EXCITATION OF ATOMIC HYDROGEN BY LITHIUM ATOMS

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In this letter we consider the excitation of atomic hydrogen in collisions with lithium atoms according to reactions of the type

$$H(1s) + Li(2s) \rightarrow H(n,\ell,m) + Li\ (\gamma)\ .\ .\ . \qquad (1)$$

If the lithium atom remains in its ground state the Born cross section, $Q(1s\text{-}n;\ 2s\text{-}2s) = \sum_{\ell,m} Q\ (1s\text{-}n,\ell,m;\ 2s\text{-}2s)$, for excitation of the hydrogen atom to a state with principal quantum number n is [1]

$$Q(1s\text{-}n;\ 2s\text{-}2s) = \frac{4\pi}{v^2}\int_{k^2_{min}}^{\infty} \frac{d(k^2)}{k^4} \left|1-F_k^{\ A}(2s,2s)\right|^2 \sum_{\ell,m} \left|F_k^{\ B}\ (1s,n\ell m)\right|^2 \ldots \qquad (2)$$

while if the lithium atom is excited to a state γ the analogous Born cross-section is

[redacted]

$$Q(1s\text{-}n;\ 2s\text{-}\gamma) = \frac{4\pi}{v^2}\int_{k^2_{min}}^{\infty} \frac{d(k^2)}{k^4} \left|F_k^{A}(2s,\ \gamma)\right|^2 \sum_{\ell,m} \left|F_k^{B}(1s,n\ell m)\right|^2 \ldots \qquad (3)$$

where

$$\left.\begin{aligned} F_k^{A}(2s,\gamma) &= \int d\underline{r}\ \mathcal{L}i_{2s}^{*}\ (\underline{r})\ \mathcal{L}i_{\gamma}(\underline{r})\ e^{i\underline{k}.\underline{r}} \\ F_k^{B}(1s,n\ell m) &= \int d\underline{r}\ \Phi_{1s}^{*}\ (\underline{r})\ \Phi_{n\ell m}\ (\underline{r})\ e^{i\underline{k}.\underline{r}} \end{aligned}\right\} \ldots \qquad (4)$$

and

$$k_{min} = \frac{1}{v}\left(\epsilon_{2s}^{A} - \epsilon_{\gamma}^{A} + \epsilon_{n}^{B} - \epsilon_{1s}^{B}\right) \quad \ldots \qquad (5)$$

Here $\mathcal{L}i_\gamma(\underline{r})$ and $\Phi_{n\ell m}(\underline{r})$ are eigenstates of lithium and hydrogen with corresponding eigenenergies ϵ_γ^A and ϵ_n^B. The superscripts A and B refer to lithium and hydrogen respectively and the energy of the incident hydrogen atom is 25 v^2 kev. The total Born cross section for excitation of the hydrogen atom to a state with principal quantum number n is obtained by summing over all possible final states of lithium atom

$$Q(1s\text{-}n;\ 2s\text{-}\Sigma) = \sum_\gamma Q\ (1s\text{-}n;\ 2s\text{-}\gamma) \quad \ldots \qquad (6)$$

Since the integrands in (2) and (3) are positive and since k_{min} is a minimum for the $\mathcal{L}i(2s) \to \mathcal{L}i(2s)$ transition we obtain an upper bound, Q^u $(1s\text{-}n;\ 2s\text{-}\Sigma)$, to $Q(1s\text{-}n;\ 2s\text{-}\Sigma)$ by application of the closure relation [1,2]

$$\sum_\gamma |F_k^{\ A}\ (2s,\ \gamma)\ |^2 = 1 \ \ldots . \qquad (7)$$

Thus

$$Q(1s\text{-}n;\ 2s\text{-}\Sigma) \le Q^{u}\ (1s\text{-}n;\ 2s\text{-}\Sigma)$$

$$= \frac{8\pi}{v^2} \int_{k_o^2}^{\infty} \frac{d(k^2)}{k^4} \left(1-\Re e\ F_k^{A}(2s,2s)\right) \sum_{\ell,m} \left|F_k^{B}(1s,n\ell m)\right|^2 \quad \ldots \qquad (8)$$

where

$$k_o = \frac{1}{2v}\left(1-\frac{1}{n^2}\right) \quad \ldots \qquad (9)$$

The evaluation of $\sum_{\ell,m} |F_k^{B}(1s,n\ell m)|^2$ proceeds without difficulty by a method analogous to that described by May [3]. We obtain

$$\sum_{\ell,m} |F_k^B(1s,n\ell m)|^2 = \frac{n^5 z^2 2^8}{3} \left(\frac{z^2+(n-1)^2}{z^2+(n+1)^2}\right)^n \frac{3z^2+n^2-1}{(z^2+(n+1)^2)^3(z^2+(n-1)^2)^3} \cdots \quad (10)$$

where $z = nka_o$ and a_o is the Bohr radius. $F_k^A(2s,2s)$ was estimated by making use of the self-consistent field wave function of Clementi et al [4]. The integrals over k^2 were evaluated numerically on the Theoretical Division's IBM-7094.

The computed values of $Q(1s\text{-}n;2s\text{-}2s)$ and $Q^u(1s\text{-}n;2s\text{-}\Sigma)$ are given in table 1 in units of $\pi a_o^2/n^3$. From equation (6) it is clear that $Q(1s\text{-}n;2s\text{-}2s)$ is a crude lower bound to $Q(1s\text{-}n;2s\text{-}\Sigma)$. However, as may be seen from table 1, it does make a large contribution to the total sum. Since contributions from other states of lithium are also expected to be significant we are led to suspect that $Q^u(1s\text{-}u;2s\text{-}\Sigma)$ may be reasonably close to $Q(1s\text{-}n;2s\text{-}\Sigma)$. This is particularly true at high energies since the k^2_{min} of equation (3) goes to zero as v^{-2}[1]

Finally, we note that application of a simple hydrogenic wave function for Li (2s) with an effective charge $Z = (1.6)^{\frac{1}{2}}$ increased the tabulated results by about 20%.

TABLE 1

Impact Energy	n	Q(1s-n;2s-2s)	Q^{u}(1s-n;2s-Σ)
kev		$\pi a_0^2/n^3$	$\pi a_0^2/n^3$
2	2	4.94	9.68
	3	2.08	4.11
	8	1.17	2.31
	15	1.09	2.16
10	2	12.6	29.9
	3	9.43	20.7
	8	7.67	16.2
	15	7.48	15.8
25	2	7.32	21.4
	3	6.15	16.2
	8	5.45	13.6
	15	5.37	13.3
50	2	3.99	13.2
	3	3.44	10.2
	8	3.10	8.65
	15	3.06	8.49
100	2	2.05	7.36
	3	1.78	5.71
	8	1.61	4.86
	15	1.59	4.78
200	2	1.03	3.89
	3	0.897	3.02
	8	0.815	2.57
	15	0.806	2.53

References

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2. H. A. Bethe, Ann. Phys. (Leipzig), 5 (1930) 325, Sec. 7.

3. R. M. May, Phys. Rev. 136 (1964) A669

4. E. Clementi, C. C. J. Roothaan and M. Yoshimine, Phys. Rev., 127 (1962) 1618.