Excitation of H-Atoms by Fast Protons

I. M. Cheshire and H. L. Kyle
Laboratory for Theoretical Studies
Goddard Space Flight Center
Greenbelt, Maryland

N66 17242

A simple formula for the total Born cross section for the excitation of ground state H-atoms to any excited state n is given and a table of cross sections is included for representative n and impact energies.

author

In this paper we consider excitation of ground state H-atoms by protons according to the reaction

$$H^+ + H(1s) \rightarrow H^+ + H(n,\ell,m) \tag{1}$$

We evaluate the total Born cross section $Q(1s,n) = \sum_{\ell,m} Q(1s,n\ell m)$ in the limit of infinitely massive protons. This latter approximation has a negligible effect on the accuracy of the calculation (Bates and Griffing 1953). May (1965) has evaluated $Q(1s,n)$ in the limit of large n while other workers (Bates and Griffing 1953 and Mittleman 1963) have evaluated $Q(1s,n\ell) = \sum_{m} Q(1s,n\ell m)$ for various values of n and ℓ up to n = 6. The relevant Born cross section is (Bates 1962)

$$Q(1s,n) = \frac{8\pi a_0^2}{v^2}\int_{k_0}^{\infty} \frac{dk}{k^3} \sum_{\ell,m} |\langle 1s|\exp(i\underline{k}.\underline{r})|n\ell m\rangle|^2 \tag{2}$$

where v is the velocity of the incident proton (we use atomic units, hence v = 1 corresponds to a proton energy of 25 kev), a_0 is the Bohr radius, k_0 is the minimum momentum change $k_0 = (1 - 1/n^2)/2v$ and

$$\langle 1s|\exp(i\underline{k}.\underline{r})|n\ell m\rangle = \int d\underline{r}\ \psi_{1s}^*(\underline{r})\ \psi_{n\ell m}(\underline{r}) \exp(i\underline{k}.\underline{r}) \tag{3}$$

where $\psi_{n\ell m}(\underline{r})$ is the hydrogenic wave function with quantum numbers n,ℓ,m. Cheshire and Kyle (1965) have shown that

$$\sum_{\ell,m} |\langle 1s|\exp(i\underline{k}.\underline{r})|n\ell m\rangle|^2$$
$$= \frac{2^8 k^2}{3n^2}\left(\frac{k^2+(1-\frac{1}{n})^2}{k^2+(1+\frac{1}{n})^2}\right)^n \frac{(3k^2+1-\frac{1}{n^2})}{(k^2+(1-\frac{1}{n})^2)^3(k^2+(1+\frac{1}{n})^2)^3} . \tag{4}$$

For large n

$$\left(\frac{k^2+(1-\frac{1}{n})^2}{k^2+(1+\frac{1}{n})^2}\right)^n = \exp\left\{-\frac{4}{1+k^2} + O\left(\frac{1}{n^2}\right)\right\} \tag{5}$$

so that (4) becomes

$$\sum_{\ell, m} |\langle 1s | \exp(i\underline{k}.\underline{r}) | n\ell m \rangle|^2 = \frac{2^8 k^2}{3n^3} \frac{(3k^2+1)}{(1+k^2)^6} \exp\left\{-\frac{4}{1+k^2}\right\} + O\left(\frac{1}{n^5}\right) \quad (6)$$

which is the result quoted by May.

Using (3) and (4) we have computed $Q(1s, n)$ for a representative set of impact energies and a reasonably comprehensive set of n's.

TABLE I

Q(1s - n) in units of $\pi a_0^2/n^3$

n \ Impact Energy (kev)	1	5	12.5	25	50	100	200	400	800
2	1.20	13.4	18.6	17.3	13.6	9.55	6.23	3.86	2.31
3	0.392	7.62	12.0	11.4	8.78	6.02	3.84	2.33	1.38
4	0.270	6.31	10.4	9.95	7.67	5.22	3.30	2.00	1.17
5	0.227	5.78	9.80	9.38	7.22	4.90	3.09	1.86	1.09
6	0.207	5.52	9.47	9.09	6.99	4.74	2.98	1.80	1.05
7	0.196	5.36	9.28	8.93	6.86	4.64	2.92	1.76	1.03
8	0.189	5.27	9.16	8.82	6.77	4.58	2.88	1.73	1.01
9	0.184	5.20	9.08	8.75	6.72	4.54	2.86	1.72	1.00
10	0.182	5.15	9.03	8.70	6.68	4.51	2.84	1.70	0.99
15	0.174	5.05	8.89	8.58	6.58	4.45	2.79	1.68	0.98
20	0.172	5.01	8.85	8.54	6.55	4.42	2.78	1.67	0.97
25	0.171	4.99	8.82	8.52	6.54	4.41	2.77	1.66	0.97

References

1. Bates, D. R., 1962, Atomic and Molecular Processes, (New York, Academic Press), pp. 549-621.
2. Bates, D. R. and Griffing, G., 1953, Proc. Phys. Soc., A66, 961-71.
3. Cheshire, I. M., and Kyle, H. L., 1965, Physics Letters, 17, 115-6.
4. May, R. M., 1965, Physics Letters, 14, 98-9.
5. Mittleman, M. H., 1963, Phys. Rev., 129, 190-3.