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ELECTRIC FIELD IONIZATION PROBABILITIES FOR THE HYDROGEN ATOM

by

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A B S T R A C T

The electric field ionization probabilities for the hydrogen atom have been calculated using the method of Lanczos and the method of Rice and Good. The results of these calculations are presented graphically for the extreme components of all levels through n = 25, and for all the individual states belonging to a particular level through n = 7. Tabulations of the ionization probabilities are presented for a few representative levels.

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C O N T E N T S

1. INTRODUCTION

The possibility of ionizing the hydrogen atom by an external electric field was first discussed by OPPENHEIMER [1], who obtained an expression for the ionization probability for the ground state. Somewhat later, LANCZOS [2] extended these calculations to include the excited states of the atom, and was able to interpret the disappearance of the spectral lines of the Balmer series in the experiments of VON TRAUBENBERG et al. [3] as being due to the electric field ionization of the excited states. The early work on the Stark effect and on electric field ionization has been reviewed by BETHE and SALPETER [4]. Recently, the problem has been reconsidered by RICE AND GOOD [5] (R G), who paid special attention to the determination of the eigenvalues and obtained an expression for the ionization probability which in some respects is more complete than that of Lanczos.

A need has arisen for explicit values of the ionization probabilities up to very high atomic levels in conjunction with studies of excited energetic hydrogen atom beams, [6,7,8], and, in the application of these atomic beams to neutral injection systems [9,10,11]. Since collision processes and radiative lifetimes of the excited levels are in general sensitive functions of the degree of excitation of the atom, it is necessary to identify the ionization thresholds with the principal quantum numbers to properly account for these processes. Explicit values in the above references have been limited to the extreme components of the $n = 4$, 5, 6 and 7 levels of hydrogen. In this paper we have used both the model of R G and what is essentially the method of Lanczos to extend these earlier calculations to include the extreme components through the $n = 25$ level and all the components of each level through $n = 7$.

2. DISCUSSION OF THE CALCULATIONS

The evaluation of the electric field ionization probabilities requires the calculation of both the energy levels and the time development of the wave function for the Schroedinger equation

$$\nabla^2 \psi + 2 [E + r^{-1} - Fz] \psi = 0$$

This equation is separable in parabolic co-ordinates [4], ξ, η, φ, with quantum numbers n_1, n_2, m, respectively, appropriate to these co-ordinates. For a non-vanishing electric field the equivalent potential in the η equation possesses a maximum which forms a barrier through which the electron can escape from the region near the proton. In the method of R G, the energy level, E_0, for a particular state is selected by requiring that the amplitude of the wave function be a minimum at the outer classical turning point of this barrier for fixed values of electric field. The time development of the wave function leading to penetration of the barrier is represented by constructing a wave packet consisting of a set of states with the same quantum numbers but with a certain range of energies, ΔE, distributed about the energy E_0. The probability of the electron remaining near the proton is found to decrease exponentially in time with a transition rate given by

$$\tau^{-1} = \Delta E/\hbar \ .$$

The method of Lanczos differs principally from that of R G in that the energy level is determined using the perturbation expansion of EPSTEIN [12] and of DOI [13]. The time development of the wave function in Lanczos' method is also traced by following the decay of the initial wave packet, but is limited to a one dimensional approximation using the η equation alone. According to R G, the full three dimensional treatment leads to an improved value for the ionization probability for certain states. On the other hand, R G have neglected a term in $(m^2 - 1)$ which is easily incorporated into the Lanczos expression, and which appears to be of importance in the sequential ordering of the thresholds for large m values. In general, the formula derived by Lanczos is simpler to use than the R G expression and for most purposes yields sufficiently accurate results.

The ionization probabilities calculated on the R G model have been evaluated using the iterative formula for the energy levels described in their paper. The ionization probabilities calculated using the Lanczos method have been evaluated using the energy and the separation parameter each of which was expanded to first, second, and third order in the electric field. These perturbation expansions for the energy up to third order and for the separation parameter up to the second order are available in BETHE and SALPETER [4]. The third order expression for the separation parameter has been derived from the equations in the original paper by DOI [13]. If the separation parameter, Z_2 , appropriate to the η equation, is expanded in powers of the field strength F,

$$Z_2 = Z_2^{(o)} + F Z_2^{(1)} + F^2 Z_2^{(2)} + F^3 Z_2^{(3)} + \dots$$

where F is in atomic units, then

$$Z_2^{(3)} = -(2^9 E^4)^{-1} (16m^4 + 246 m^3 n_2 + 996 m^2 n_2^2 + 1500 m n_2^3 + 750 m_2^4 + 123 m^3 + 996 m^2 n_2 + 2250 m n_2^2 + 1500 n_2^3 + 346 m^2 + 1584 m n_2 + 1584 n_2^2 + 417 m + 834 n_2 + 178) ;$$

here E is the unperturbed energy expressed in atomic units.

In Figs.1, 2, and 3 some comparisons are made of the ionization probabilities obtained using both methods for the $n = 1$ level and for the extreme states of the $n = 7$ and $n = 20$ level. On each figure the results obtained by the R G method are indicated by crosses and those obtained by the Lanczos method are shown as solid curves. The order of the perturbation theory expansions used to calculate E and Z_2 are shown as small numbers against each curve. In the case of $n = 1$ the first and third order terms for E vanish, but this is not the case for the terms in Z_2 so that there is some meaning to 'first' and 'third' order calculations. The effect of increasing the order of the expansions for E and Z_2 for the extreme components can be seen in Fig.2 for $n = 7$. On the high field side very good agreement is achieved but on the low field side the Lanczos results for higher orders are moving away from the R G results. This tendency for higher orders to move away from the R G results, occurs on both sides in the case of $n = 20$, Fig.3. The discrepancies between the third order Lanczos results and those of R G are due to differences in the values for both E and Z_2. These discrepancies, however, are less than experimental uncertainties [3,6,7,8].

The R G ionization probabilities versus electric field are plotted in Figs.4 5 and 6 for the extreme Stark components of all levels through n = 25. The thresholds for the successive levels are seen to be distinct through n = 6, the first overlap occurring at n = 7, 8. The overlapping becomes successively more pronounced for the higher levels, at n = 20 the ionization probabilities of as many as eight levels lie within the range of the extreme components of n = 20.

To facilitate the use of the figures we have listed in Table I the ionization probabilities of the extreme components at several electric field values for levels n = 1, 5, 10, 15, 20 and 25. The ionization probabilities are listed in double entry, the first column giving the R G results, the second column the third order Lanczos results.

In Figs.7 through 12 are plotted the ionization probabilities for all components of each particular level for n = 2 through n = 7. These figures are based on the R G expression for the ionization probability. Notice that for the higher n levels there is a tendency for the ionization probabilities to cluster toward the low field side of the electric field range. Upon comparing the results of Figs.5 and 6 with earlier estimates [11] of the ionization probabilities based on the Lanczos method, the previous calculations are seen to have over-estimated the requisite electric fields by approximately twenty per cent for levels n = 5, 6 and 7, and by approximately thirty to forty per cent for levels n = 9 and 10.

The ionization probabilities for all states of n = 7 calculated using the Lanczos method are plotted in Fig.13. A comparison of Fig.12 and Fig.13 shows that the ordering of the ionization probabilities is the same in either case with the exception of two of the three states with the largest m values. In Fig.12 the states follow the sequence $n_1 n_2 m$ = 114, 006, 321, 213, 105, 420, 312 and in

Fig.13 the sequence $n_1 n_2 m$ = 114, 321, 213, 006, 420, 312, 105. This difference in sequence has been traced to the neglect of the term $(m^2 - 1)/4$ in the R G expression for the ionization probability. This term has been included in the Lanczos expression used here although Lanczos did in fact neglect it in his original calculations. An examination of the sequence for n = 6 has shown a similar behaviour; the neglect of this term would be expected to be more pronounced for the higher levels.

Ionization has been observed by various workers for levels n = 5 through n = 23. In the experiments of VON TRAUBENBERG et al. [3], the quenching of the Balmer lines by an electric field allows for a correlation between ionization probability and principal quantum number for levels n = 5, 6 and 7. The experiment of BERKNER et al [6] identifies the ionization probabilities for levels 6, 7, 8 and 9, and the experiment of RIVIERE and SWEETMAN [7] for those levels n = 9 through n = 23. The correlation of these experimental ionization probabilities with the theoretical values reported here allows for an unambiguous identification of ionization threshold with principal quantum number for levels n = 5 through n = 23.

ACKNOWLEDGEMENT

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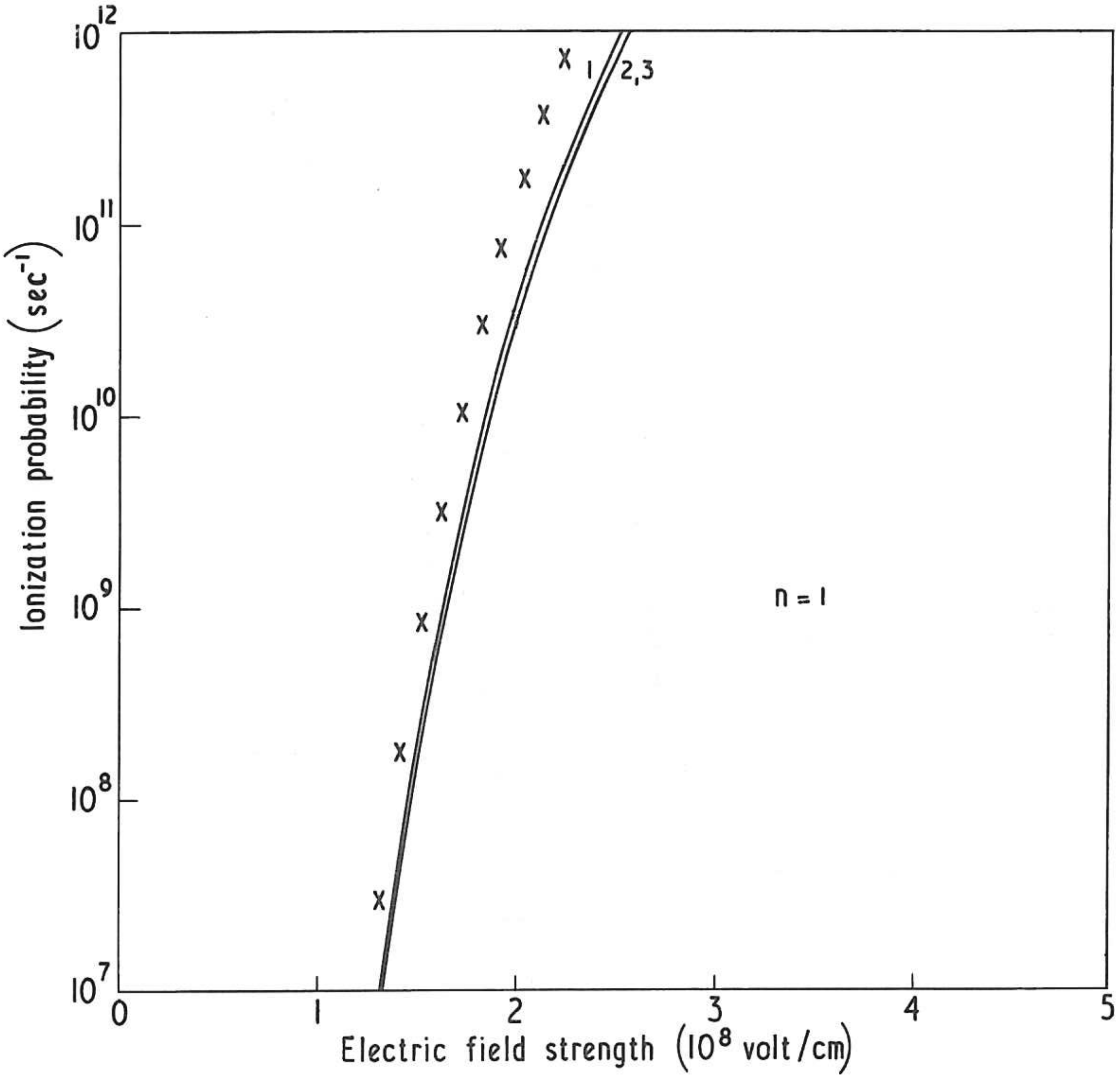
TABLE I

n	n_1, n_2, m	Field Strength volt/cm	Transition Probability sec^{-1} (Rice and Good)	(Lanczos with ($m^2 - 1$) Term)
1	0, 0, 0	1.209 + 8	3.632 + 6	8.433 + 5
		1.617 + 8	3.198 + 9	7.399 + 8
		2.027 + 8	1.732 + 11	3.935 + 10
		2.440 + 8	2.347 + 12	5.226 + 11
		2.857 + 8	1.449 + 13	3.159 + 12
5	0, 4, 0	5.444 + 5	1.899 + 6	2.561 + 5
		6.280 + 5	3.088 + 8	4.146 + 7
		7.142 + 5	1.298 + 10	1.744 + 9
		8.283 + 5	3.873 + 11	5.240 + 10
		9.308 + 5	2.822 + 12	3.966 + 11
5	4, 0, 0	8.042 + 5	3.240 + 6	2.892 + 6
		9.675 + 5	5.611 + 8	4.896 + 8
		1.133 + 6	1.959 + 10	1.673 + 10
		1.302 + 6	2.513 + 11	2.091 + 11
		1.477 + 6	1.646 + 12	1.319 + 12
10	0, 9, 0	4.058 + 4	7.406 + 3	8.236 + 2
		4.603 + 4	7.460 + 6	8.016 + 5
		5.178 + 4	1.389 + 9	1.425 + 8
		5.814 + 4	7.479 + 10	7.560 + 9
		6.710 + 4	1.379 + 12	1.934 + 11
10	9, 0, 0	8.082 + 4	8.535 + 6	1.539 + 7
		9.134 + 4	4.668 + 8	8.525 + 8
		1.021 + 5	9.894 + 9	1.802 + 10
		1.252 + 5	6.266 + 11	9.821 + 11
		1.643 + 5	6.196 + 12	1.909 + 12
15	0, 14, 0	9.790 + 3	7.751 + 5	6.394 + 4
		1.038 + 4	2.791 + 7	2.155 + 6
		1.101 + 4	6.399 + 8	4.851 + 7
		1.168 + 4	9.829 + 9	7.156 + 8
		1.246 + 4	1.030 + 11	8.181 + 9

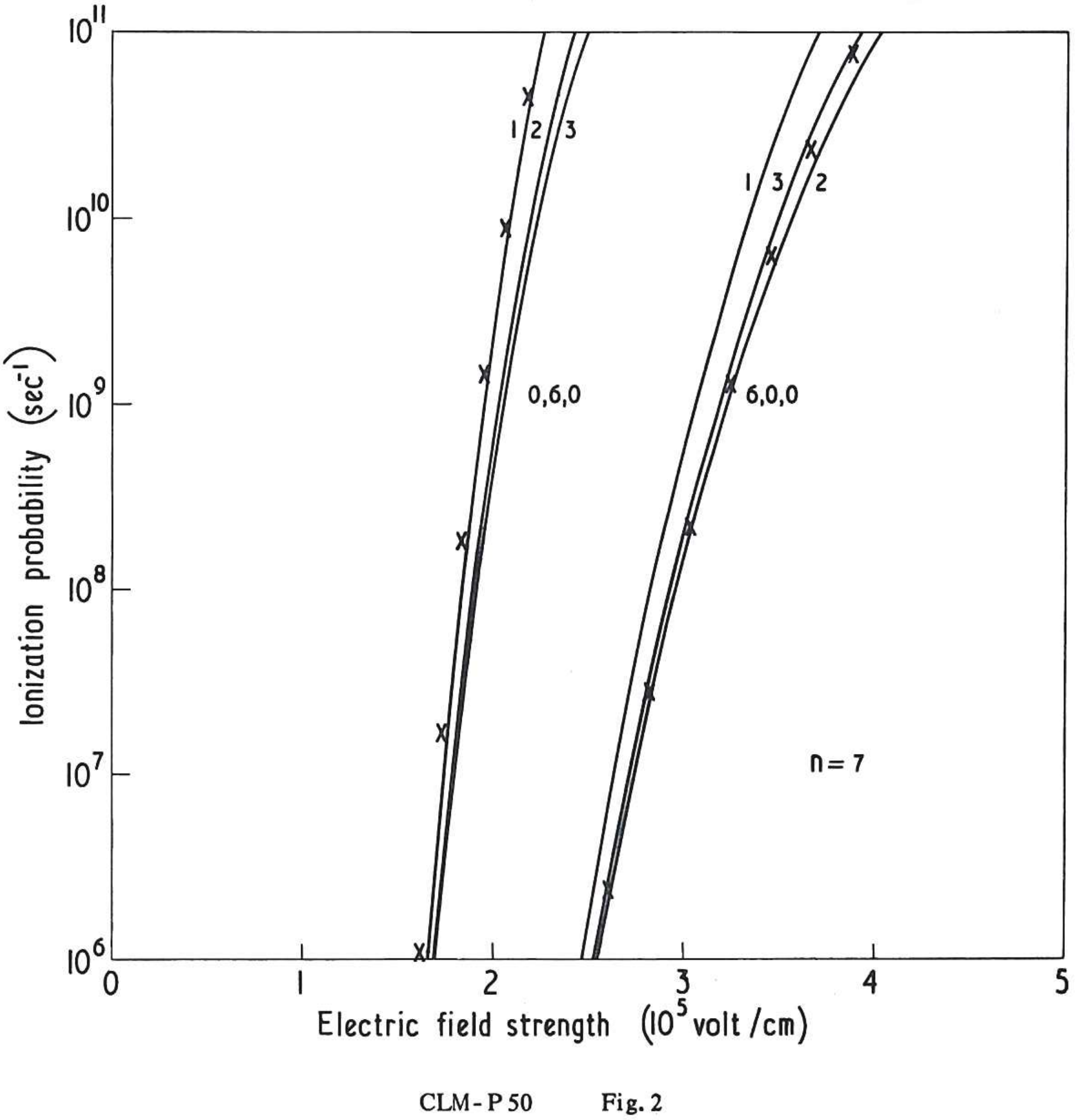
TABLE I
(continued)

n	n_1, n_2, m	Field Strength volt/cm	Transition Probability sec^{-1} (Rice and Good)	(Lanczos with (m^2-1) Term)
15	14, 0, 0	1.877 + 4	1.457 + 6	4.670 + 6
		2.038 + 4	4.161 + 7	1.386 + 8
		2.202 + 4	6.658 + 8	2.259 + 9
		2.429 + 4	1.296 + 10	4.361 + 10
		2.670 + 4	1.264 + 11	3.576 + 11
20	0, 19, 0	3.270 + 3	3.073 + 5	1.896 + 4
		3.393 + 3	4.767 + 6	2.786 + 5
		3.588 + 3	1.932 + 8	1.063 + 7
		3.801 + 3	4.970 + 9	2.660 + 8
		4.063 + 3	7.987 + 10	5.367 + 9
20	19, 0, 0	6.572 + 3	4.417 + 5	2.418 + 6
		7.065 + 3	1.350 + 7	7.840 + 7
		7.570 + 3	2.393 + 8	1.442 + 9
		8.090 + 3	2.663 + 9	1.586 + 10
		8.818 + 3	3.510 + 10	1.676 + 11
25	0, 24, 0	1.401 + 3	3.453 + 5	1.484 + 4
		1.460 + 3	1.025 + 7	4.224 + 5
		1.522 + 3	2.247 + 8	8.689 + 6
		1.591 + 3	3.676 + 9	1.470 + 8
		1.723 + 3	8.453 + 10	7.612 + 9
25	24, 0, 0	2.973 + 3	8.623 + 5	8.206 + 6
		3.199 + 3	3.379 + 7	3.438 + 8
		3.432 + 3	7.031 + 8	7.080 + 9
		3.675 + 3	8.350 + 9	6.931 + 10
		3.869 + 3	3.773 + 10	1.501 + 11



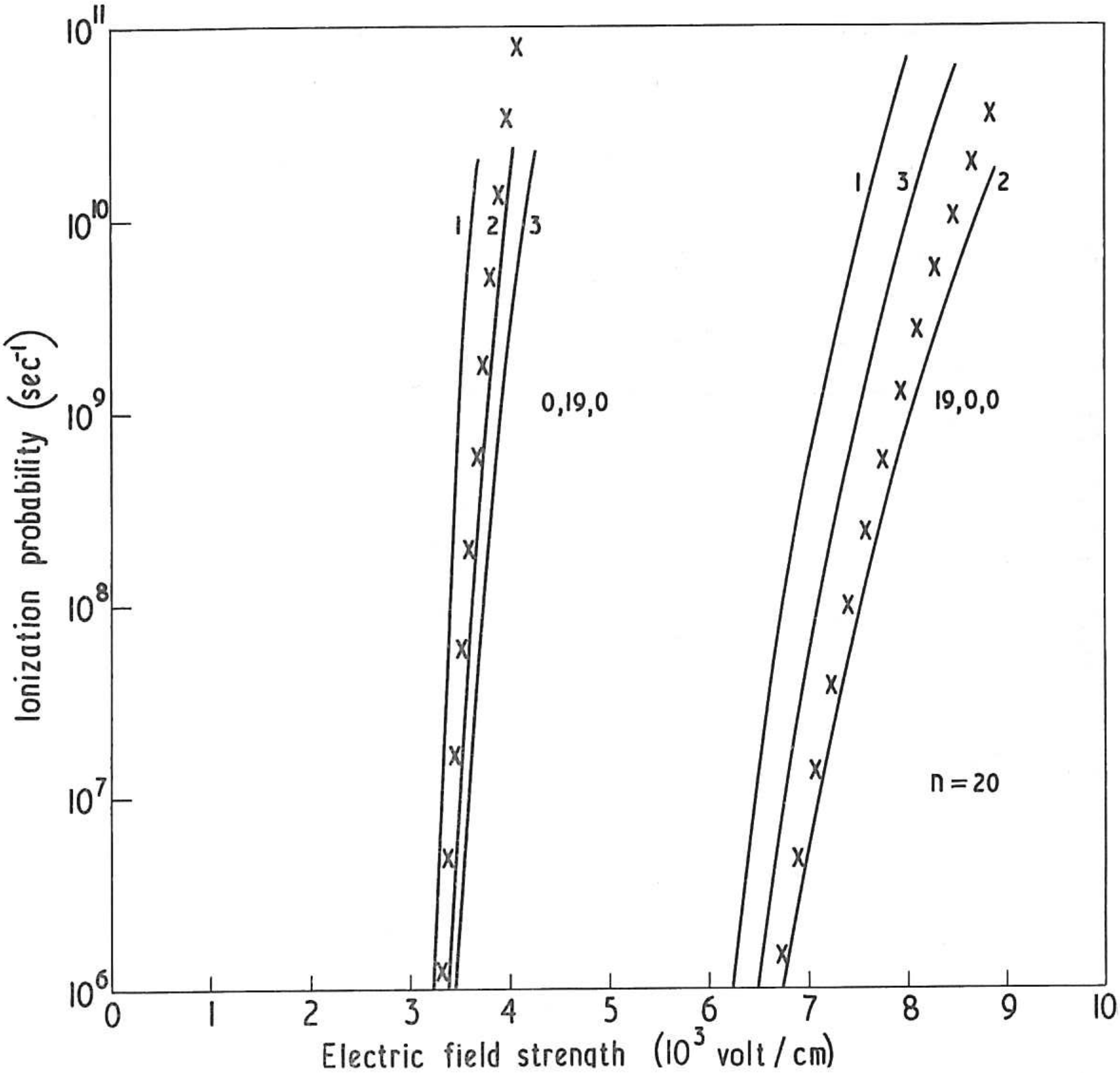
CLM-P 50 Fig. 1

Comparison of the ionization probability for n = 1 calculated using the method of Lanczos (solid curves) in successive orders with that calculated using the method of Rice and Good (crosses).



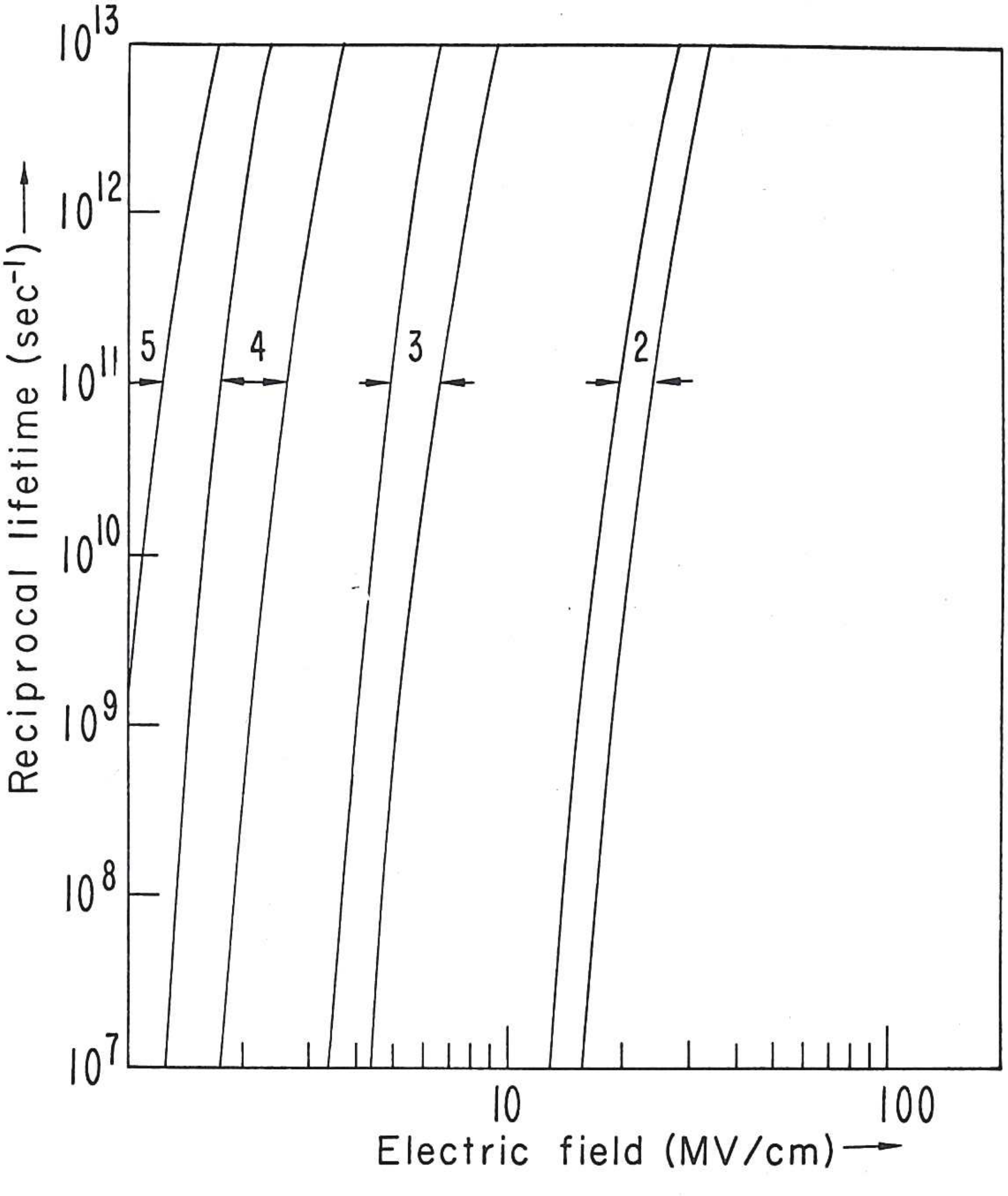
CLM-P 50 Fig. 2

Comparison of the ionization probabilities for the extreme components of n = 7 calculated in successive orders using the method of Lanczos (solid curves) with those calculated using the method of Rice and Good (crosses)



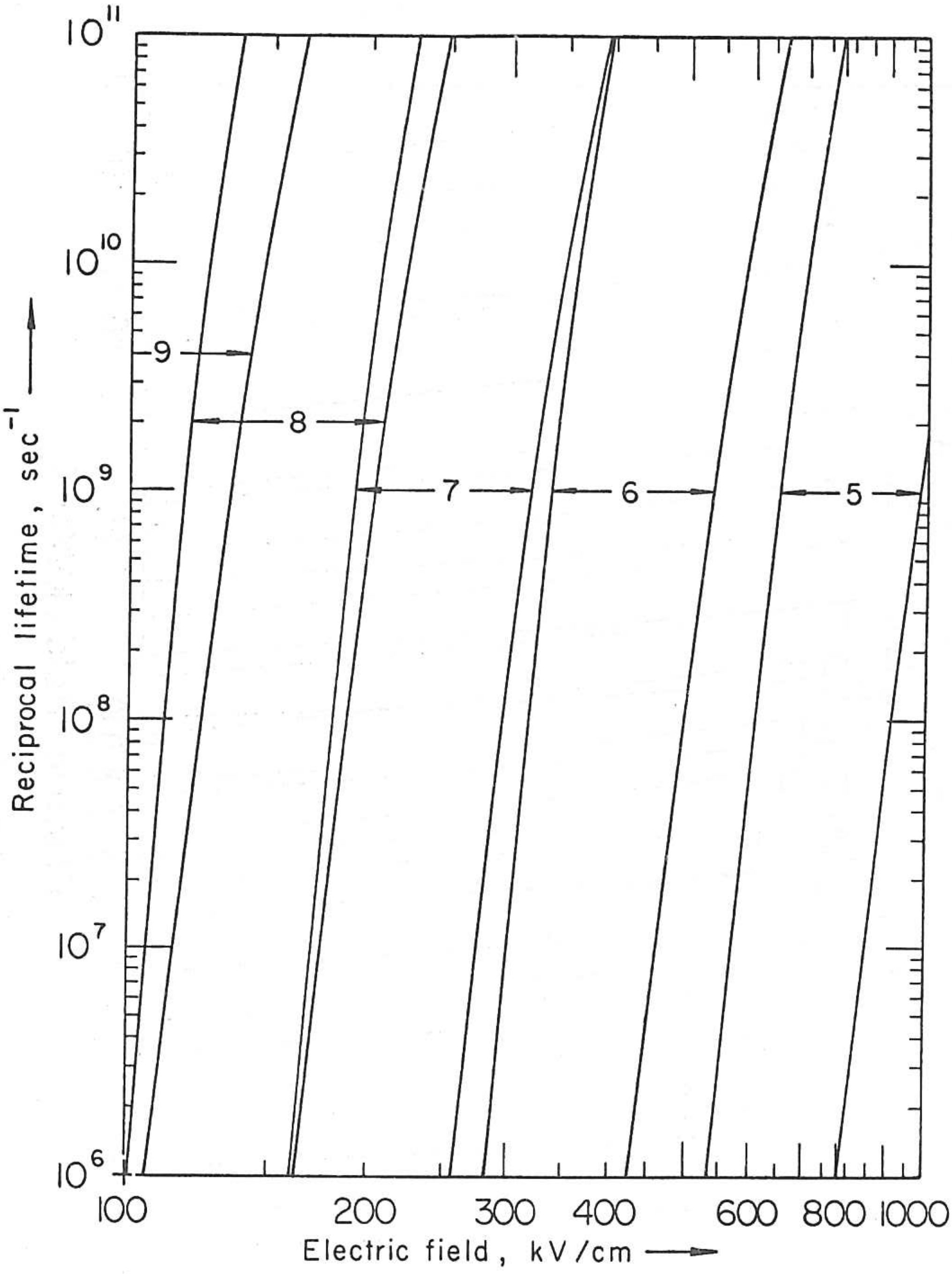
CLM-P 50 Fig. 3

Comparison of the ionization probabilities for the extreme components of n = 20 calculated in successive orders using the method of Lanczos (solid curves) with those calculated using the method of Rice and Good (crosses)



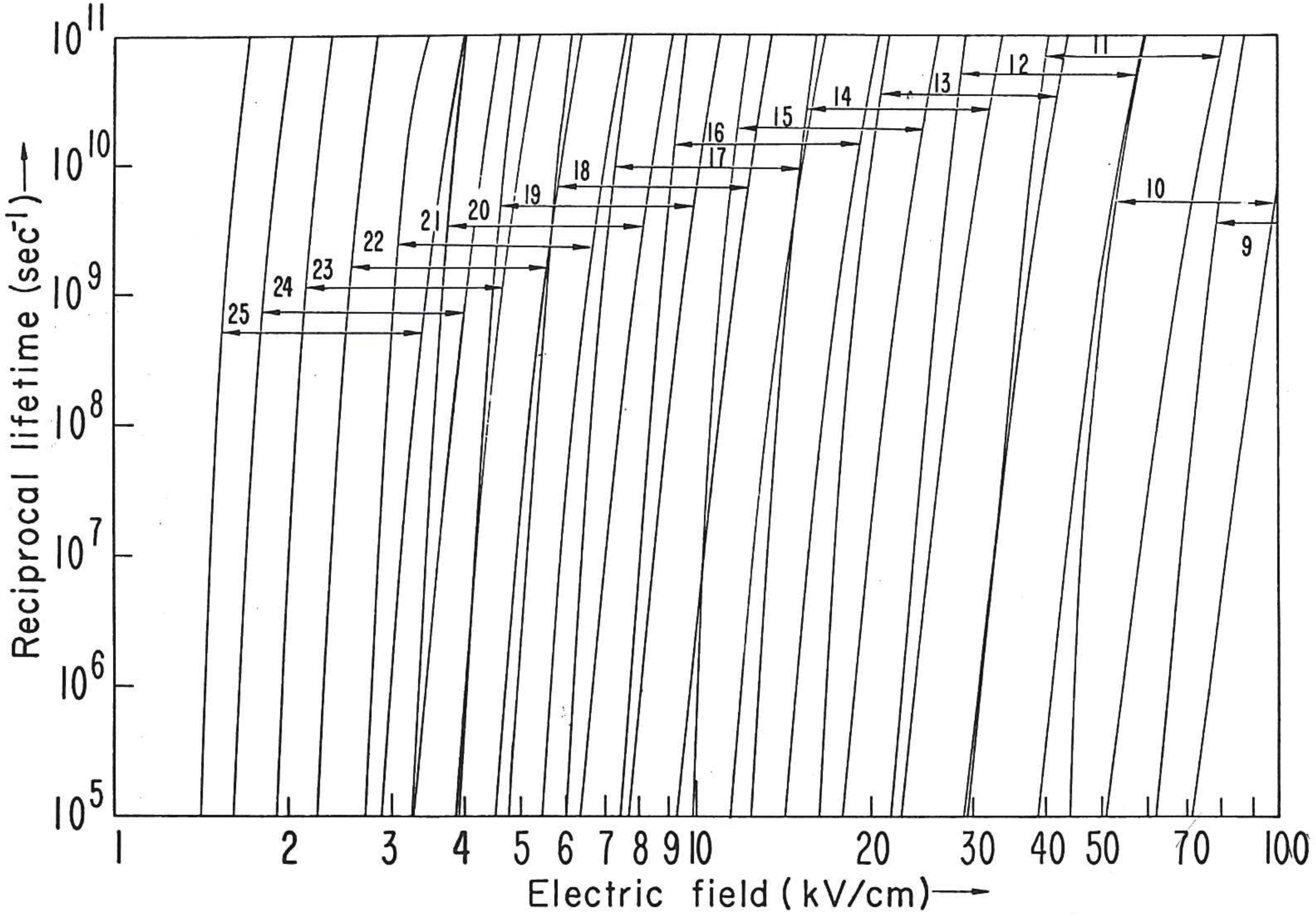
CLM-P 50 Fig. 4

Ionization probabilities versus electric field, in units of 10^6 volts/cm, for the extreme components of levels n = 2, 3, 4 and 5 using the R G method



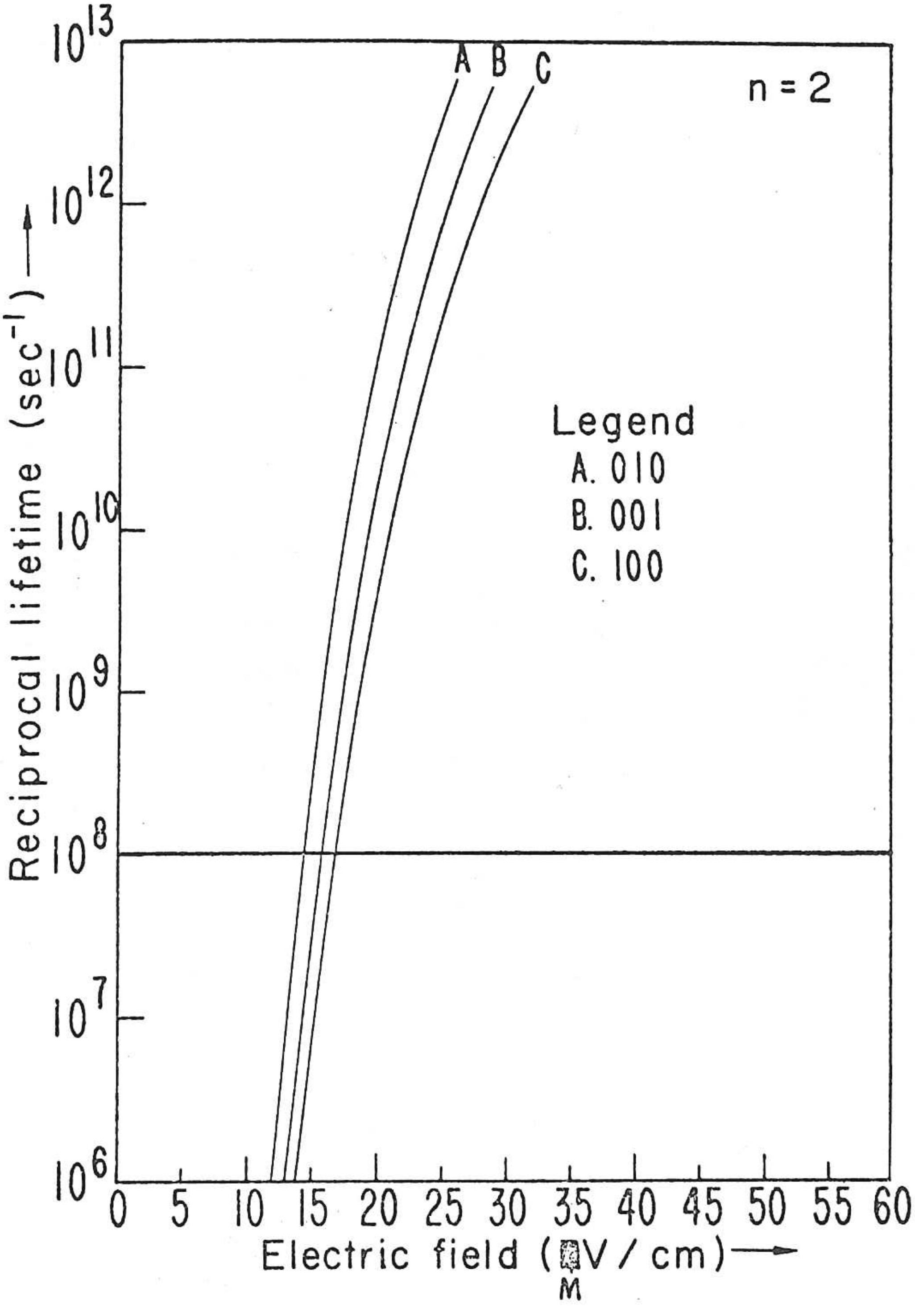
CLM-P 50 Fig. 5

Ionization probabilities versus electric field, in units of 10^3 volts/cm, for the extreme components of levels n = 5, 6, 7, 8 and 9 using the R G method



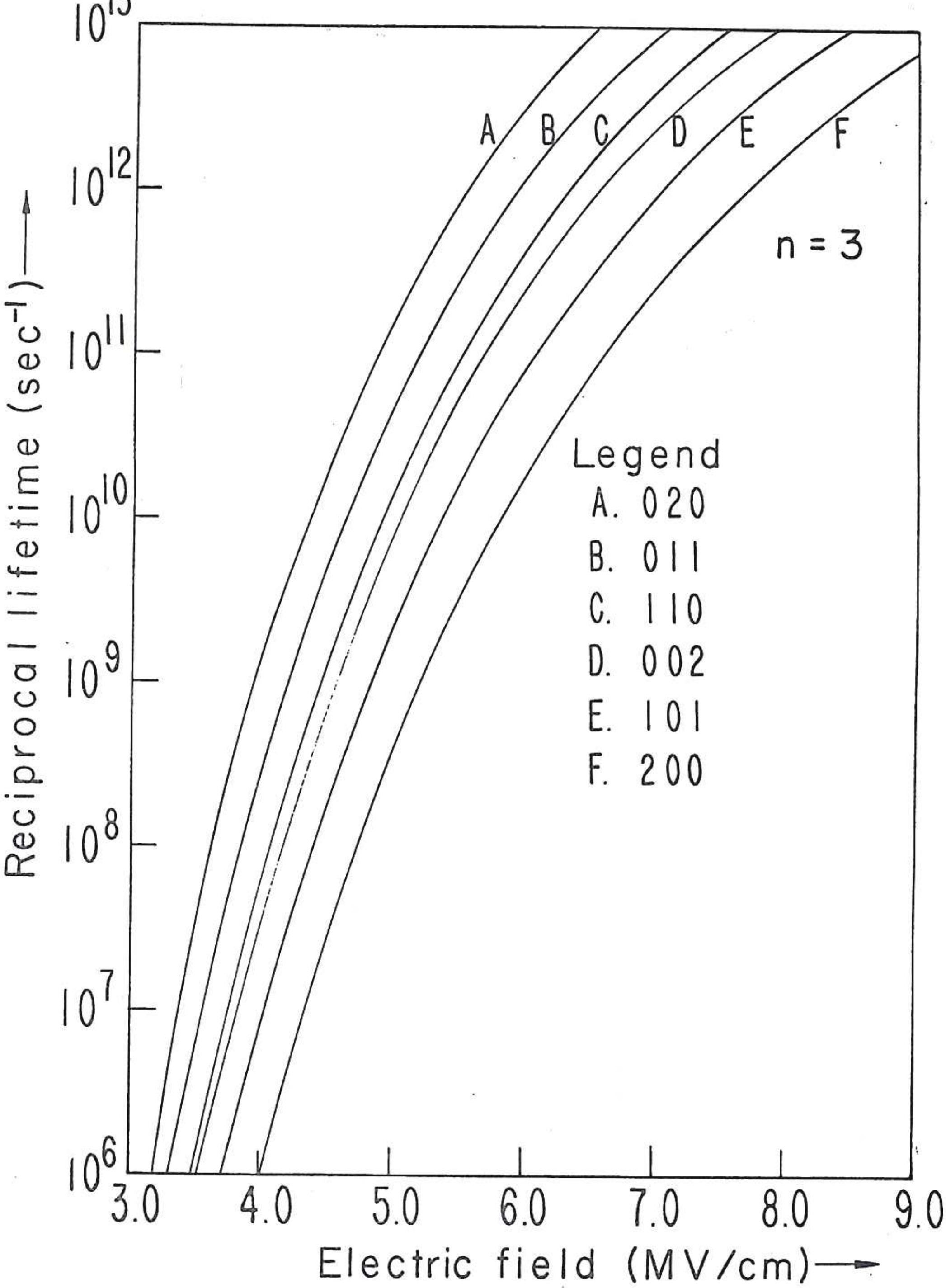
CLM-P 50 Fig. 6

Ionization probabilities versus electric field, in units of 10^3 volts/cm, for the extreme components of levels n = 9 through n = 25 using the R G method



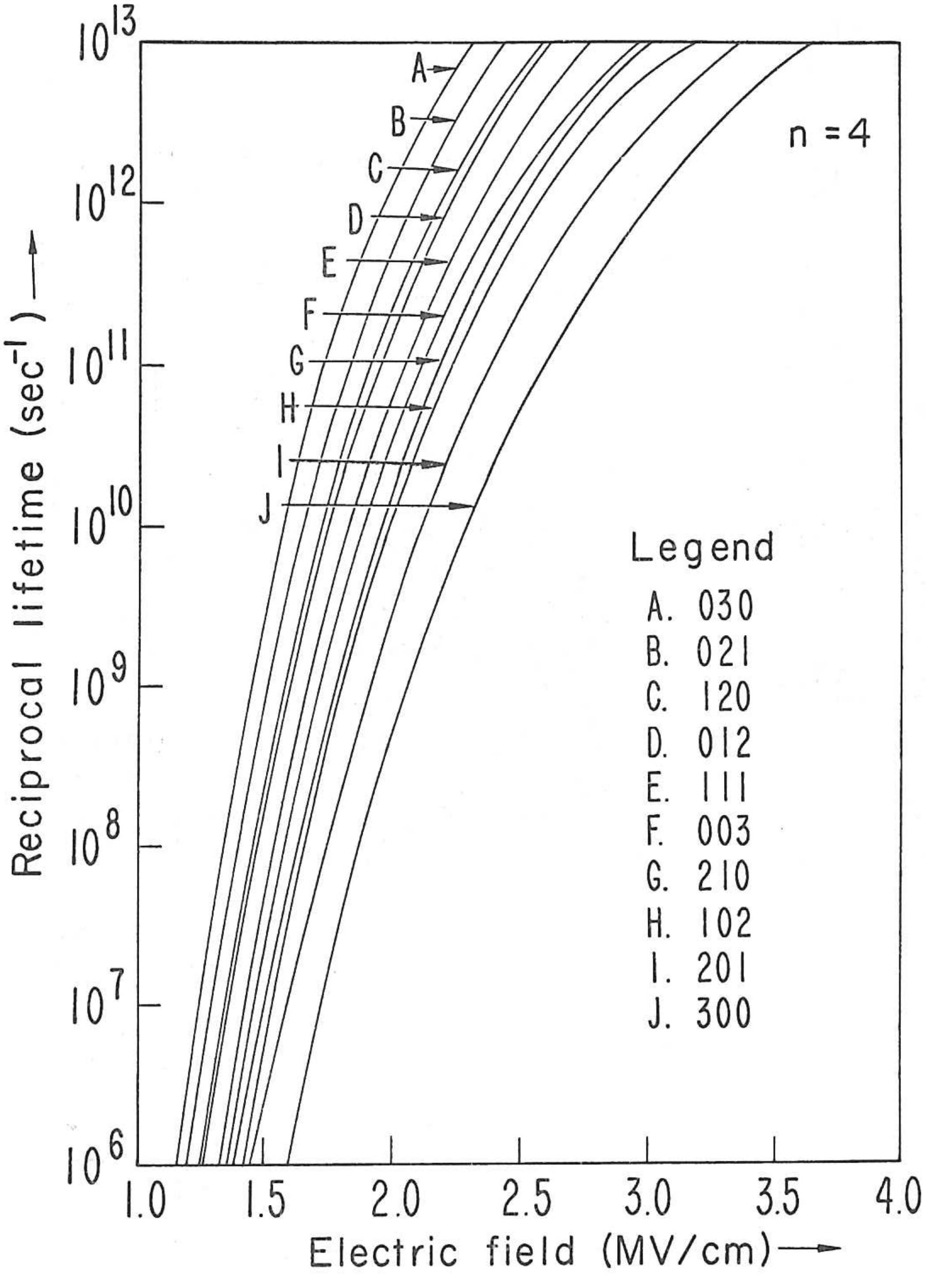
CLM-P 50 Fig. 7

Ionization probabilities versus electric field, in units of 10^6 volts/cm, for the different Stark states, $n_1\ n_2\ m$, belonging to the $n = 2$ level using the R G method



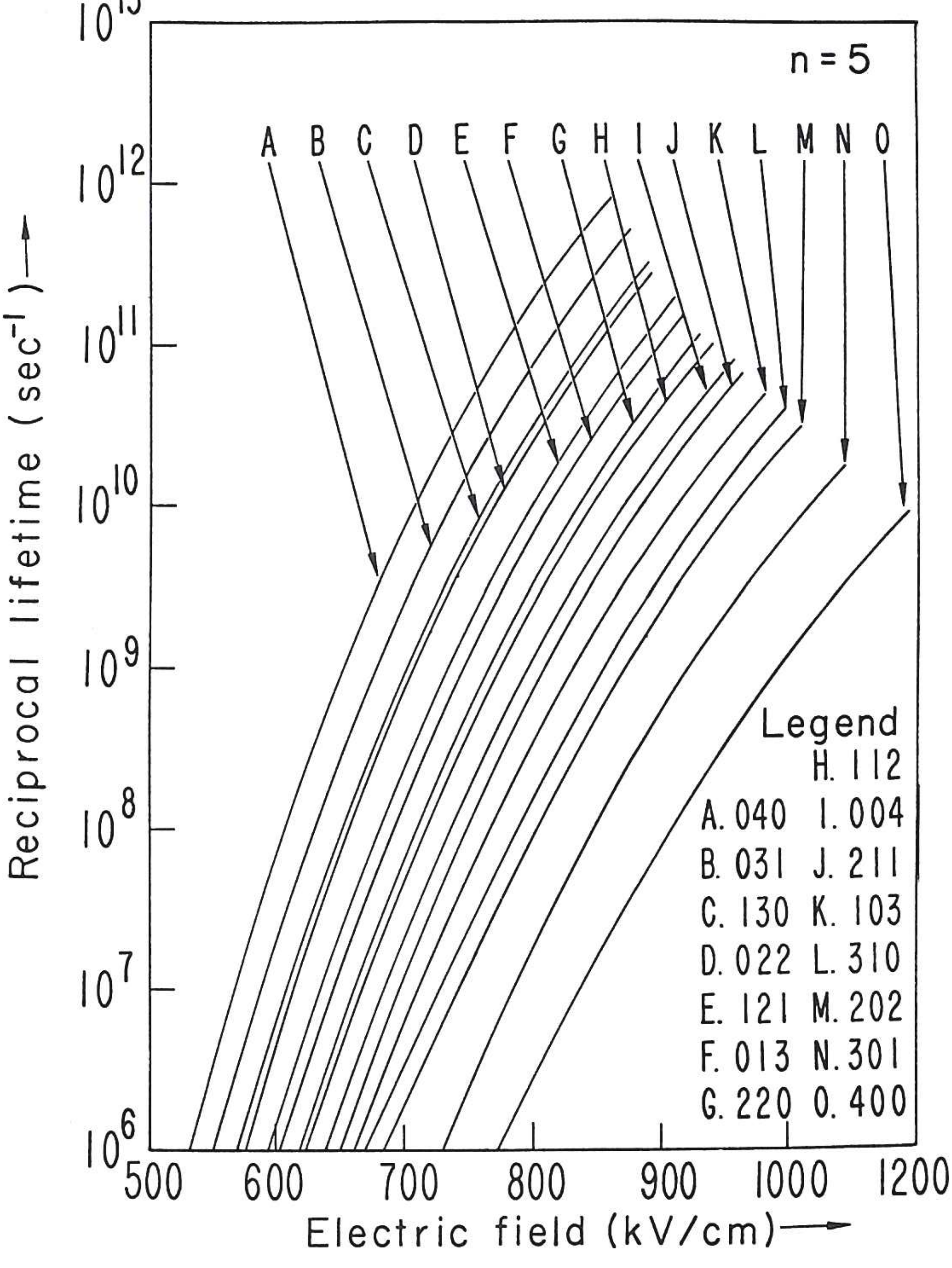
CLM-P 50 Fig. 8

Ionization probabilities versus electric field, in units of 10^6 volts/cm, for the different Stark states, n_1 n_2 m, belonging to the n = 3 level using the RG method



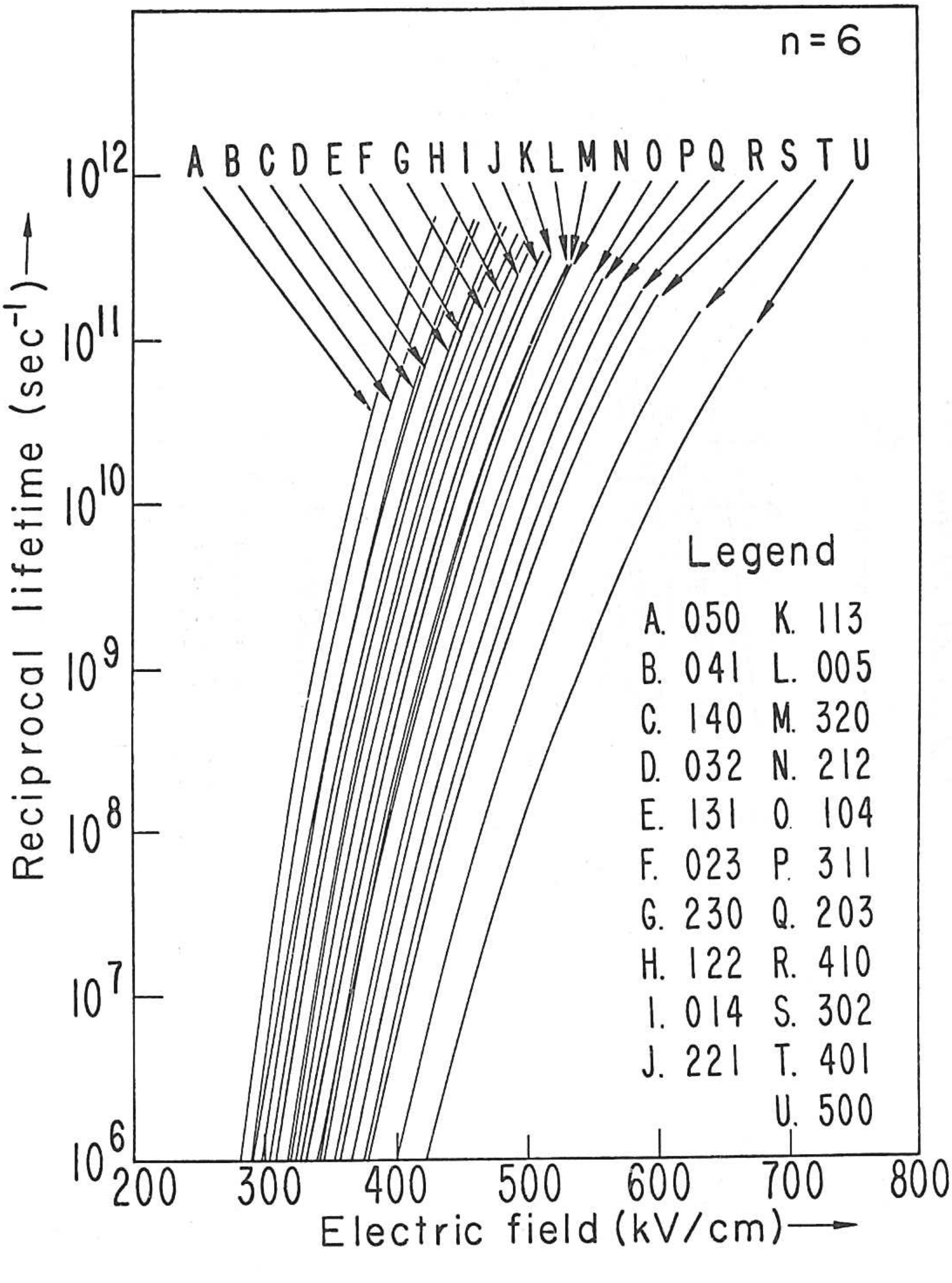
CLM-P 50 Fig. 9

Ionization probabilities versus electric field, in units of 10^6 volts/cm, for the different Stark states, $n_1\, n_2\, m$, belonging to the n = 4 level using the RG method



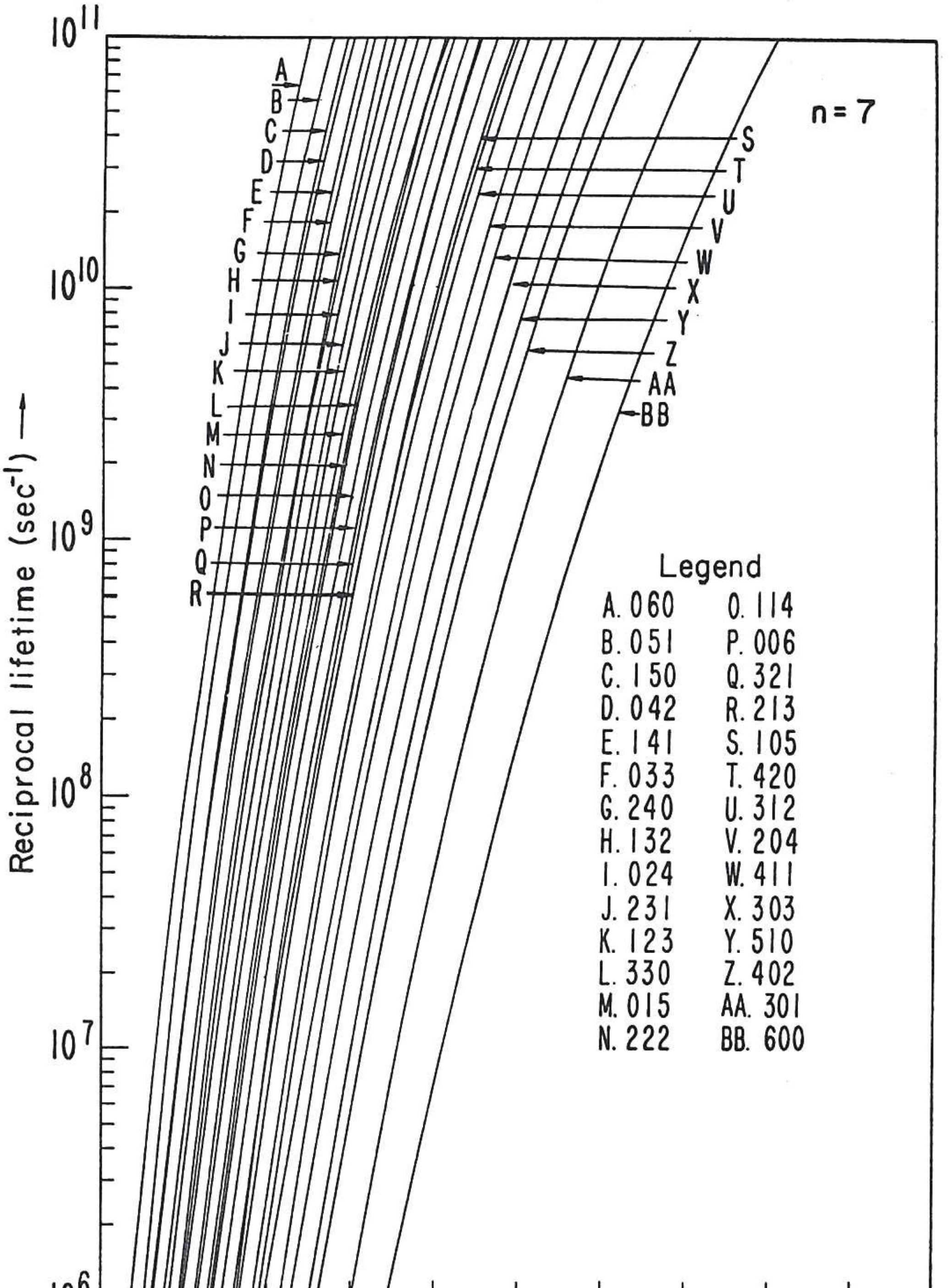
CLM-P 50 Fig. 10

Ionization probabilities versus electric field, in units of 10^3 volts/cm, for the different Stark states, $n_1 n_2 m$, belonging to the $n = 5$ level using the RG method



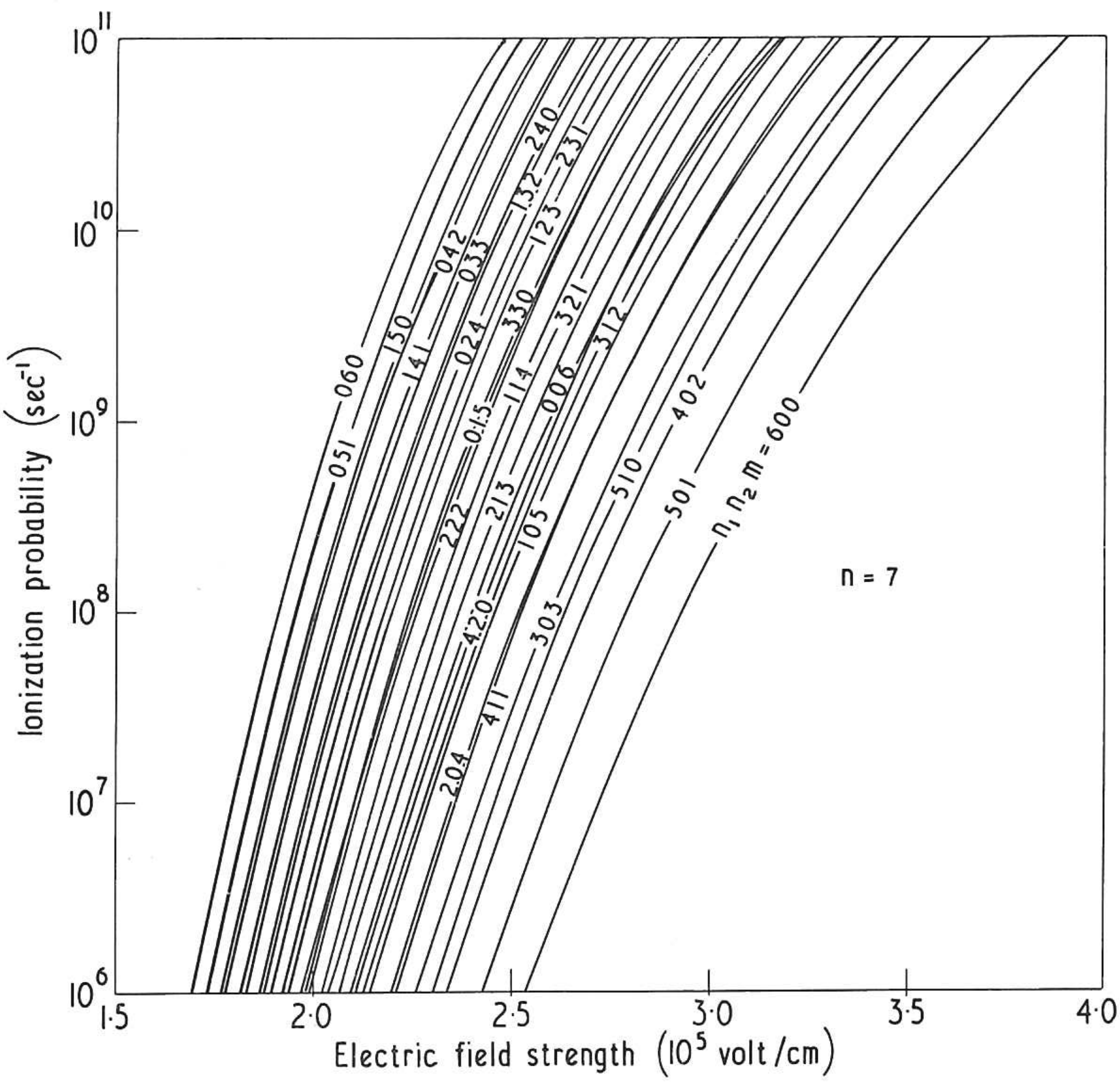
CLM-P 50 Fig. 11

Ionization probabilities versus electric field, in units of 10^3 volts/cm, for the different Stark states, n_1 n_2 m, belonging to the n = 6 level using the R G method



CLM-P 50 Fig. 12

Ionization probabilities versus electric field, in units of 10^3 volts/cm, for the different Stark states, $n_1 n_2 m$, belonging to the $n = 7$ level using the RG method



CLM-P 50 Fig. 13

Ionization probabilities versus electric field, in units of 10^5 volts/cm, for the different Stark states, $n_1\ n_2\ m$, belonging to the $n = 7$ level calculated using the Lanczos method in third order