$$G^1(\vec{r}_1,\vec{r}_2)=-\frac{1}{4\pi}\frac{e^{-Zr_{12}}}{r_{12}}+\frac{Z}{2\pi}e^{-Z(r_1+r_2)}\times\left(\gamma-\tfrac{5}{2}+Z(r_1+r_2)+\ln Z(r_1+r_2+r_{12})-\int_0^{Z(r_1+r_2-r_{12})}\frac{e^t-1}{t}dt\right) \quad (10)$$

in agreement with the result derived by Hostler.[2]

[1]H. F. Hameka, J. Chem. Phys. 47, 2728 (1967); 48, 4810 (1968).

[2]L. C. Hostler, Phys. Rev. 178, 126 (1969).

[3]These variables are also of importance for the full Coulomb Green's function as shown by L. C. Hostler and R. H. Pratt, Phys. Rev. Letters 10, 469 (1963).

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Photodetachment Cross Section of the Negative Ion of Lithium

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The photodetachment cross section for the negative ion of lithium is calculated following Geltman using an improved value of the electron affinity (0.62 eV) obtained by Weiss.

The photodetachment cross section of the negative ion of lithium was calculated by Geltman[1] employing a value 0.384 eV for the electron affinity of the lithium atom (or the binding energy of the negative lithium ion). This value was obtained by Geltman by extrapolating along the isoelectronic sequence and seemed to be considerably smaller than various other theoretical determinations. Thus, Moiseiwitsch[2] obtained 0.74 eV, Weiss[3] obtained 0.62 eV and Edlén[4] obtained 0.8 eV. Recently, experiments with electrically exploded lithium wires[5] indicated that the affinity of lithium is about 0.6 eV, close to the value calculated by Weiss.[3] The latter's method of calculation seems to be the most direct and elaborate and since it best agrees with the experiment, it will be adopted here as the best value of the electron affinity of lithium. A revised calculation of the photodetachment cross section seems appropriate. The much larger value of electron affinity, as compared with that of Geltman, would shift the photodetachment threshold and the continuum associated with the inverse process to much shorter wavelengths of the spectrum.

The photodetachment cross section of Li^- has not been measured. However, Geltman's calculations, as applied to the hydrogen negative ion, yielded good agreement with other methods and with the experiment. It can, thus, be expected that following the simple procedure employed by Geltman and using an improved value of the electron affinity would give reliable results.

It is assumed that the lithium (and the hydrogen) negative ion has only one bound state and therefore the total absorption coefficient (per unit density of negative ions) and the photodetachment cross section coincide. A further assumption is that the two 1s electron merge with the nucleus or that the lithium negative ion is likened to a hydrogen negative ion with the two electrons in the 2s orbital.

Geltman constructs eigenfunctions out of bound and free one-electron functions and assumes the potential in the one-electron Schrödinger equation to be a cutoff Coulomb potential

$$V(r)=1/r_0-1/r, \quad r\leqslant 0$$
$$=0, \quad r\geqslant 0. \quad (1)$$

The potential is chosen such as to give one bound state of energy equal to the electron affinity of the neutral atom. The choice of functions assures the fulfillment of certain necessary conditions on the absorption coefficient[1] but not that of minimal energy. The photodetachment cross section is then obtained as

$$\sigma(k)=\tfrac{1}{3}(32\pi^2)\alpha a_0^{\,2}(k_0^{\,2}+k^2)/k$$

TABLE I. Calculated continuous absorption coefficients of Li^-.

k^2 (a.u.)	λ (Å)	k_λ (10^{-17} cm^2)
0	19 996	0
0.0025	18 957	0.93
0.005	18 021	2.11
0.0075	17 172	3.16
0.01	16 400	4.03
0.015	15 047	5.32
0.02	13 900	6.15
0.025	12 916	6.65
0.03	12 061	6.95
0.035	11 313	7.11
0.04	10 652	7.18
0.05	9 538	7.13
0.06	8 635	6.95
0.08	7 260	6.41
0.10	6 263	5.79
0.12	5 506	5.16
0.16	4 435	3.98
0.20	3 713	2.99

$$\times \left| \int_0^\infty \varphi_0 \chi_1 r^2 dr \right|^2 , \qquad (2)$$

where α is the fine-structure constant, a_0 the Bohr radius, and k the wave number in atomic units. φ_0 is the one-electron bound-state solution. χ_1 is the radial part of the p wave of a free electron.

First, r_0 is computed using the requirements that φ_0 and its derivative be continuous at r_0, and φ_0 should have one node inside the well (to be an appropriate $2s$ function). With the adopted value of 0.62 eV for the electron affinity of lithium we obtain $r_0 = 9.66$, as compared with $r_0 = 8.78$ obtained by Geltman. Further, the phase shift $\delta_1(k)$ appearing in χ_1 is obtained from the requirements that χ_1 and its derivative be continuous at r_0 and that

$$\lim_{k \to \infty} \delta_1(k) = 0 .$$

The continuous absorption cross section is then obtained by computing the integral in Eq. (2) numerically from 0 to r_0 and analytically from r_0 to ∞. The results are given in Table I and Fig. 1.

By adopting an improved value of the electron affinity, as compared with that adopted by Geltman, the absorption threshold has shifted from 32 293 to 19 996 Å and the wavelength of maximum absorption from about 17 000 to about 10 500 Å. Such a shift was necessary to be assumed to account for the very high intensity of continuous radiation emitted in the red part of the visible spectrum when exploding lithium wires.[5]

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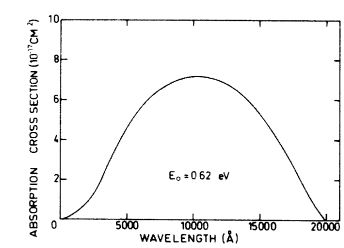

FIG. 1. Calculated photodetachment cross section of Li^- (or continuous absorption coefficient per unit density of negative ions).

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