## **ERRATA**

## Erratum: Absolute partial and total electron-impact-ionization cross sections for $CF_4$ from threshold up to 500 eV [Phys. Rev. A 44, 2921 (1991)]

Ce Ma, M. R. Bruce, and R. A. Bonham

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While the results for the ion trajectories as a function of initial kinetic energy and direction as presented in Figs. 3 and 4 of our original paper are correct as calculated, they do not present a true picture of the actual situation. In an attempt to model the effects of using grids, the grid wires were placed at every fourth field sampling point in a SIMION trajectory calculation. This yields a grid transmission of 75% and leads to severe focusing and defocusing effects as shown in inset (a) in Fig. 1 of this Erratum. That such effects might be the artifact of an insufficient number of field sampling points was called to our attention by Professor G. G. B. de Souza of the Federal University of Rio de Janeiro. His group repeated our calculations using 100% dense grids (0% transmission) and found that for the parameters employed in our original Figs. 3 and 4 the maximum initial kinetic energy for which all singly charged ions could be collected was 4 eV. We have repeated the calculations of de Souza and co-workers and confirm their results as shown in Fig. 1 with an enlargement of the trajectories in the extraction region given in inset (b). In addition we have modeled the extraction grids by employing a grid wire for every ten field sampling points (90% grid transmission) and find that the results are

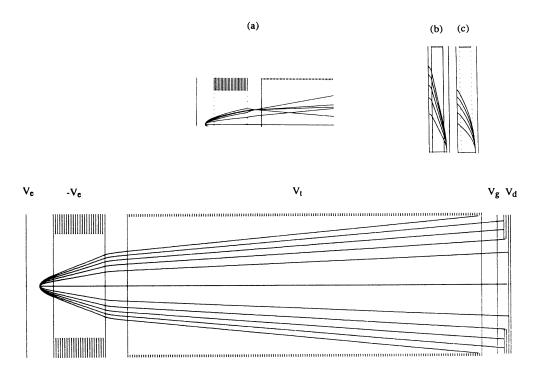


FIG. 1. SIMION calculation of ion trajectories in simulated time-of-flight mass spectrometer. The potential voltages were  $V_e = 60$  V,  $V_t = V_g = -1000$  V, and  $V_d = -2250$  V; the initial trajectory angle is 90° with respect to the axial axis (other angles will have less radial dispersion than the 90° angle); the initial kinetic energies of the ions are 0, 2, 4, 6, 8, and 10 eV, where the plotted trajectories have increasing radial dispersion with respective increasing energy (ion trajectories move left to right). Note that the trajectories are independent of the mass for single charged ions. One-half of the extraction region has been enlarged in insets (a)-(c). Inset (a): SIMION calculations for 75% transmission grids with only three field sampling points between electrode grid points. Inset (b): SIMION calculations with an ideal grid (all field sampling points are electrode points, hence the small area in  $-V_e$  is completely shielded from  $V_t$ ). These trajectories correspond to those in the main figure. Inset (c): SIMION calculations with a 90% transmission grid, with nine field sampling points between grid electrode points. Note that in the case for insets (b) and (c), the radial axis has been exaggerated by a factor of 12 in order to realistically model the grids in the extraction region (trajectories move right to left in these insets).

closer to the nongrid results with a very much smaller grid-focusing effect than in our original calculation as shown in inset (c) of Fig. 1. The net effect is that in case (c) the punch through fields increases the maximum energy that can be collected with 100% efficiency (excluding grid transmission losses) by the detector from 4 to 5 eV. Also note that the more realistic simulations of insets (b) and (c) have a well-defined maximum energy that can be detected, while for case (a) the trajectories tend to be randomized by the grids.

The problem with modeling grid-focusing effects should not have any bearing on the results reported by us on  $CF_4$  with the possible exception of the partial ionization cross section for  $F^+$  since that is the only ion which is believed to have initial kinetic energies capable of exceeding our upper collection limit. Hence our published results in the case of  $F^+$  can be regarded as a lower bound on the true result. Our model calculations indicate that for our geometry using an extraction field of 167 V/cm (200 V across 12 mm) it is necessary to employ a drift potential between 1500 and 2000 V in order to guarantee 100% collection of ions with an initial kinetic energy of 10 eV. However, experimentally we find that there is less than a 5% change in the  $F^+$  count rate at 80-, 150-, and 500-eV electron impact energies for extraction voltages  $(V_e)$  between 50 and 90 V and drift voltages  $(V_t)$  between -600 and -1000 V, while there is a considerable loss in count rate for lower voltages. From the SIMION calculations, this implies that most of the  $F^+$  ions must dissociate with less than 5 eV of kinetic energy. The experimental conditions in the original paper were 60 V for the extraction and -800 V for the drift tube, therefore we expect the  $F^+$  cross sections in Table I of the original paper to be well within their stated 15% uncertainties (that is to say, the 15% uncertainty has built into it the uncertainties in the effects of the kinetic energies of the ions). Recently new results have appeared for  $CF_4$  [1] which are in agreement with our published results although the  $F^+$  cross section, still within our error bars, was systematically larger than ours. It may be that the problem discussed above is related to this last observation.

One additional correction is that on p. 2934 of the original article, in the sentence beginning 9 lines from the bottom of the left-hand column, the range over which the relative efficiency of the detector was tested for ion impact energy should read 2-3 keV, and not 2-4 keV as stated. That this range is too narrow to get a valid test of the sensitivity to detector impact energy is discussed elsewhere [2]. The implications of this problem do not lead to significant corrections to any of our singly charged cross sections, but do have some influence on the results for the doubly charged cross sections although not nearly enough to explain the disagreement between our results and those of [1].

In conclusion we would like to emphasize that it is important to model grid-focusing effects, but that problems can arise by using SIMION to do this if insufficient field sampling points are employed. It is also important to point out that a shorter extraction tube can increase the maximum collectable initial ion energy, but if it is too short a field punch through may alter the course of the incoming electron pulse. Fast ions can be focused by the use of electrostatic lenses but ions with low kinetic energy may be lost in the process. In the present approach all ion energies less than the maximum detectable are collected.

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- [1] H. U. Poll, C. Winkler, D. Margreiter, V. Grill, and T. D. Mark, Int. J. Mass Spectrom. Ion Proc. 112, 1 (1992).
- [2] M. R. Bruce and R. A. Bonham (unpublished).

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## Erratum: Asymptotic expansion for $\delta$ -function matrix elements of helium [Phys. Rev. A 45, 70 (1992)]

G. W. F. Drake

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The line labeled  $\epsilon$  in Table I of this paper is incorrect. The corrected values are given below. The numerical values in the other tables are correct.

TABLE I. Asymptotic expansion coefficients for the energy  $(\xi)$  and  $\delta$  function  $(\Delta \xi)$ . For each line,  $\xi$  stands for the coefficient in the first column.

Coeff. $(\xi)$	ξ	Δξ	Δξ'	Δξ''
<i>€</i>	4329	131 393	122 035	140 751
	$32Z^{10}$	$64Z^{12}$	$128Z^{12}$	$128Z^{12}$