

## Electron capture from lithium by protons and helium ions

S. L. Varghese,\* W. Waggoner, and C. L. Cocke

*J. R. Macdonald Laboratory, Physics Department, Kansas State University, Manhattan, Kansas 66506*

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Experimental cross sections are reported for single-electron capture by protons,  $\text{He}^+$  and  $\text{He}^{2+}$  ions from lithium at projectile energies between 0.257 and 8.2 keV. For proton projectiles the results are in agreement with recent theoretical predictions from both molecular- and atomic-orbital expansions, as well as with older data. For  $\text{He}^{2+}$  projectiles the results are in agreement with recent atomic- and molecular-orbital expansion results, but some disagreement is found with earlier experimental and theoretical results.

### INTRODUCTION

Electron capture by light projectiles from lithium has frequently been studied because of the simplicity of the system and its consequent suitability as a testing ground for theoretical descriptions of the capture process. At a low projectile velocity compared to that characterizing the  $1s$  electrons in Li, capture of the single  $2s$  electron dominates, with the population proceeding usually to excited states of even singly-charged projectiles. For proton and  $\text{He}^{2+}$  projectiles, the process may be described within a particularly clean quasi-one-electron picture. With potential applications in view, electron capture from Li by alpha particles has recently received attention because of proposals that such a process could be useful in diagnosing properties of hot plasmas. While the most frequently addressed proposal involves double capture to diagnose velocities and densities of hot  $\alpha$  particles from thermonuclear burning in magnetic confinement fusion reactors,<sup>1</sup> schemes involving detection of radiation from single capture from Li have also been proposed.<sup>2</sup>

For the case of proton bombardment, the capture at low velocity is mainly into the  $n=2$  state of hydrogen and is nearly resonant. The molecular-orbital calculations of Allan *et al.*<sup>3</sup> are in agreement with the modified atomic-orbital (AO+) results of Fritsch and Lin,<sup>4</sup> although they differ somewhat from the molecular-orbital results of Sato and Kimura<sup>5</sup> and with the atomic-orbital results of Ermolaev.<sup>6</sup> All theoretical results are in fair agreement with the experimental data of Grüebler *et al.*<sup>7</sup> and Il'in *et al.*,<sup>8</sup> although the error bars quoted on the experiment are so large as to accommodate a considerable range of possibilities.

For  $\text{He}^{2+}$  projectiles, the capture feeds primarily  $n=3$  on the  $\text{He}^+$  final ion. Above a  ${}^4\text{He}^{2+}$  energy of 20 keV, the data of McCullough *et al.*,<sup>9</sup> Murray *et al.*,<sup>10</sup> and Kadota *et al.*<sup>11</sup> are in fair agreement with each other and with the atomic-expansion results of Fritsch and Lin.<sup>4</sup> At lower energies, the molecular-orbital calculation of Shipsey *et al.*<sup>12</sup> and the atomic-expansion calculation of Ermolaev and Bransden<sup>13</sup> descend rather steeply, while the more recent molecular-orbital calculation of Sato and Kimura<sup>5</sup> and the AO+ results of Fritsch and Lin<sup>4</sup> both predict that the cross section stays high down to much

lower velocities. Prior to the present work, the only experimental guidance in this discrepancy was provided by the results of Murray *et al.*<sup>10</sup> and McCullough *et al.*<sup>9</sup> which seemed to indicate that the cross section descended immediately below 10 keV. In view of the relative simplicity of this collision system, one would expect that either a molecular- or atomic-expansion approach, with an adequate basis set, should do well, and thus the major disagreement among theories and apparently with experiment is of particular concern. A major goal of the present work is to establish experimentally what the cross section really does at lower energy.

This paper reports total cross sections for electron capture from lithium by protons and doubly and singly charged helium ions in a velocity range extending from approximately (5–35)% of the orbital velocity of the  $2s$  target electron. The major purpose has been to test recent theoretical work for the bare projectiles and to resolve the discrepancy among theories at low energy for  $\text{He}^{2+}$  projectiles. The experimental arrangement invited the measurement of cross sections for capture by  $\text{He}^+$  projectiles as well, although no theoretical results have appeared in the literature yet for this case.

TABLE I. Cross sections for single capture by protons from Li.

Proton energy (eV)	Cross section for electron capture $\sigma_{10}$ (units of $10^{-16}$ cm <sup>2</sup> )
257	1.8±2.4
385	3.9±1.4
520	5.7±1.4
718	11.7±2.0
848	14.7±2.5
985	13.5±2.2
1150	15.1±2.4
1290	17.0±2.7
1460	22.0±3.2
1943	25.0±3.5
2412	39.0±5.4
2900	42.0±5.8
3395	43.0±5.8
3850	44.0±5.9

TABLE II. Cross sections for single capture by  $({}^4\text{He})^{2+}$  ions from Li.

$({}^4\text{He})^{2+}$ ion energy (keV)	Cross section for electron capture $\sigma_{21}$ (units of $10^{-15} \text{ cm}^2$ )
8.2	$11.71 \pm 1.63$
7.2	$11.18 \pm 1.55$
6.0	$11.40 \pm 1.86$
5.0	$10.28 \pm 1.87$
4.0	$11.90 \pm 1.64$
3.0	$10.79 \pm 1.53$
2.0	$10.18 \pm 1.50$
1.55	$9.49 \pm 1.71$
1.0	$8.0 \pm 1.34$
0.83	$6.89 \pm 1.15$
0.64	$6.28 \pm 1.41$
0.50	$4.83 \pm 0.69$
0.42	$4.23 \pm 0.63$

### EXPERIMENT

The protons and helium ions used in this experiment were obtained from a secondary ion recoil source pumped by a fast fluorine beam from the Kansas State University (KSU) tandem Van de Graaff. The source has previously been used for the study of electron capture by slow multiply charged ions from gaseous targets, and is described in other publications.<sup>15,16</sup> It is particularly well suited to the production of very low energy ions. The exact configuration used for this case has been described previously,<sup>17</sup> and will only be summarized here. The ions extracted from the source were passed through a resistively heated Li oven extending 1.90 cm along the ion path, with entrance and exit apertures 1.0 and 2.0 mm in diameter. Exiting ions were charge state analyzed by a spherical-sector electrostatic analyzer and detected by a channeltron. The Li target thickness was determined by measuring the cell temperature with two Chromel-Alumel thermocouples silver soldered to either end of the cell and using the vapor-pressure data of Douglas *et al.*<sup>18</sup> (These values are slightly lower, by approximately 6% over the temperature

TABLE III. Cross sections for single capture by  $({}^4\text{He})^+$  ions from Li.

$({}^4\text{He})^+$ ion energy (eV)	Cross section for electron capture $\sigma_{10}$ (units of $10^{-16} \text{ cm}^2$ )
256	$7.8 \pm 1.5$
510	$23.8 \pm 3.4$
728	$29.4 \pm 4.1$
966	$38.6 \pm 5.3$
1211	$43.9 \pm 6.0$
1421	$40.1 \pm 5.4$
1659	$50.5 \pm 6.8$
1876	$51.2 \pm 6.9$
2121	$55.9 \pm 7.6$
2394	$54.7 \pm 7.4$
2597	$54.2 \pm 7.3$
2821	$55.0 \pm 7.4$
3073	$55.3 \pm 7.5$

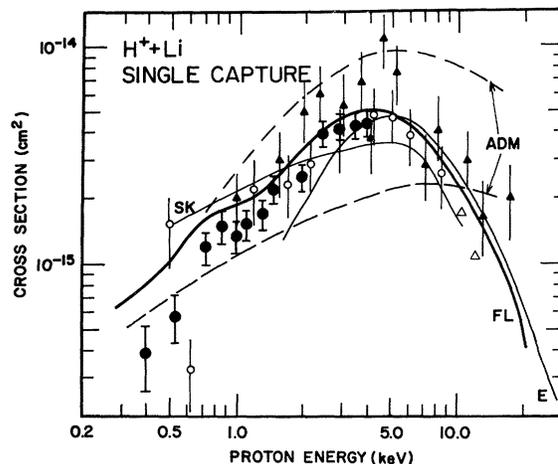


FIG. 1. Cross sections for single capture by protons from lithium. Data points are the following: ●, present; ▲ and ○, Grüebler *et al.* (Ref. 7) with proton and deuteron projectiles, respectively; △, Il'in *et al.* (Ref. 8). Theoretical curves are the following: — (FL) Fritsch and Lin (Ref. 4); - - - (ADM) Allan *et al.* (Ref. 3); — (E) Ermolaev (Ref. 6); — (SK) Sato and Kimura (Ref. 5).

range used here, than those given by Hultgren *et al.*<sup>19</sup> The latter set were used in Refs. 9 and 10.) By using a pulsed fluorine beam and time-of-flight analysis on the slow projectiles the initial charge state of each ion was determined, allowing distinction between, for example,  $\text{He}^+$  and  $\text{He}^{2+}$  ions. For the detection of neutral ions produced in capture by the single-charged projectiles, a 4-mm-diam aperture was made in the back plate of the spherical-sector analyzer to allow the passage of neutral particles into a second "on-line" channeltron.

Before making measurements, the Li oven was outgassed at a high temperature for typically 1–2 h. Once the target thickness stabilized, it remained stable and reproducible for the duration of the run, typically several days. Counting rates were typically 1000–5000 counts/sec in the direct beam and of order 10–100 counts/sec in the charge-exchange groups. Measurements were made for several cell temperatures, corresponding to target thicknesses up to  $2 \times 10^{13}$  atoms/cm<sup>2</sup>. Charge exchange with residual gas in the systems, when the cell was at room temperature, contributed a background which was usually less than 10% of the signal obtained with the warm oven. The fraction of ions undergoing charge exchange was typically 5% or less; corrections for second-order processes were quite small.

For the  $\text{He}^{2+}$  case, cross sections were obtained from the ratio between  $\text{He}^+$  and  $\text{He}^{2+}$  yields after charge-state analysis by the electrostatic analyzer. In the case of singly charged projectiles, the corresponding ratio of neutrals to singly charged ion yields was obtained from the on-line detector, with analyzer voltage on and off, respectively.

### RESULTS AND DISCUSSION

The results are shown in Tables I–III and in Figs. 1–3. Helium ion energies are given for  ${}^4\text{He}$ , and are in the labo-

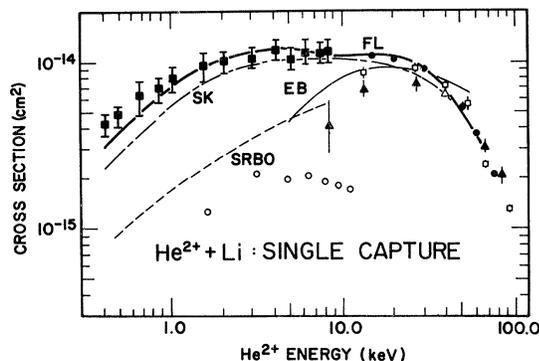


FIG. 2. Cross sections for single capture by  $\text{He}^{2+}$  ions from lithium vs  ${}^4\text{He}^{2+}$  laboratory energy. Data points are the following:  $\blacksquare$ , present;  $\bullet$ , Kadota *et al.* (Ref. 11);  $\blacktriangle$ , Murray *et al.* (Ref. 10);  $\square$ , McCullough *et al.* (Ref. 9);  $\circ$ , Barrett and Leventhal (Ref. 20). Theoretical curves are the following: — (FL) Fritsch and Lin (Ref. 4); --- (SK) Sato and Kimura (Ref. 5); — (EB) Ermolaev and Bransden (Ref. 13); - - - (SRBO) Shipsey *et al.* (Ref. 12).

ratory system. Uncertainties given in the figures and the tables include those due to counting statistics and to an estimated overall uncertainty in the absolute scale. The latter, which usually dominates, was due mainly to uncertainty in the absolute Li target thickness. It was estimated from the reproducibility of results over a series of modifications to the cell and to the thermocouple attachments, including replacement of the entire cell. An additional uncertainty attends the correction for end effects, made here by adding the sum of the aperture radii to the physical length of the cell. The error bars quoted correspond to an absolute uncertainty of 13%.

For  $\text{He}^+$  on Li, a rather complete picture of the energy dependence emerges from the data. Although overlap does not exist between our data and the earlier results, it appears that a smooth curve can reasonably join our results with those of McCullough *et al.*<sup>9</sup> To our knowledge, no theoretical results on this process have yet appeared in the literature.

The results for protons on Li are quite consistent with the previous results of Grüebler *et al.*<sup>7</sup> The agreement of the data with both the AO + results of Fritsch and Lin<sup>4</sup> and the molecular-orbital calculations of Allan *et al.*<sup>3</sup> is excellent, except perhaps for the lowest two data points. It should be pointed out that these are the most problematic points from the experimental side, involving appreciable background corrections. There is the further possibility that some reaction products for the lowest energies scatter outside the angular acceptance of our apparatus (approximately  $\pm 3.5^\circ$  by  $\pm 1.7^\circ$  here). The calculations by Allan *et al.* span a range, since instead of explicitly including electron translation factors in their calculations, they chose to present separate results for calculations done with their coordinate-system origin placed at the target and at the projectile. The data lie within this

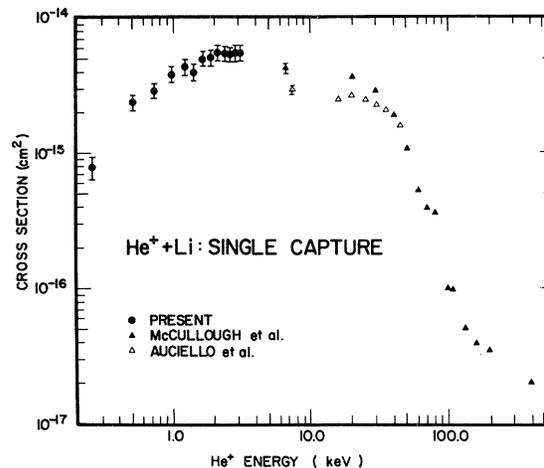


FIG. 3. Cross sections for single capture by  $\text{He}^+$  ions from lithium vs  ${}^4\text{He}^+$  laboratory energy. Data points are the following:  $\bullet$ , present;  $\triangle$ , Auciello *et al.* (Ref. 14);  $\blacktriangle$ , McCullough *et al.* (Ref. 9).

range. The molecular-orbital results of Sato and Kimura<sup>5</sup> give somewhat less satisfactory agreement, especially at low energy, as is also the case for the atomic-expansion calculation of Ermolaev.<sup>6</sup> The AO + calculation avoids the electron translation factor problem by using a large basis of atomic states with plane-wave translation factors, yet includes, in the basis, states of the united atom system which should take into account some molecular features of the process. Such an approach should span the energy region from well below to well above velocity matching. The agreement it gives with all available data is quite encouraging.

For the case of  $\text{He}^{2+}$  on Li, our results clearly support the theoretical calculations of Fritsch and Lin<sup>4</sup> and of Sato and Kimura.<sup>5</sup> With the exception of the data of Barrett and Leventhal,<sup>20</sup> which appear too low by a factor near 5, and the lowest two data points of Murray *et al.*,<sup>10</sup> the data give a rather consistent picture of the energy dependence for this process. In particular, agreement of our results with those of Kadota *et al.*<sup>11</sup> is excellent. We note that the results of Barrett and Leventhal<sup>20</sup> and of Kadota *et al.*<sup>11</sup> are from optical measurements which generally involve greater difficulties in establishing the absolute cross-section scale than do direct measurements such as those of Refs. 9 and 10. The earlier molecular-orbital calculations apparently suffer from not including an adequate number of couplings as is shown most clearly by comparison with the more recent results of Sato and Kimura.<sup>5</sup> Again, the ability of the AO + model to cover a large energy range is noted to be excellent.

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\*Permanent address: Physics Department, University of South Alabama, Mobile, AL 36688.

<sup>1</sup>D. E. Post, *Phys. Scr.* **23**, 122 (1981).

<sup>2</sup>H. Winter, *Comments At. Mol. Phys.* **12**, 165 (1982).

<sup>3</sup>R. J. Allan, A. S. Dickinson, and R. McCarroll, *J. Phys. B* **16**, 467 (1983).

<sup>4</sup>W. Fritsch and C. D. Lin, *J. Phys. B* **16**, 1595 (1983).

<sup>5</sup>H. Sato and M. Kimura, *Phys. Lett.* **96A**, 286 (1983).

<sup>6</sup>A. M. Ermolaev, in *Abstracts of Contributed Papers, Thirteenth International Conference on the Physics of Electronic and Atomic Collisions, Berlin, 1983*, edited by J. Eichler, W. Fritsch, I. V. Hertel, N. Stolterfoht, and U. Wille (ICPEAC, Berlin, 1983), p. 514.

<sup>7</sup>W. Grüebler, P. A. Schmelbach, U. König, and P. Marmier, *Helv. Phys. Acta* **43**, 254 (1970).

<sup>8</sup>R. N. Il'in, V. A. Oparin, E. S. Solov'ev, and N. V. Fedorenko, *JETP Lett.* **2**, 197 (1965).

<sup>9</sup>R. W. McCullough, T. V. Goffe, M. B. Shah, M. Lennon, and H. B. Gilbody, *J. Phys. B* **15**, 111 (1982).

<sup>10</sup>G. A. Murray, J. Stone, M. Mayo, and T. J. Morgan, *Phys. Rev. A* **25**, 1805 (1982).

<sup>11</sup>K. Kadota, D. Dijkkamp, R. Van der Woude, Pan Guang

Yan, and F. J. deHeer, *J. Phys. B* **15**, 3275 (1982).

<sup>12</sup>E. J. Shipsey, L. T. Redmon, J. C. Browne, and R. E. Olson, *Phys. Rev. A* **18**, 1961 (1978).

<sup>13</sup>A. M. Ermolaev and B. H. Bransden, in *Abstracts of Contributed Papers, Thirteenth International Conference on the Physics of Electronic and Atomic Collisions, Berlin, 1983*, edited by J. Eichler, W. Fritsch, I. V. Hertel, N. Stolterfoht, and U. Wille (ICPEAC, Berlin, 1983), p. 567.

<sup>14</sup>O. Auciello, E. V. Alonso, and R. A. Baragiola, *Phys. Rev. A* **13**, 985 (1976).

<sup>15</sup>C. L. Cocke, R. DuBois, T. J. Gray, and E. Justiniano, *IEEE Trans. Nucl. Sci.* **NS-28**, 1032 (1981).

<sup>16</sup>E. Justiniano, C. L. Cocke, T. J. Gray, R. D. Dubois, and C. Can, *Phys. Rev. A* **24**, 2953 (1981).

<sup>17</sup>W. Waggoner, C. L. Cocke, S. L. Varghese, and M. Stockli, *Phys. Rev. A* **29**, 2457 (1984).

<sup>18</sup>T. B. Douglas, L. F. Epstein, J. L. Dever, and W. H. Howland, *J. Am. Chem. Soc.* **77**, 2144 (1955).

<sup>19</sup>R. R. Hultgren, R. L. Orr, P. D. Anderson, and K. K. Kelly, *Selected Values of Thermodynamic Properties of Metals and Alloys* (Wiley, New York, 1963), p. 153.

<sup>20</sup>J. L. Barrett and J. J. Leventhal, *Phys. Rev. A* **23**, 485 (1981).