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Comments and Addenda

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Resonant contributions to single charge transfer between He^{2+} and He

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Energy levels and lifetimes are calculated for the resonant states that are important in radiative single charge transfer in He^{2+}-He collisions at thermal energies. The resonant contribution to the charge-transfer rate decreases with increasing temperature and is approximately 12% of the total rate at 300 K.

Calculations of the rate of radiative charge transfer in low-energy He^{2+}-He collisions have recently been reported[1] and compared with experimental results.[2] In those calculations the motion of the nuclei was treated by a semiclassical method in which the effects of shape resonances were not assessed accurately. Since the formation and decay of these resonant states involves tunneling through the centrifugal potential barrier, they can be described most easily within a fully quantum-mechanical formalism.

The emission of a photon during heavy-particle collisions can be described by the addition of an imaginary part to the ion-atom interaction potential.[1,3] The resulting complex partial-wave phase shifts can be computed by direct numerical integration using the Numerov technique, and the charge-transfer cross section can then be obtained from the imaginary parts of the phase shifts.[3]

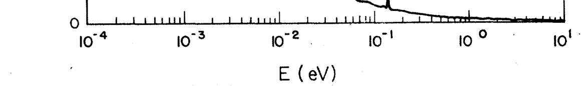

FIG. 1. Radiative single-charge-transfer cross section for He^{2+}-He collisions as a function of the relative energy. The positions of the predissociating states with quantum numbers (v, J) are indicated by arrows. The lowest peak is associated with the partial wave $J=13$. The very narrow resonances are not shown on this figure.

The complex phase shifts were first computed at 82 values of the relative energy E, spanning the range between 0.5 and 160 meV. All significant partial waves at $E \gtrsim 160$ meV and the lower partial waves at $10 \lesssim E \lesssim 160$ meV were essentially the same in the fully quantum and the JWKB calculations and consequently did not have to be recalculated. The resultant cross section, shown in Fig. 1, exhibits considerable structure. Many of the peaks can be identified with predissociating levels of the $B^1\Sigma_u^+$ state of He_2^{2+} that is formed in the He^{2+}-He collisions. The broader and less prominent structures are associated with the onset of significant contributions from each odd partial wave. For example, the centrifugal barrier in the partial wave $J=13$ can be surmounted classically if the energy is above 2 meV and thus the contribution from that partial wave increases significantly near that energy. Some of these peaks can be associated with resonant states near the top of the barrier, but are not well described by the Breit-Wigner form. For most of the structures seen in Fig. 1, the contributions to the thermal charge-transfer rate were computed by numerical integration of the cross section across the structure.

In addition to the peaks seen in Fig. 1 there are narrower peaks, associated with predissociating states with longer lifetimes, in which the cross section rises as much as two orders of magnitude. The contribution from each of these resonances can

TABLE I. Parameters for resonant levels of $He_2^{2+}(B\,^1\Sigma_u^+)$. [a]

v	J	E_{vJ} (a.u.)[b]	$\Gamma_{vJ}^{>}$ (a.u.)[b]	$\Gamma_{vJ}^{<}$ (a.u.)[b]
0	41	3.84^{-3}	1.6^{-7}	7.1^{-9}
1	37	2.40^{-3}	7.5^{-9}	7.2^{-9}
2	35	2.28^{-3}	2.3^{-6}	5.4^{-9}
3	31	1.30^{-3}	8.4^{-8}	5.7^{-9}
5	25	6.10^{-4}	6.1^{-7}	3.5^{-9}
7	19	1.90^{-4}	1.4^{-7}	1.5^{-9}
8	17	1.47^{-4}	3.1^{-6}	1.6^{-9}

[a] The states listed are those with widths between 10^{-9} and 10^{-5} a.u., corresponding to lifetimes between 2×10^{-8} sec and 2×10^{-12} sec.
[b] The superscript numbers indicate powers of 10.

be calculated by fitting the cross section to a Breit-Wigner profile and integrating analytically across the resonance. Radiative charge transfer occurs when these resonant states decay by emitting a photon rather than by predissociation.

Within each partial wave the narrow resonances were located by looking for the appearance of an additional node in the wave function or an increased phase shift as the energy was increased across the resonance. To facilitate this search, estimates of the resonant energies were first obtained by extrapolation from the bound-state energies for a given v to higher J. The complex phase shift and the corresponding contribution to the radiative charge-transfer cross section were then evaluated at a series of energies close to each estimated resonance. Each resonant contribution to the cross section was fitted to the form

$$\sigma_{\rm res}(E)=\frac{\pi}{2ME}(2J+1)\frac{\Gamma_{vJ}^{r}\Gamma_{vJ}^{d}}{(E-E_{vJ})^2+(\frac{1}{2}\Gamma_{vJ}^{t})^2}\,,$$

in which M is the reduced mass and E is the relative energy of the colliding particles, E_{vJ} is the resonant energy and Γ_{vJ}^{r}, Γ_{vJ}^{d}, and Γ_{vJ}^{t} are the widths corresponding to radiative decay, predissociation, and the total decay ($\Gamma_{vJ}^{t}=\Gamma_{vJ}^{r}+\Gamma_{vJ}^{d}$) of the He_2^{2+} states with vibrational and rotational quantum numbers v and J. It should be noted that,

TABLE II. Rate constants for radiative charge transfer in thermal He^{2+}-He collisions, calculated by the quantum and JWKB methods, in units of 10^{-14} $cm^3\,sec^{-1}$.

T(K)	100	300	600	1000	2000	3000
Quantum	4.43	4.24	4.02	3.79	3.43	3.25
JWKB	3.73	3.66	3.58	3.47	3.26	3.15

by fitting this form to the computed cross sections, one can obtain the two values of the partial widths, Γ_{vJ}^{r} and Γ_{vJ}^{d}, but cannot assign the values to each decay mode. We will thus designate the two partial widths for each resonance as $\Gamma_{vJ}^{>}$ and $\Gamma_{vJ}^{<}$.

The radiative decay widths are expected to be of the order of 10^{-9} a.u., whereas the predissociation widths vary by many orders of magnitude. Since the contribution of each resonance to the reaction rate is mainly determined by the smaller partial width $\Gamma_{vJ}^{<}$, we are mostly concerned with the states for which $\Gamma_{vJ}^{d}>\Gamma_{vJ}^{r}$. The positions and widths of the important resonances are given in Table I.

The reaction rates computed with allowance for the resonant effects are compared with the previous calculations in Table II. At 300 K resonant effects represent about 12% of the total reaction rate. Our calculated rate constant of 4.2×10^{-14} $cm^3\,sec^{-1}$ compares well with the measured value[2] of $(4.8\pm0.5)\times10^{-14}$ $cm^3\,sec^{-1}$.

A determination of the $B\,^1\Sigma_u^+$- and $E\,^1\Sigma_g^+$-state potential curves for He_2^{2+} from measurements of the relative elastic differential scattering cross section for the $He^{2+}+He$ system has been drawn to our attention by Champion.[4] The experimentally deduced potentials and the corresponding energy difference are in good agreement with our results.[1]

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[1] J. S. Cohen and J. N. Bardsley, Phys. Rev. A 18, 1004 (1978).
[2] R. Johnsen and M. A. Biondi, Phys. Rev. A 18, 996 (1978).
[3] J. S. Cohen and N. F. Lane, J. Chem. Phys. 66, 586 (1977).
[4] S. K. Lam, L. D. Doverspike, and R. L. Champion, Phys. Rev. A 7, 1595 (1973).