarded in the present work. The energy- and momentum-selected ions were crossed with a supersonic target beam, and then the scattered ions were energy-analyzed by an electrostatic analyzer with a position-sensitive detection system to distinguish from the background ions.

The angular distribution was determined from the energy spectrum obtained by rotating the detector with a 0.3° step in the laboratory frame. The counting rate for the signal was about 2 s^{-1} around θ_{cm} = 0.45 rad. The accumulation time was 4000 s at each angle setting. The measured signal was then converted to the DCS in the center-of-mass system with a standard manner. The overall angular resolution at the full width at half maximum (FWHM), about ± 1.0°, corresponds to that in the center-of-mass system about ± 0.07 rad at θ_{cm} = 0.45 rad. To determine the collision energy accurately, the measured energy- and angular-dependences of the scattered ions were compared with the calculated ones by changing the impact energy so as to reproduce the results. The accuracy of the collision energy was estimated to be better than ± 0.5 eV in the laboratory frame.

The DCS determined is shown in Fig. 1 by circles. As we made relative measurements, the measured values are shifted vertically by arbitrary amounts. The error bar shows the sum of the statistical error and the systematic error mainly due to the fluctuation of the primary-beam intensity. The DCS decreases with the increase in the scattering angle showing a shoulder at θ_{cm} = 0.45 rad, and then decreases monotonically.

To interpret the behavior of the measured DCS, we applied the phase-shift analysis using the JWKB approximation. Atomic units are used hereafter unless indicated otherwise. The JWKB phase-shifts for the potential $V(r)$ at the center-of-mass energy E is given by

$$\eta_l = \int_{r_0}^{\infty} \sqrt{F(r) - U(r)}\,\mathrm{d}r - \int_{(l+1/2)/k}^{\infty} \sqrt{F(r)}\,\mathrm{d}r\,, \tag{1}$$

where $F(r) = k^2 - (l + 1/2)^2 / r^2$ and $U(r) = 2\mu\, V(r)$, μ is the reduced mass of the system, r_0 is the classical turning point, and the wave number is $k = \sqrt{2\mu E}$. The orbital angular momentum quantum number is l. [5]

We used the potential energies obtained in the *ab initio* calculation reported by Castillo *et al.* [6] for the phase-shift analysis. Reported values were read from the figure 1(a) of their publication and then fitted to a Morse-type potential: $V(r) = 0.0265\, X(r)[X(r) - 2]$, where $X(r) = \exp\,[1.094(2.9 - r)]$. This model potential is displayed in Fig. 2(a).

The phase-shifts were calculated using the following equation in the case of $r_0 \le (l + 1/2)/k$:

$$\eta_l = \int_{r_0}^{(l+1/2)/k} \sqrt{F(r) - U(r)}\,\mathrm{d}r + \int_{(l+1/2)/k}^{\infty} [\sqrt{F(r) - U(r)} - \sqrt{F(r)}\,]\mathrm{d}r\,, \tag{2}$$

and eq. (3) is used in the case of $r_0 > (l + 1/2)/k$:

$$\eta_l = \int_{r_0}^{(l+1/2)/k} \sqrt{F(r)}\,\mathrm{d}r + \int_{r_0}^{\infty} [\sqrt{F(r) - U(r)} - \sqrt{F(r)}]\mathrm{d}r. \tag{3}$$

The double exponential method [7] was used to evaluate the integrals in eqs. (2) and (3). The maximum number of the partial waves involved was $l = 800$, and the phase-shift η_{800} was about 5×10^{-7} rad. The phase-shifts were then used to calculate the scattering amplitude, and the DCS, $\mathrm{d}\sigma/\mathrm{d}\Omega$, was determined.

The calculated DCSs are shown in Fig. 1 by dots. The cross section shows typical rainbow structures and rapid oscillations.[1] As the experimental angular resolution was insufficient to resolve the rapid oscillations, we smoothed the calculated results by taking account of the angular resolution of the apparatus, as displayed in Fig. 1 with a bold curve. An overall agreement between the measured and calculated results is found to be satisfactory; hence, the observed structure around θ_{cm} = 0.45 rad is assigned to rainbow scattering. It should be noted that the measured peak position exceeds the calculated one. The dashed curve shown in Fig. 1 is calculated using an *ab initio* potential proposed by Ohtsuki.[8] This potential, shown in Fig. 2(b), $V(r) = 0.0305\, X(r)[X(r) - 2]$ where $X(r) = \exp[1.043(2.9 - r)]$, has a well located at an equal position to that obtained by Castillo *et al.*[6] but is deeper by about 15 %. Note that the absolute value of the DCS is multiplied by 2.5 in Fig. 1. One can observe that the agreement between the measured and calculated positions of the rainbow scattering is improved. However, the measured position is still slightly more distant than the theoretical one. Hence, the actual well depth of the interaction potential is expected to be deeper than 0.0305. This is the first conclusion of the present analysis.

The rapid oscillations in the DCSs is well known to be due to the interference between the paths of the ions deflected by the attractive and repulsive parts of the interaction potential to result in a nearly equal scattering angle. The oscillation disappears when the scattering angle θ_{cm} exceeds 0.7 rad. This means that the deflection of the ion trajectory caused by the repulsive potential exceeds that by the attractive potential, and that the repulsive potential mainly determines the scattering. The repulsive parts of the potentials reported by Castello *et al.* [6] and that proposed by

Ohtsuki [8)] agree well with each other. When we use the relation between the phase-shift and the classical deflection angle, $\theta = 2\ \mathrm{d}\eta/\mathrm{d}l$, the largest scattering angle θ_{cm} = 1.9 rad in the present measurements, is interpreted to be the scattering of the partial wave with $l \approx 35$, and this partial wave corresponds to the classical closest approach, $r_0 \approx 1.9$. The angular dependence of the measured DCS beyond θ_{cm} = 0.7 rad agrees well with the theoretical ones. This leads to the second conclusion that the repulsive part of the potential used for the present analysis is accurate up to the internuclear distance of 1.9.

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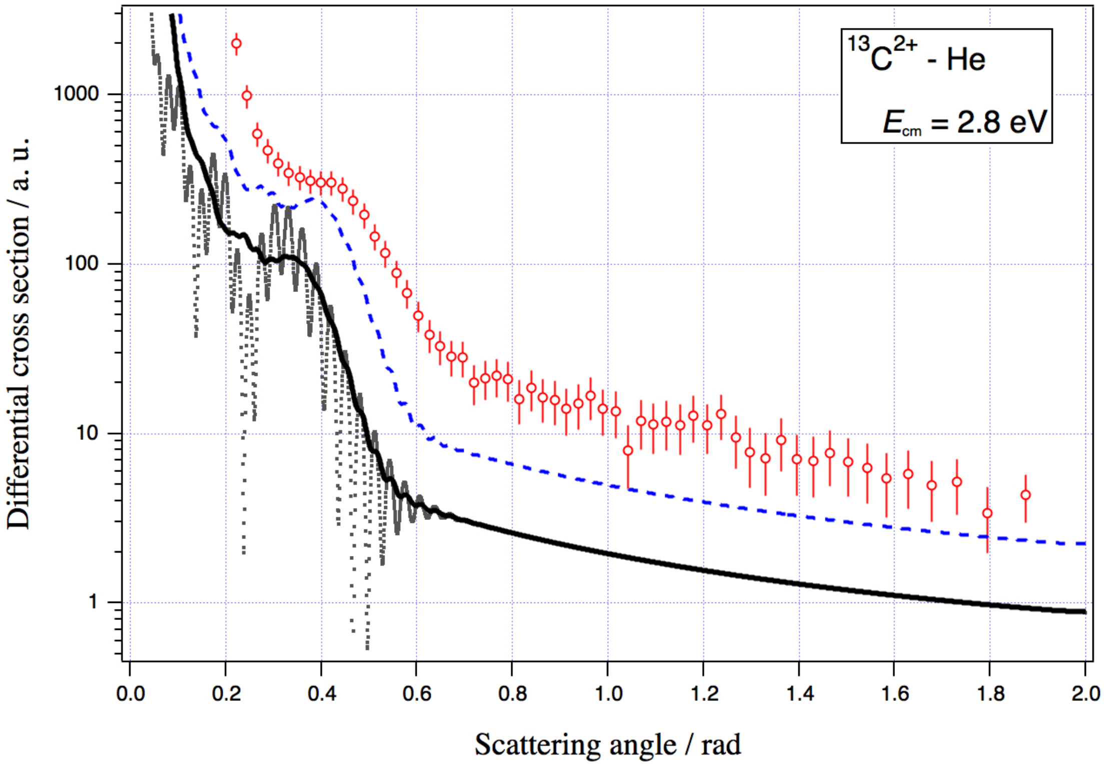
Figure captions:

Fig. 1. Measured and calculated DCSs. Experimental results are shown by circles. Calculated DCSs using the potential parameter deduced from the work of Castillo *et al.*[6] are shown by dots, and the smoothed result is shown by a bold curve. A dashed curve indicates the calculated result, which is multiplied by factor 2.5, adopting the potential parameter proposed by Ohtsuki. [8]

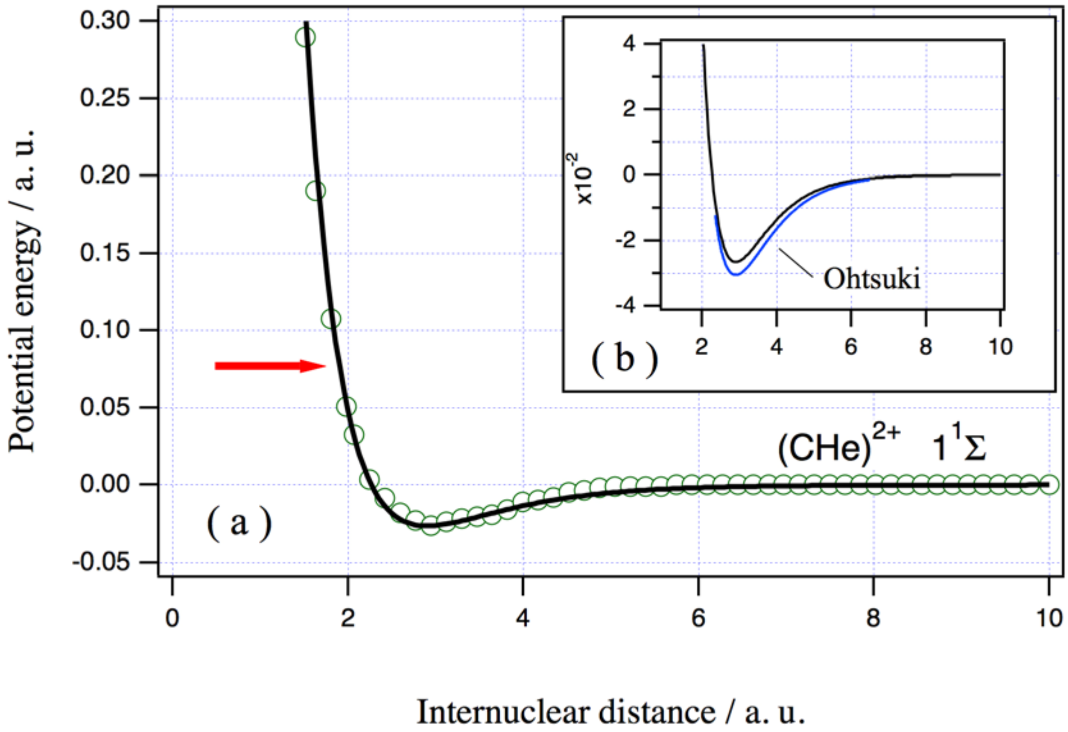
Fig. 2. Interaction potentials used for the phase-shift analysis. (a) The circles show the theoretical results reported by Castillo *et al.*[6] The Morse potential fitted to those points is shown by a curve. The arrow indicates the shortest internuclear distance probed by the present measurement. (b) The potential curve proposed by Ohtsuki. [8]

Fig.1:



$^{13}C^{2+}$ - He
E_{cm} = 2.8 eV
Differential cross section / a. u.
Scattering angle / rad
1000
100
10
1
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0

Fig. 2(a), (b)


0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
Potential energy / a. u.
0
2
4
6
8
10
Internuclear distance / a. u.
(a)
(CHe)2+ 1 1Σ
(b)
x10-2
4
2
0
-2
-4
2
4
6
8
10
Ohtsuki