and the Morse Potential

$$\varphi(r) = \varphi_o \left\{ \exp\left[ -2\frac{C}{\sigma}(r-r_e) \right] - 2\exp\left[ -\frac{C}{\sigma}(r-r_e) \right] \right\} \tag{5}$$

In the latter there are only three adjustable constants since $C = \sigma \ell n 2/(r_e - \sigma)$

Average cross sections (or their equivalent[2] $\Omega^{(\ell,s)*}$) have been computed for the potential of Eq. (3)[3], of Eq. (4)[4] and of Eq. (5)[5,6] The methods used for the Morse potential differed somewhat, leading to slightly different values for the cross sections. Smith and Munn[5] use the potential as in Eq. (5) for all values of r, noting that it has a finite value at r=0 and thus is not a good representation of the true potential for small r. For this reason they terminated their tables at low values of $T^* = kT/\varphi_o$ for small C. Samuylov and Tsitelauri,[6] on the other hand, replaced the Morse potential by an infinite potential when

$$r \leq 0.3\sigma \tag{6}$$

in order to prevent unrealistic particle trajectories through r=0. They are thus able to extend their calculations to lower values of C than is possible with the pure Morse potential. Their values were used in the present work.*

The computed results for the above potentials are given in tabular form, and it is necessary to interpolate between entries to obtain cross sections for parameters of the actual potential. This was accomplished with a Lagrange 3-point formula for Eqs. (3) and (4). Two interpolations are necessary for the Morse potential; a linear formula was found adequate for the T*-interpolation while linear interpolation vs. $\ell n \beta (= C + \ell n\ 2)$ was deemed sufficiently accurate for the C-interpolation.

The constants used in the computation of the cross sections for the atom-atom and atom-ion elastic interactions are collected in Table I. Extensive comparison with

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*Some additional information on the Morse potential is included in Appendix A.

other work for Ar-Ar has been given in Ref. 7 and papers referred to therein. Inasmuch as the data on which the $Ar^+$-Ar potentials are based are the first theoretical computation it is difficult to assess their accuracy. One check is possible, namely on the depth $\varphi_o$ of potential minimum for the $^2\Sigma_u$ state, which corresponds to the $Ar_2^+$ molecular ion. The current knowledge of the potential depth for the rare-gas molecular ions has been reviewed by Mulliken,[9] from which we can conclude that $\varphi_o = 1.25$eV is reasonable. The potentials for the Ar-$Ar^+$ interaction are actually not very important in determining the transport coefficients, since they are used only in computing average cross sections with $\ell$ even.[10] Cross sections for $\ell$ odd are computed from the charge-transfer cross sections, which are much larger than the elastic cross sections and hence dominant.

Since they could be useful in computations of properties of a two-temperature partially ionized gas, some of the average cross sections computed for this work are collected in Table II. It should be noted that $\bar{Q}^{(2,2)}$ for Ar-$Ar^+$ is computed by first calculating the cross section for each of the four potentials in Table I and then averaging with the appropriate, in this case equal, statistical weight .[10] The Ar-Ar cross sections can be used to compute the pure atom thermal conductivity for argon. Comparing the values so computed with those of Amdur and Mason,[11] we find that the latter report values somewhat lower at low temperatures (ca. 10% at 2000°K), about the same at 5500°K and slightly higher above this temperature.

For the ion-atom cross sections with $\ell$-odd, charge transfer is the dominant process. A very good approximation for the energies of interest here is[12]

$$Q^{(\ell)} = 2\, Q_{Tr} \tag{7}$$

Over a limited range of energies we can also relate $Q_{Tr}$ to the relative speed g by the expression[12]

$$Q_{Tr} = \frac{1}{2}\,(A - B\ell n g)^2 \tag{8}$$