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Population Inversions in He I and C III
in Recombining Plasmas

by

Raied M. Nasser

Submitted to School of Graduate Studies in
partial fulfillment of the requirements
for the degree of Ph.D. in Physics

Department of Physics
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1986



Raied M. Nasser, Ottawa, Canada, 1987.

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UNIVERSITÉ D'OTTAWA
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To my wife Hana, and my daughters Sherreen and Reem.....

Abstract

In the present thesis a number of investigations on population inversions in He I and C III in recombining plasmas are reported. Model calculations for laser action in He I are carried out using Collisional-Radiative model, when helium plasma is rapidly cooled by expansion. In this model 61 excited levels of He I are considered, and excitation, de-excitation, ionization and three-body recombination by electronic collision, spontaneous transition and radiative recombination have been included. The best available rate coefficients for the processes involved are utilized. The quasi-steady state approximation is used in calculating the population densities of 62 discrete levels of He I. Population inversions have been found to occur in many of transitions of He I. We have concentrated our attention on transitions between levels with $n \leq 4$ which give rise to emission lines in the visible region of the spectrum and show large population inversion. Results are presented for four transitions: $3^1S \rightarrow 2^1P$ ($\lambda 7281$), $3^1D \rightarrow 2^1P$ ($\lambda 6678$), $4^1S \rightarrow 2^1P$ ($\lambda 5047$) and $4^1D \rightarrow 2^1P$ ($\lambda 4922$). Available observational evidence for possible laser action in the He I $\lambda\lambda 7281, 6678$ lines in Wolf-Rayet and emission line stars is summarized and discussed.

A similar model calculation for laser action in C III is carried out. A total of 59 states of C III are considered in the Collisional-Radiative model. All the elementary processes mentioned above are included, in addition, we include the dielectronic recombination. Accurate oscillator strengths for the allowed electric dipole transitions between 40 lowest terms in C III required in the calculations have been calculated. The method of calculation and the results of these oscillator strengths are given and compared with previous results and experimental values, where available. Also, a modified ionization equilibrium model for carbon, applicable to high and low electron densities, is used to calculate the relative concentrations of various ions. Appreciable population inversion is found to occur only in

two lines $2s3p\ ^3P^o \rightarrow 2s3s\ ^3S$ ($\lambda 4650$) and $2p3p\ ^3S \rightarrow 2p3s\ ^3P^o$ ($\lambda 5263$) in the visible region. The results are presented in the form of n_e - T_e digram. The relevance of these results in resolving the problem of intensity anomalies in the spectra of Wolf-Rayet stars is pointed out.

Extending the model calculation for He I, the sudden cooling assumption is removed and the plasma is allowed to expand in finite time. The initial population densities of excited states of He I are calculated using steady-state assumption. The differential equations for the population relaxation, electron density, ions densities and electron temperature are solved jointly using Runge-Kutta-Gill method. The variations of population densities with time are presented and discussed. The effect of initial conditions of the helium plasma on the population inversion is studied. A similar model is applied to carbon plasma. The evolution of the densities of the levels of C III are investigated in detail. The calculation is carried out for three sets of initial conditions to study the dependence of the population inversion in C III ion on the initial plasma parameters.

Results of a theoretical model are presented, which describes a stationary He I plasma brought into contact with cool and dense hydrogen gas. The model includes elastic collision interaction and the detailed kinetic excited levels of helium and hydrogen atom. Atom-atom collision processes are included. The quasi-steady state approximation is used only for levels i lying above certain level i^* which is greater or equal to 11 in He I and 5 in H I. Effective electron cooling is found to occur in a short time. It is found that the population inversions which occur between levels of hydrogen atom are realized only in the quasi-steady state following the transient phase, while those in helium are realized in the transient phase. The calculations have shown that the magnitude of the population inversion which occurs between levels of helium is much greater than that obtained previously by expansion.

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Chapter 1

Introduction

A) An overview of the previous work

For some time past there has been considerable interest in using the plasma as an amplifying medium of radiation and a large number of schemes by which this might be achieved have been proposed. Gudzenko and Shelepin (1963, 1965) were the first to point out the possibility of radiation amplification in a rapidly cooled (recombining) plasma. This scheme is capable of generating intense laser action and it is known as the plasma laser or recombination laser. The work of Gudzenko and Shelepin has been amplified and extended by Gudzenko *et al.* (1966, 1967). Reviews of the subject have been published by Gudzenko *et al.* (1974, 1975). Short reviews have been given by Otsuka (1980) and Bunkin *et al.* (1981). Laser using recombination plasma has the following advantages over lasers using other media:

- 1- broad range of frequencies (from infrared to soft X-rays) capable of being amplified in different types of plasma.
- 2- the possibility of obtaining in principle a high efficiency.

Production of an efficient amplifying medium is the result of the simultaneous action of two mechanisms, one of which fills the upper working level of the atom (ion), the other of which empties the lower level. Several methods of cooling the plasma have been suggested. Two of these which are of importance in astrophysics are considered in this work and these the following:

(1) Rapid expansion into a vacuum

Cooling of the free electrons by rapid expansion into vacuum was first investigated by Gudzenko *et al.* (1966) in magnetized and unmagnetized plasma. A moving plasma with rapidly changing density and temperature is a medium in which substantial electronic

nonequilibrium phenomena is realized. A rapid recombination that occurs with sharp reduction of the temperature of the free electrons in a plasma which initially exhibits a high degree of ionization, can lead to overpopulate the upper levels. The populations in the lower levels are depopulated by radiative or collisional processes; the nonequilibrium situation that is obtained in this way, if one achieves sufficiently rapid cooling of the free electrons, can lead to strong population inversion, thus making it possible to use this plasma as lasing medium. The significance of using the rapid expansion into a vacuum of a plasma stream is primarily to cool the medium rapidly and thereby create the recombination conditions. In addition, since the decay of different parts of an expanding plasma takes place at different times, the recombination process unfolds in time and the radiating medium is carried out of the active zone. Thus, it is possible to obtain continuous high power lasing in a plasma stream flowing constantly out of a nozzle or of a star. Experimental evidence of population inversion due to the rapid expansion into vacuum of highly ionized hydrogen or hydrogenic plasma has been given by Gol'dfarb *et al.* (1966), Gol'dfarb *et al.* (1969), Hoffmann and Bohn (1972), Irons and Peacock (1974), Dewhurst *et al.* (1976), Dixon *et al.* (1978), Korukhov *et al.* (1982), and of helium by Goldfarb *et al.* (1969), Zhinzhikov *et al.* (1978), Hara *et al.* (1985). Theoretical studies on plasma dynamic laser have been carried out by Kuznetsov *et al.* (1965), Gudzenko *et al.* (1970), Bowen and Park (1971), Stupitskii *et al.* (1972), and Reshetnyak and Shelepin (1973). The numerical calculations of Bowen and Park (1971) and Stupitskii *et al.* (1972), respectively, have demonstrated the possibility of obtaining a population inversion on a neutral nitrogen line ($\lambda 1745 \text{ \AA}$) and on xenon atomic lines ($7p \rightarrow 5d$, $4f \rightarrow 5d$). Reshetnyak and Shelepin (1973) showed the possibility of obtaining a population inversion in a lithium transition ($10792 \text{ \AA}$), and a helium transition ($21120 \text{ \AA}$). Calculations by Varshni and Lam (1976) showed population inversion in a He II line ($\lambda 4686$) under stellar conditions, and Millette and Varshni (1980) have shown several transitions in C IV, N V, and O VI ions to have inverted population

under similar conditions.

(2) Contact with a neutral gas

Rapid cooling of the free electrons by collisions with a cool gas can be achieved in a high density plasma. The advantage of this method is that the charge particle density does not decrease as in an expanding plasma, and thus there is the possibility of obtaining higher gain and VUV laser. Theoretical calculations have shown that inverted population can be realized in a high density plasma interacting with a cool gas (Gudzenko and Yakovlenko, 1970; Gudzenko *et al.*, 1975; Wagli and Bohn, 1980; Furukane and Oda, 1984). Population inversion between low-lying levels of He II was observed by Sato *et al.* (1977), and Sato (1977), in a stationary plasma interacting with a neutral gas.

There are several physical situations in which a plasma expands into a vacuum or a low density gas, and where laser action may be important to different degrees. Some important examples of such physical situations are as follows:

- (a) Rapid mass loss from Wolf-Rayet stars.
- (b) Novae and supernovae.
- (c) Explosion of an atomic bomb or hydrogen bomb in outer space.
- (d) When a laser pulse strikes the surface of a solid target.
- (e) Electrical explosion of thin wires in vacuum (Tyulina 1965).
- (f) When high-energy meteorites strike the surface of a planet that has no atmosphere.

In principle, any analysis of the prospects for recombining plasma is closely associated with a discussion of relaxation processes involving a large number of discrete electronic levels. For a given electron temperature and density, the population densities of a large number of excited states and ions densities are required. The population densities of discrete electronic levels in non-LTE plasmas must be obtained from the rate coefficients of the individual collisional and radiative processes occurring within the plasma. Several

models which take into account some or most useful of these processes have been proposed; of these, the most useful and general is the Collisional-Radiative (CR) model (Bates et al., 1962a,b). This model is based on the following assumptions:

1. The free electrons have a Maxwellian velocity distribution.
2. Ionization is by electron collision from any bound level (in complex composition plasma, one must, of course, include the ionization by heavy particles collision) and is partially balanced by three-body recombination into any level.
3. Transitions between any pair of bound levels are induced by electron collisions (heavy particles collisions must be included in the case of complex composition plasma).
4. Radiation is emitted when an electron in an upper bound level makes a spontaneous transition to a lower level and when a free electron recombines into a bound level.
5. The plasma is optically thin, such that all radiation emitted within the plasma escapes without being absorbed; this assumption is less realistic since some degree of radiation reabsorption is likely to occur in the plasma (especially in high density plasma). In some cases, one can use the effective probability of the radiative transition, in order to allow for radiation absorption (Bates et al., 1962b; Gordiets et al., 1968a,b; Drawin, 1969, 1970; Drawin and Emard, 1970, 1972, 1973, 1974).

With these assumptions, an infinite number of the coupled equations which describe the population densities of all the discrete levels are obtained. To avoid dealing with impossibly large number of coupled equations, it can be reduced to a limited number by the fact that because with increasing quantum number the level spacing become closer, the probability of collisional processes becomes greater while at the same time the probability of radiative processes becomes smaller. Thus to any desired accuracy there is always some level above which the effect of the radiative processes may be neglected. Under these circumstances, the population density of these upper levels obeys the Saha-Boltzmann distribution law. Further there is a cutoff in the number of excited states because of

the reduced ionization limit in a plasma. The principal quantum number, n_s , at which summations may be curtailed is given by (Griem, 1974)

$$n_s = (z^2 E_H / \Delta E^{z-1})^{1/2} \quad (1-1)$$

Here $z = 1$ for neutral atoms, $z = 2$ for singly charged ions, etc. and E_H is the ionization energy of hydrogen, and

$$\Delta E^{z-1} = \frac{ze^2}{\rho_D} \quad (1-2)$$

with ρ_D being the Debye radius.

This model was first proposed and applied to hydrogen-like ions by Bates *et al.* (1962a, b). These authors considered a plasma containing hydrogen ions, bare nuclei, and electrons, not necessarily in a steady state and showed that the population densities of the excited bound levels of hydrogenic ions come into equilibrium effectively instantaneously with the relatively slowly varying ground level population. Thus, the rate equation can be set equal to zero for all levels other than the ground state. This approximation is known as the quasi-steady state (QSS) approximation. Following Bates *et al.*, the population densities of hydrogenic ions in the ground level N_1^{+m} and bare nuclei N^{m+1} are described by the equation

$$\frac{dN_1^{+m}}{dt} = -\frac{dN^{m+1}}{dt} = \alpha_{CR} N^{m+1} n_e - S_{CR} N_1^{+m} n_e \quad (1-3)$$

The two coefficients α_{CR} and S_{CR} are the CR recombination and ionization coefficients, respectively. They may be regarded as net recombination and ionization rates. In steady-state plasma this equation reduces to ($N_1^{+m} \gg N_i^{+m}$)

$$N^{m+1} / N^{+m} = S_{CR} / \alpha_{CR} \quad (1-4)$$

Numerical solutions for hydrogen and hydrogen-like ions have been obtained by Bates *et al.* (1962a,b) and by McWhirter and Hearn (1963) and they list representative sets of values of the various coefficients.

Since then, much work has been done on and with the CR model using the QSS approximation. Hydrogen and hydrogen-like ions, being simple systems have been extensively investigated. Theoretical studies have been carried out by Bates and Kingston (1963), Gordiets *et al.* (1968, 1968a), Bohn (1971, 1974, 1978), Fujimoto *et al.* (1972), Skorupski and Suckewer (1974, 1974a), Pert and Ramsden (1974) Reshetnyak and Shelepin (1975), Pert (1976, 1979), Luk'yanov (1977), Tallents (1977, 1978), Otsuka (1978), Furukane *et al.* (1979), Furukane and Yamamoto (1980), Pert and Tallents (1981), Furukane *et al.* (1982, 1983), Boiko *et al.* (1982), and Oda and Furukane (1983).

Experimental observations of population inversion in hydrogen have been made in hydrogen by Hoffmann and Bohn (1972), Suckewer *et al.* (1976), Lukyanov *et al.* (1978), Hara *et al.* (1980, 1980a), Trebes *et al.* (1981), and Miyake *et al.* (1983), in He II by Suckewer *et al.* (1976), Sato *et al.* (1977), and Hara *et al.* (1982), in C VI by Irons and Peacock (1974), Dewhurst *et al.* (1976), Dixon *et al.* (1978), Key *et al.* (1979), and Jacoby *et al.* (1981), and in O VIII by Korukhov *et al.* (1982). Suckewer *et al.* (1986) (Milchberg *et al.*, 1985; Suckewer, 1985) have observed gain in plasma for the C VI $\lambda 812$ line. The model has been applied to other atoms also. Work on helium atom has been summarized in Chapter 2. The model was first applied to lithium by Gordiets *et al.* (1968b), and to cesium by Norcross and Stone (1968)

An alternative theoretical approach which does not invoke the quasi-steady state approximation is to seek the solution of the time-dependent relaxation equations. This approach has the advantage that one can then study the temporal evolution of the plasma by integrating the relaxation equations numerically (Gordiets, Gudzenko and Shelepin 1968b; Limbaugh and Mason, 1971). On the other hand this approach has the disadvantage that

the integration consumes much computing time, because the system of equations is stiff, so that the integration step-length has to be kept very small. Also, the number of differential equations involved is large, one equation being required for each of the bound states.

Jones and Ali (1975, 1977, 1978) (Ali and Jones, 1976) have carried out calculations on hydrogen and hydrogen-like ions from a detailed time-dependent numerical model. Starting with completely stripped ions, the plasma is allowed to recombine and the time histories of the excited states are followed.

In the laboratory, there is a serious limitation in the production of short-wavelength lasers. As the wavelength decreases, it becomes increasingly difficult to device suitable mirrors for multiple passes. The reflectivity of such mirrors which are possible is $\sim 10\%$ (Sobel'man and Vinogradov, 1985). For wavelength $\leq 400 \text{ \AA}$, in soft X-rays, lasing can be achieved only by amplified spontaneous emission (ASE) i.e. single pass lasers. In stellar sources, ordinarily, one can only consider single pass lasers. Thus both for stellar sources (at any wavelength) and laboratory sources at short wavelengths one has to consider the best conditions for ASE. The intensity of the laser radiation is proportional to $e^{g\ell}$, where g is the gain coefficient and ℓ is the length. The main difference between laboratory and astronomical plasmas is physical size. This difference in size means that the demands on g are different in the two cases. In astronomical sources, ℓ is very large, thus even a very small value of g can lead to an intense line, but in laboratory sources, the small value of ℓ means that g must be very large for the production of an intense line.

The plasma laser is also of importance for military applications. One of the possibilities which is being explored in the X-ray laser program of the Strategic Defense Initiative (SDI) research, is essentially based on laser action in a recombining plasma. (Robinson 1984, Eder et al. 1985; Richardson 1985; Hagelstein et al. 1985; Smith 1985).

According to two short reports that appeared in 1981 (Robinson, 1981; Walbridge, 1981) an X-ray laser action has been demonstrated for the first time in experiments con-

ducted in the Nevada desert. The device pumped by X-rays from a small nuclear bomb, produced a nanosecond long pulse of several hundred terawatts at 14 Å. Obvious potential military applications cover any other details of this experiment by total secrecy. Estimates by a Russian group (Bunkin *et al.*, 1981) have shown that it is possible to achieve a quasi-steady state amplification in the 10–20 Å range in a recombination plasma of an element with $Z \simeq 30$ (for example, the $6 \rightarrow 5$ transition in Zinc yields $\lambda = 14.2$ Å).

B) This thesis

In the present thesis a number of investigations are reported with the aim of finding appropriate transitions in He I and C III in which population inversion may occur in a recombining plasma. Whereever possible the results obtained are compared with astrophysical observations or laboratory experimental results.

In Chapter 2, the population densities of the discrete levels of He I in optically thin plasma cooled by adiabatic expansion are calculated with the Collisional–Radiative model. Population inversion of varying degrees is found to occur in several transition. Results for four such transitions which lie in the visible region of the spectrum, and for which laser action is possible, are presented in the form of n_e – T_e diagram. The evidence available on Wolf-Rayet spectra for two of the lines $\lambda\lambda 7281, 6678$ is summarized and the behaviour of these lines is compared with the expectations of the model calculations.

In Chapter 3, the assumption of sudden cooling which was used in chapter 2 is removed and the helium plasma is allowed to expand in vacuum in a finite time. The evolution of the population densities is investigated in detail. The dependence of population inversion on the initial conditions is studied.

We wanted investigate population inversion in C III levels. For this purpose a great many cross-sections are needed. It was found that for many of the transitions which would enter into the calculation, no theoretical as experimental data were available. Con-

sequently a substantial project on the calculation of oscillator strengths of C III transitions was undertaken. Calculation of oscillator strength for all allowed electric dipole transition between the 40 lowest terms in C III ion is described in Chapter 4. Configuration interaction wavefunction are used. The results are used in subsequent chapters.

Model calculations for laser action in C III, similar to those in chapter 2, are presented in chapter 5. Two transitions are found to show appreciable population inversion. The results are presented in the form of n_e - T_e diagram. The behaviour of these lines are compared with that in the spectra of Wolf-Rayet stars. In chapter 6, a model similar to that presented in chapter 3 is applied to carbon plasma expanding in vacuum, and the population densities of the levels of C III are studied in detail.

Finally in chapter 7, the processes leading to the population inversion are investigated in a recombining plasma when a stationary helium plasma is brought into contact with a dense and cool hydrogen gas. The population densities for the levels of He I and H I are calculated using the rate equations on the basis of a Collisional-Radiative model and the energy equations of electrons and neutral particles.

Two papers, based on chapters 2 and 4, have been published:

1. Y. P. Varshni and R. M. Nasser: Laser Action in Stellar Envelopes, *Astrophys. Space Sci.* **125**, 341 (1986).
2. R. M. Nasser and Y. P. Varshni: Oscillator strengths for C III lines, *Astron. Astrophys. Suppl.* **60**, 325 (1985).

Chapter 2

Laser action in stellar envelopes. He I

A) Introduction

Several types of stars (e.g., Wolf-Rayet, Of) are known to undergo mass loss, and if the mass loss is rapid enough, it can lead to rapid cooling. In the astrophysical context, the term laser action actually means amplified spontaneous emission as there are no mirrors.

Varshni and Lam (1976) presented calculations on population inversion and laser action in He II in the context of stellar envelopes. In this chapter model calculations for laser action in certain transitions of He I, using the CR model, are reported. First we summarize the work which has been done on population densities and population inversion in He I in laboratory plasma.

An early discussion of the possibility of producing population inversion in helium is due to Gordiets *et al.* (1968b). Theoretical calculations on population densities of He I levels under different conditions have been made by Johnson (1967), Drawin (1969), Brocklehurst (1972), Limbaugh and Mason (1971), Drawin *et al.* (1973), Filippov and Yevstigneyev (1975), Hess and Burrell (1979), Fujimoto (1979), and Ilmas and Nugis (1982).

The experiments of Goldfarb *et al.* (1969) on axisymmetric supersonic jets of a helium plasma revealed a deviation from an equilibrium energy distribution of He atoms at the end of the nozzle of a plasmatron and showed that a population inversion of levels with principal quantum numbers $n = 4$ and 3 occurs at some finite distance from the nozzle.

Johnson (1967) and Johnson and Hinnov (1969) give the results on the measurement of population densities of excited states of neutral helium in afterglow discharges. The data show population inversion between certain levels with $n = 4$ and 3 and also between certain levels with $n = 5$ and 3 .

Zhinzikov *et al.* (1978) have studied the population inversion in He I levels with $n = 4$ and 3 in the supersonic expansion of helium plasma from circular and plane nozzles into a low density medium. In an axisymmetric jet the population inversion occurred at some finite distance from the nozzle; in plane jets the inversion occurred immediately beyond the slit nozzle. The experimental results were compared with theoretical calculations; the experimental results confirm the operation of a recombination mechanism.

Recently Hara *et al.* (1985) have observed population inversions in a freely expanding helium plasma. Experimental results showed that population inversions for $n = 3 - 4$ and 3 - 5 levels of He singlet system are larger than the triplet system.

B) The Theoretical Model

We consider what happens when the plasma in the outer layers of a star rapidly expands. To focus our discussion we consider Wolf-Rayet stars. The atmospheres of these stars depart seriously from a condition of local thermodynamic equilibrium (LTE). We consider the state of plasma at the base of the extended atmosphere of a Wolf-Rayet star, roughly where its 'photosphere' would lie. We make the reasonable assumption that the conditions there will also correspond to non-LTE. Hence to obtain the relative concentrations of He, He^+ , and He^{++} at a particular electron density (n_e) and electron temperature (T_e) we use the non-LTE method of House (1964) (see Appendix A). It is well known that Wolf-Rayet stars are undergoing a high-speed mass loss. We assume that this plasma expands adiabatically, for which the plasma density N and T_e are related by $TN^{1-\gamma} = \text{const.}$ We assume $\gamma = 5/3$; for the actual plasma the value will be slightly smaller. The flow is supersonic and to a first approximation, the plasma is assumed to be 'frozen' during the rapid fall of temperature, for which a factor of 5 is assumed. (The same factor for the fall in the temperature has been used by Gudzenko

et al., 1966, and Varshni and Lam, 1976.) Rapid recombinations will occur in this cooled plasma. The populations of the atomic levels can be calculated from the CR model. The time development of the population density N_i of a level i is described by the differential equation

$$\begin{aligned} \dot{N}_i \equiv \frac{dN_i}{dt} = & -n_e N_i S_i - n_e N_i \sum_{j \neq i}^{\infty} C_{ij} - N_i \sum_{j=1}^{i-1} A_{ij} \\ & + n_e \sum_{j \neq i}^{\infty} N_j C_{ji} + \sum_{j=i+1}^{\infty} N_j A_{ji} + \{\beta_i + \alpha_i n_e\} n_e N^{+m}, \end{aligned} \quad (2-1)$$

where i and j symbolically represent energy states available to the bound electron. The meanings of other symbols in Equation (2-1) as follows:

N^{+m} = the density of the next ionization stage,

n_e = electron density,

C_{ij} = rate coefficient for excitation ($i < j$) or de-excitation ($i > j$) from level i to j by electronic collision,

A_{ij} = Einstein coefficient for radiative transition from level i to j ,

S_i = rate coefficient for ionization from level i by electron collision,

α_i = that for three-body recombination to level i ,

β_i = that for radiative recombination.

Other atomic processes are possible to occur in the plasma, but since they occur less frequently or they are not effective at the temperatures and densities considered in this calculation, they are not included in the CR model. For example: proton-atom, atom-atom collision, photoionization, dielectronic recombination.

There is such an equation for each and every discrete level $i = 1, 2, 3, \dots, \infty$. Thus, we obtain an infinite number of coupled differential equations describing the population

densities of all the discrete levels.

The normalized population density of level i is defined by

$$\rho_i = \frac{N_i}{N_i^E}, \quad (2-2)$$

where N_i^E is the Saha equilibrium population density of level i ,

$$N_i^E \equiv Z_i n_e N^{+m} \quad (2-3)$$

and

$$Z_i = \{\omega_i / 2\omega^+\} (h^2 / 2\pi m_e k T_e)^{3/2} \exp(\chi_i / k T_e), \quad (2-4)$$

where ω_i and ω^+ are the statistical weight and the partition function of the ion, respectively, χ_i is the ionization potential of the level i , and the other symbols have the usual meaning.

Dividing eq.(2-1) by N_i^E and using eq.(2-2), the set of equations (2-1) becomes

$$\begin{aligned} \dot{\rho}_i \equiv \frac{\dot{N}_i}{N_i^E} = & - \left(n_e S_i + n_e \sum_{j \neq i}^{\infty} C_{ij} + \sum_{j=1}^{i-1} A_{ij} \right) \rho_i \\ & + \sum_{j=i+1}^{\infty} \{ C_{ij} n_e + \frac{Z_j}{Z_i} A_{ji} \} \rho_j + \frac{1}{Z_i} \{ \alpha_i n_e + \beta_i \}, \end{aligned} \quad (2-5)$$

with $i = 1, 2, 3, \dots, \infty$. To solve this set of equations, the following assumptions are used.

First, for all levels i located above a sufficiently high lying level, r , the population density is assumed to be given by the Saha-Boltzmann equilibrium equation instead of by Eq.

(2-1). Thus, in this case, we have $\rho_{i>r} = 1$. The infinite set of equations (2-5) thus become

a finite set of r coupled equations which can be solved for ρ_i , $i = 1, 2, \dots, r$. The infinite

sums appearing in Eq. (2-5) can be cut off at a sufficiently high-lying level $s > r$ above

which the rate coefficients involving these states contribute little to the infinite sums of

Eq. (2-5). Second, the time derivative, Eq. (2-5), can be put equal to zero for all the levels $i \leq r$ except the ground state (1^1S) without causing significant error. This leads to coupled linear equations for the levels $2 \leq i \leq r$ instead of the coupled differential equations. Using these assumptions, Equation (2-5) reduces to

$$\begin{aligned} \dot{\rho}_i = & - \left(n_e S_i + n_e \sum_{j \neq i}^s C_{ij} + \sum_{j=1}^{i-1} A_{ij} \right) \rho_i + \sum_{j=i+1}^r \left\{ C_{ij} n_e + \frac{Z_j}{Z_i} A_{ji} \right\} \rho_j \\ & + \sum_{j>r}^s \left\{ C_{ij} n_e + \frac{Z_j}{Z_i} A_{ji} \right\} + \frac{1}{Z_i} \{ \alpha_i n_e + \beta_i \} = 0, \quad (i = 2, 3, \dots, r) \end{aligned} \quad (2-6)$$

The solution of $r - 1$ linear simultaneous equation, in term of local ground state population density, may be written as follows

$$\rho_i = r_i^{(0)} + r_i^{(1)} \rho_1 \quad \text{for } 2 \leq i \leq r, \quad (2-7)$$

$r_i^{(0)}$ is the contribution from the continuum towards ρ_i , and $r_i^{(1)} \rho_1$ is the contribution from the ground state towards ρ_i . Substituting Equation (2-7) into Equation (2-6), we have two set of $r - 1$ equations for $r_i^{(0)}$ and $r_i^{(1)}$ with $2 \leq i \leq r$. The solutions $r_i^{(0)}$ and $r_i^{(1)}$ obtained from these two sets of equations give the population density,

$$N_i = Z_i r_i^{(0)} N^{+m} n_e + \frac{Z_i}{Z_1} r_i^{(1)} N_1. \quad (2-8)$$

The atomic data used in the calculations are summarized in the next section.

C) Atomic Data

(a) Energy levels.

The excitation energy of each level is based on Martin (1973). All of the levels having a principal quantum number $n \leq 8$ are treated as individual levels except for the levels

having the orbital angular momentum $\ell \geq 4$, which for the same n , are grouped together to form a single level. For the levels with $n > 8$ all of the S,P,D,... levels are grouped together in one level, which was approximated by a hydrogenic level having a statistical weight twice that of hydrogen. The upper limit of the levels, r and s in CR model calculation are taken as $n_r = 15$ and $n_s = 22$, respectively. Therefore we have 69 distinct levels in the main system, and the total number of levels whose population densities is calculated is 62. The labelling, energies and weight factors for these levels are given in Table 2-1.

(b) *Radiative Transitions.* The rates of spontaneous radiative transitions are determined by Einstein coefficients $A_{n\ell, n'\ell'}$. Einstein coefficients were calculated using the formula (Menzel and Pekeris, 1935)

$$A_{n\ell, n'\ell'} = \frac{8\pi^2 e^2 \omega_{n'\ell'}}{mc^3 \omega_{n\ell}} \nu_{n\ell, n'\ell'}^2 f_{n'\ell', n\ell}, \quad (2-9)$$

where $\omega_{n'\ell'}$ and $\omega_{n\ell}$ are the statistical weights of the level $n'\ell'$ and $n\ell$, respectively, $\nu_{n\ell, n'\ell'}$ the frequency of the photon emitted as result of the transition and $f_{n'\ell', n\ell}$ is the absorption oscillator strength for the transition, and the other symbols have their usual meaning. When the angular momentum states ℓ or ℓ' are grouped together then,

$$A_{n\ell_i, \dots, \ell_k, n'\ell'_i, \dots, \ell'_k} = \frac{8\pi^2 e^2 \nu^2 \sum_{\ell_i}^{\ell_k} \sum_{\ell'_i}^{\ell'_k} \omega_{n'\ell'} f_{n'\ell', n\ell}}{mc^3 \sum_{\ell_i}^{\ell_k} \omega_{n\ell}}, \quad (2-10)$$

Oscillator strengths for all the allowed transitions between the states n^1S , n^1P , n^1D , n^3S , n^3P , and n^3D , $n \leq 8$ were taken from Kono and Hattori (1984). These authors used variational wave function and they estimate the accuracy of their results to be better than 1% for most of the transitions and better than 0.1% for about a third of the transitions. The error estimate is based on numerical convergence as the number of expansion terms in the wave function is increased.

TABLE 2-1. Energy levels of He I used in the model.

Level No. (i)	State	Energy $E_i(\text{cm}^{-1})$	g_i	Level No. (i)	State	Energy $E_i(\text{cm}^{-1})$	g_i
1	1 ¹ S	0.0	1	32	6 ³ D	195260.49	15
2	2 ³ S	159856.07	3	33	6 ¹ D	195260.86	5
3	2 ¹ S	166277.55	1	34	6 ³ F	195262.49	21
4	2 ³ P	169086.94	9	35	6 ¹ F	195262.50	7
5	2 ¹ P	171135.00	3	36	6 ^{1,3} L	195262.85	80
6	3 ³ S	183236.89	3	37	6 ¹ P	195273.04	3
7	3 ¹ S	184864.55	1	38	7 ³ S	195868.35	3
8	3 ³ P	185564.68	9	39	7 ¹ S	195979.04	1
9	3 ³ D	186101.65	15	40	7 ³ P	196027.40	9
10	3 ¹ D	186105.07	5	41	7 ³ D	196069.73	15
11	3 ¹ P	186209.47	3	42	7 ¹ D	196070.22	5
12	4 ³ S	190298.21	3	43	7 ³ F	196071.27	21
13	4 ¹ S	190940.33	1	44	7 ¹ F	196071.28	7
14	4 ³ P	191217.13	9	45	7 ^{1,3} L	196072	132
15	4 ³ D	191444.59	15	46	7 ¹ P	196079.24	3
16	4 ¹ D	191446.56	5	47	8 ³ S	196461.42	3
17	4 ³ F	191451.98	21	48	8 ¹ S	196534.88	1
18	4 ¹ F	191451.99	7	49	8 ³ P	196566.82	9
19	4 ¹ P	191492.82	3	50	8 ³ D	196595.18	15
20	5 ³ S	193347.09	3	51	8 ¹ D	196595.54	5
21	5 ¹ S	193663.63	1	52	8 ³ F	196596.17	21
22	5 ³ P	193800.80	9	53	8 ¹ F	196596.17	7
23	5 ³ D	193917.24	15	54	8 ^{1,3} L	196597	192
24	5 ¹ D	193918.39	5	55	8 ¹ P	196601.51	3
25	5 ³ F	193921.18	21	56	9	196955	324
26	5 ¹ F	193921.19	7	57	10	197213	400
27	5 ^{1,3} L	193922	36	58	11	197403	484
28	5 ¹ P	193942.57	3	59	12	197548	576
29	6 ³ S	194936.23	3	60	13	197661	676
30	6 ¹ S	195115.00	1	61	14	197750	784
31	6 ³ P	195192.91	9	62	15	197822	900

For the allowed transitions between the states $n^{1,3}D$ and $n^{1,3}F$, we used the Coulomb approximation method proposed by Bates and Damgaard (1949) to calculate the oscillator strength (see Appendix B). It is based on the fact that for most transitions, the main contribution to the radial matrix element comes from a region in which the deviation of the potential of an atom or ion from its asymptotic Coulomb form is so small that the deviation can altogether be neglected and the potential replaced by its asymptotic Coulomb form. This method gives satisfactory results for transitions in He I (Bates and Damgaard, 1949). For transitions between unresolved levels and between resolved and unresolved levels, hydrogenic formula was used to calculate the oscillator strength (Kramers, 1923).

$$f_{n',n} = \frac{2^2}{3\sqrt{3}\pi\omega'_{n'}} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right)^{-3} \left(\frac{1}{n^3 n'^3} \right) g_I(n', n) \quad (2-11)$$

where $\omega'_{n'}$ is the statistical weight of the level n' , and $g_I(n', n)$ is the bound-bound Kramers-Gaunt factor. Analytic form for $g_I(n', n)$ has been given by Menzel and Pekeris (1935),

$$g_I(n, n') = \frac{\pi\sqrt{3}[(n - n')/(n + n')]^{2n+2n'} n n'}{(n - n')} |\Delta(n, n')| \quad (2-12)$$

where

$$\Delta(n, n') = \left[{}_2F_1 \left(-n + 1, -n; 1; \frac{-4nn'}{(n - n')^2} \right) \right]^2 - \left[{}_2F_1 \left(-n' + 1, -n; 1; \frac{-4nn'}{(n - n')^2} \right) \right]^2 \quad (2-13)$$

and the ${}_2F_1$ are hypergeometric functions.

For the optically forbidden transition, $1^1S \rightarrow 2^3P$, the calculated transition probability by Garstang (1967) was adopted, while experimental values are used for $1^1S \rightarrow 2^1S$ (van Dyck et al., 1970) and for $1^1S \rightarrow 2^3S$ (Moos et al., 1973).

(c) *Collisional excitation and de-excitation rate coefficients.*

The rate coefficient for collisional excitation of the $n'\ell' \rightarrow n\ell$ transition by electron impact is given by

$$C_{n'\ell',n\ell} = \int_v \sigma_{n'\ell',n\ell}(v) v f(v) dv \quad (2-14)$$

where v is the velocity and $f(v)$ the velocity distribution of the incident electrons. Using the Maxwellian velocity distribution

$$\frac{dn_e}{n_e} = f(v) dv = \frac{4v^2}{\sqrt{\pi}(2kT/m)^{3/2}} e^{-\frac{mv^2}{2kT}} dv \quad (2-15)$$

and expressing Equations (2-14) and (2-15) in terms of the kinetic energy E of the incident electron, we obtain

$$C_{n'\ell',n\ell} = \frac{1}{\sqrt{\pi m}} \left(\frac{2}{kT} \right)^{3/2} \int_E \sigma_{n'\ell',n\ell}(E) E e^{-\frac{E}{kT}} dE \quad (2-16)$$

with threshold energy units $U = E/E_{n'\ell',n\ell}$, Equation (2-16) becomes

$$C_{n'\ell',n\ell} = \sqrt{\frac{8}{\pi m k^3}} \frac{E_{n'\ell',n\ell}}{T^{3/2}} \int_1^\infty \sigma_{n'\ell',n\ell}(U) e^{-\frac{E_{n'\ell',n\ell}}{kT} U} U dU \quad (2-17)$$

where $E_{n'\ell',n\ell}$ is the threshold energy for the excitation of the $n'\ell' \rightarrow n\ell$ transition in Rydberg.

A very large number of excitation cross sections is required in this work. Unfortunately, the available data are but a very small fraction of the required cross sections. Most of the available data from theoretical calculations and experimental work are on the excitation from the ground state and low lying excited states. For all of the cross sections for which data exist the best experimental and theoretical data were fitted to semi-empirical formulas.

For allowed transitions between low-lying levels, the modified form of the Drawin formula (1963, 1964, 1967) proposed by Millette and Varshni (1980) was used:

$$\sigma_{n'\ell',n\ell}(U) = 4\pi a_0^2 \alpha \frac{f_{n'\ell',n\ell}}{E_{n'\ell',n\ell}^2} \frac{U - \phi}{U^2} \ln(1.25\beta U), \quad (2-18)$$

$f_{n'\ell',n\ell}$ is the absorption oscillator strength, α , β and ϕ are the fitting parameters which depend on the transition. This formula was fitted to the following cross sections:

$1^1S \rightarrow 2^1P$ and $1^1S \rightarrow 3^1P$: Experimental cross sections of Westerveld *et al.* (1979).

$1^1S \rightarrow 4^1P$: Experimental cross sections of Donaldson *et al.* (1972).

$1^1S \rightarrow 5^1P$: Experimental cross sections of Moustafa Moussa *et al.* (1969).

$2^1S \rightarrow 2^1P$ and $2^3S \rightarrow 2^3P$: Theoretical cross sections of Burk *et al.* (1969).

$2^1S \rightarrow 3^1P$: Theoretical cross sections of Flannery and McCann (1975).

$2^1S \rightarrow 4^1P$: Theoretical cross sections of Flannery *et al.* (1974).

$2^3S \rightarrow 3^3P$, $2^3S \rightarrow 4^3P$ and $2^3S \rightarrow 5^3P$: Theoretical cross sections of Ton-That *et al.* (1977).

We used the least squares method in fitting these data to Equation (2-18). The sum of the square of the relative differences between the actual and the fit values of the cross sections is minimized with respect to the fit parameters. The resulting minimization conditions are non-linear equations in the parameters α , β , and ϕ for Equation (2-18). These equations are solved by an iterative procedure. The fitting parameters α , β and ϕ of the above allowed transitions are given in Table 2-2.

For the remaining allowed transitions with $\Delta n \leq 3$, the excitation cross sections were calculated from the semi-classical impact parameter theory (IP) developed by Seaton (1962) for neutrals and later extended to ions by Burgess (1964a). The cross section is defined as:

$$\sigma_{n'\ell',n\ell} = \int P_{n'\ell',n\ell}(R) 2\pi R dR \quad (2-19)$$

where $P_{n'\ell',n\ell}(R)$ is the probability that the incident (perturbing) electron with impact parameter R will induce in the emitter a transition from the state $n'\ell'$ to $n\ell$. The integration is extended over all impact parameters. In this formalism, the $P_{n'\ell',n\ell}(R)$ are symmetrized to ensure reciprocity [$P_{n'\ell',n\ell}(R_{n'\ell'}) = P_{n'\ell',n\ell}(R_{n\ell})$] at low energies and adjusted to corre-

spond with the Born approximation at high energies.

At small impact parameters, the integral in Equation (2-19) diverges vitiating the perturbation treatment. Therefore, it is necessary to introduce a cutoff parameter R_0 , of the order of atomic dimensions, independent of perturber energy but subject to the constraint $P_{n'\ell',n\ell}(R_0) \leq 1$. This procedure yields good results in the weak coupling case (Davis and Roberts, 1968), i.e. when the interaction matrix element $R_{n'\ell',n\ell}$ is small. When the interaction causes strong coupling, a new cutoff $R_1 > R_0$ and weakly dependent on perturber energy is chosen so that $P_{n'\ell',n\ell}(R \leq R_1) = \frac{1}{2}$.

The cross section in the weak coupling case is given by (Roberts and Davis, 1968)

$$\sigma_{n'\ell',n\ell} = \frac{8\pi}{3} \left(\frac{h}{2\pi m} \right)^2 \frac{R_{n'\ell',n\ell}}{v_i^2} Y(\zeta, \delta_0) \quad (2-20)$$

where

$$\delta_0 = |v_i - v_f| R_0 \frac{h}{2\pi e^2} \quad (2-21)$$

$$\zeta = \left| \frac{1}{v_i} - \frac{1}{v_f} \right| \frac{2\pi z e^2}{h} \quad (2-22)$$

and

$$R_{n'\ell',n\ell} = \frac{S_{n'\ell',n\ell}}{\omega_{n'\ell'}} \quad (2-23)$$

$R_{n'\ell',n\ell}$ is the dipole matrix element connecting state $n'\ell'$ and $n\ell$, $\omega_{n'\ell'}$ is the statistical weight of the state $n'\ell'$, $S_{n'\ell',n\ell}$ is the line strength, z is the initial charge number of ion ($z = 0$ for neutral, $=1$ for He II etc.). ζ is a symmetrizing parameter which accounts approximately for the back reaction, the function $Y(\zeta, \delta_0)$ is given by Burgess (1964a),

$$Y(\zeta, \delta) = \exp(\pi\zeta) K_{i\zeta}(\zeta + \delta) K'_{i\zeta}(\zeta + \delta) (\zeta + \delta) \quad (2-24)$$

The initial and final velocities, v_i and v_f , are related by the energy conservation condition, [i.e. $\frac{1}{2}mv_f^2 = \frac{1}{2}mv_i^2 - \Delta E$, where ΔE is the energy separation between levels $n'\ell'$

and $n\ell$], and set R_o equal to the average mean radius of the state $n'\ell'$ or $n\ell$, whichever is the smaller. It is taken as

$$R_o = \frac{3n_\ell^{*2} - \ell(\ell+1)}{2(z+1)} \quad (2-25)$$

for resolved state, and for unresolved state it is taken as

$$R_o = \frac{5n^{*2} + 1}{4(z+1)} \quad (2-26)$$

where n^* is the effective principal quantum number. R_o is measured in atomic units.

For those cases where strong coupling applies, the cross section is obtained from:

$$\sigma_{n'\ell',n\ell} = \pi \left(\frac{h}{2\pi m} \right)^2 \frac{1}{v_i^2} \left[\frac{8}{3} R_{n;\ell',n\ell} Y(\zeta, \delta_1) + zR_1 + \frac{1}{2} \left(\frac{h}{2\pi e^2} \right)^2 v_i v_f R_1^2 \right] \quad (2-27)$$

where R_1 is the strong collision cutoff in atomic units. The cutoff R_1 is chosen so that:

$$\frac{8}{3} R_{n;\ell',n\ell} \frac{4\pi^2 e^4}{h^2} \frac{v_i v_f}{\left(\frac{4\pi^2 z e^2}{h^2} + v_i v_f R_1 \right)^2} X(\zeta, \delta_1) = 1 \quad (2-29)$$

where the function $X(\zeta, \delta_1)$ is given by Burgess and Summers (1976),

$$X(\zeta, \delta) = \exp(\pi\zeta) (\zeta + \delta)^2 \left(K_{i\zeta}'^2(\zeta + \delta) + \left(1 - \frac{\zeta^2}{(\zeta + \delta)^2} \right) K_{i\zeta}^2(\zeta + \delta) \right) \quad (2-30)$$

$K_{i\zeta}$ and $K_{i\zeta}'$ are modified Bessel functions of the second kind and the prime denotes a derivative with respect to the argument.

TABLE 2-2. Fit parameters for the cross sections of the allowed transitions (Eq. 2-18) of He I.

Transition	α	β	ϕ
$1s^2 \ ^1S \rightarrow 1s2p \ ^1P$	0.948	0.812	0.882
$1s^2 \ ^1S \rightarrow 1s3p \ ^1P$	1.00	0.891	0.961
$1s^2 \ ^1S \rightarrow 1s4p \ ^1P$	1.030	0.901	0.880
$1s^2 \ ^1S \rightarrow 1s5p \ ^1P$	1.05	0.870	1.00
$1s2s \ ^1S \rightarrow 1s2p \ ^1P$	0.30	6.380	0.65
$1s2s \ ^1S \rightarrow 1s3p \ ^1P$	0.27	0.800	0.903
$1s2s \ ^1S \rightarrow 1s4p \ ^1P$	0.28	0.800	0.79
$1s2s \ ^3S \rightarrow 1s2p \ ^3P$	0.27	6.710	0.570
$1s2s \ ^3S \rightarrow 1s3p \ ^3P$	0.21	1.00	0.294
$1s2s \ ^3S \rightarrow 1s4p \ ^3P$	0.20	1.150	0.380
$1s2s \ ^3S \rightarrow 1s5p \ ^3P$	0.20	1.17	0.430

TABLE 2-3. Fit parameters for the cross sections of the forbidden transitions (Eq. 2-32) without change in spin of He I.

Transition	α	ϕ
$1s^2 \ ^1S \rightarrow 1s2s \ ^1S$	0.130	0.80
$1s^2 \ ^1S \rightarrow 1s3s \ ^1S$	0.32	0.82
$1s^2 \ ^1S \rightarrow 1s4s \ ^1S$	0.330	0.85
$1s^2 \ ^1S \rightarrow 1s5s \ ^1S$	0.31	0.86
$1s^2 \ ^1S \rightarrow 1s3d \ ^1D$	0.172	0.24
$1s^2 \ ^1S \rightarrow 1s4d \ ^1D$	0.26	0.86
$1s^2 \ ^1S \rightarrow 1s5d \ ^1D$	0.290	0.88
$1s^2 \ ^1S \rightarrow 1s4f \ ^1F$	0.92×10^{-3}	1.00
$1s^2 \ ^1S \rightarrow 1s5f \ ^1F$	0.15×10^{-3}	1.00
$1s2s \ ^1S \rightarrow 1s3s \ ^1S$	0.57	0.71
$1s2s \ ^1S \rightarrow 1s3d \ ^1D$	1.62	0.66
$1s2s \ ^3S \rightarrow 1s3s \ ^3S$	0.51	0.68
$1s2s \ ^3S \rightarrow 1s4s \ ^3S$	0.32	0.66
$1s2s \ ^3S \rightarrow 1s5s \ ^3S$	0.27	0.68
$1s2s \ ^3S \rightarrow 1s3d \ ^3D$	1.15	0.72
$1s2s \ ^3S \rightarrow 1s4d \ ^3D$	0.81	0.64
$1s2s \ ^3S \rightarrow 1s5d \ ^3D$	0.70	0.64
$1s2s \ ^3S \rightarrow 1s4f \ ^3F$	0.12	0.50
$1s2s \ ^3S \rightarrow 1s5f \ ^3F$	0.80×10^{-2}	0.50

In practice, both the weak and strong coupling cross sections are evaluated for a particular transition and the smaller of the two is adopted.

For transitions with $\Delta n > 3$, we used the the effective Gaunt factor or $\bar{g}$ approximation developed by Van Regemorter (1962) for calculating the cross sections. In this approximation, the cross section for excitation of an ion or atom from state $n'\ell'$ to state $n\ell$ is given by the simple expression

$$\sigma_{n'\ell',n\ell} = \frac{8\pi}{\sqrt{3}} \frac{1}{E} \frac{f_{n'\ell',n\ell}}{E_{n'\ell',n\ell}} \bar{g}(E) \quad (\text{in units of } \pi a_0^2) \quad (2-31)$$

E and $E_{n'\ell',n\ell}$ are the incident electron energy and the energy separation between levels $n'\ell'$, and $n\ell$, respectively, and $f_{n'\ell',n\ell}$ is the absorption oscillator strength for the transition. $\bar{g}$ is the effective Gaunt factor (Van Regemorter, 1962, gives a simple expressions for $\bar{g}$).

For optically forbidden transitions without change in spin, we used the modified form of Drawin, proposed by Millette and Varshni (1980):

$$\sigma_{n'\ell',n\ell}(U) = 4\pi a_0^2 (n'/n)^3 \frac{\alpha}{E_{n'\ell',n\ell}^2} \frac{U - \phi}{U^2}, \quad (2-32)$$

where the symbols have their usual meaning. This formula was fitted to the following cross sections:

$1^1S \rightarrow 2^1S$: Experimental cross sections of Rice *et al.* (1972).

$1^1S \rightarrow 3^1S, 1^1S \rightarrow 3^1D, 1^1S \rightarrow 4^1D$ and $1^1S \rightarrow 5^1D$: Experimental cross sections of Moustafa Moussa *et al.* (1969).

$1^1S \rightarrow 4^1S$: Experimental cross sections of Van Rann *et al.* (1971).

$1^1S \rightarrow 5^1S$: Experimental cross sections of Pochat *et al.* (1972).

$2^1S \rightarrow 3^1S$ and $2^1S \rightarrow 3^1D$: Theoretical cross sections of Flannery and McCann (1975).

$2^3S \rightarrow 3^3S$: Theoretical cross sections of Khayrallah *et al.* (1978).

$2^3S \rightarrow 3^3D, 2^3S \rightarrow 4^3S, 2^3S \rightarrow 4^3D, 2^3S \rightarrow 4^3F, 2^3S \rightarrow 5^3S, 2^3S \rightarrow 5^3D$ and $2^3S \rightarrow 5^3F$:
Theoretical cross sections of Ton-That et al. (1977).

$1^1S \rightarrow 4^1F$: Theoretical cross sections of Van den Bos (1969).

$1^1S \rightarrow 5^1F$: Theoretical cross sections of Moiseiwitsch and Smith (1968).

The fitting parameters α and ϕ for above transitions are given in Table 2-3.

For other optically forbidden transitions without change in spin between levels with $n \leq 8$ cross sections were calculated using the symmetrized binary encounter theory (Burgess, 1964a,b). The basic idea of the binary-encounter collision theory is that excitation of atoms by electrons is described approximately as a collision between two free electrons. In the derivation of cross section formulas it is further assumed that the atomic electrons initially have an isotropic velocity direction distribution with one constant magnitude of the velocity. This theory has been developed by Thomson (1912) and Gryziński (1959). Mathematical corrections and discussions of the theory are given by Stabler (1964) and Vriens (1964a,b).

Burgess (1964a,b) introduced a new model with a symmetrical treatment of the two interacting electrons; the binary encounter may be treated as a quantum mechanical collision between identical particles with proper symmetrization and treatment of interference between direct and exchange scattering. The initial and final atomic states are treated classically in terms of an orbiting electron with definite initial and final kinetic energy, the change in kinetic energy being related to the angle of scattering. Burgess also allowed for the acceleration of the incident electron in the same way as Thomas (1927), the kinetic energy of the incident electron before the binary encounter being set equal to $E_1 + E_2 + U$, where E_1 is the initial kinetic energy of the incident electron, E_2 is the initial kinetic energy of the atomic electron, and U is the ionization energy. In this way, Burgess showed that cross sections for direct and exchange excitation could be calculated, together with the ef-

fect of interference between direct and exchange scattering. Vriens (1966) obtained simpler formulas for the cross section than those Burgess has given, using the same transformations in Burgess's collision model,

$$\sigma(\varepsilon_1, \varepsilon_2) = (\sigma_d + \sigma_{ex} + \sigma_{int}) F \quad (2-33)$$

where σ_d is the cross section for direct excitation,

$$\sigma_d = \frac{\pi e^4}{E_1 + E_2 + U} \left[\frac{1}{\varepsilon_1} - \frac{1}{\varepsilon_2} + \frac{2E_2}{3} \left(\frac{1}{\varepsilon_1^2} - \frac{1}{\varepsilon_2^2} \right) \right] \quad (2-34)$$

σ_{ex} is the cross section for exchange excitation,

$$\begin{aligned} \sigma_{ex} = \frac{\pi e^4}{E_1 + E_2 + U} & \left[\frac{1}{E_1 + U - \varepsilon_2} - \frac{1}{E_1 + U - \varepsilon_1} \right. \\ & \left. + \frac{2E_2}{3} \left(\frac{1}{(E_1 + U - \varepsilon_2)^2} - \frac{1}{(E_1 + U - \varepsilon_1)^2} \right) \right] \end{aligned} \quad (2-35)$$

σ_{int} gives the influence of interference between direct and exchange scattering:

$$\sigma_{int} = -\frac{\pi e^4}{E_1 + E_2 - U} \frac{1}{E_1 + U} \ln \left[\frac{(E_1 + U - \varepsilon_1)\varepsilon_2}{\varepsilon_1(E_1 + U - \varepsilon_2)} \right] \quad (2-36)$$

F is the focussing factor, which was introduced by Burgess (1964a,b) to account for electron-positive ion collision, and is given by

$$F = 1 + (ze^4/E_1\bar{r}) \quad (2-37)$$

where $\bar{r}$ is the mean radius and z is the charge number of the ion.

Equations (2-34)-(2-36) are valid for $E_1 \geq \varepsilon_2$, while ε_2 should be replaced by E_1 for $\varepsilon_1 \leq E_1 \leq \varepsilon_2$. The appropriate classical energy band specified by ε_1 and ε_2 is not well defined; in this calculations ε_1 has been taken as the excitation energy of the transition

$n'\ell' \rightarrow n\ell$ and ε_2 as the excitation energy to the next higher level with the same L or S (Cacciatore and Capitelli, 1976).

For optically forbidden transitions with change in spin, we used the following semi-empirical formula:

$$\sigma_{n'\ell',n\ell} = 4\pi a_0^2 (n'/n)^3 \frac{1}{E_{n'\ell',n\ell}^2} \left(\alpha \frac{U^2 - \phi}{U^k} + \frac{\beta}{\sqrt{U}} \right), \quad (2-38)$$

where the symbols have their usual meaning. $k = 5$ in all cases except for $2^1S \rightarrow 2^3P$, $2^3S \rightarrow 2^1P$ and $2^3S \rightarrow 2^1S$ transitions, for which k was taken equal to 3. This formula was fitted to the following cross sections :

$1^1S \rightarrow 2^3P$: Experimental cross sections of Jobe and St-John (1967).

$1^1S \rightarrow 2^3S$: Theoretical cross sections of Lin de Barros et al.(1975).

$1^1S \rightarrow 3^3S$, $1^1S \rightarrow 4^3S$, $1^1S \rightarrow 5^3S$, $1^1S \rightarrow 3^3P$, $1^1S \rightarrow 4^3P$, $1^1S \rightarrow 5^3P$, $1^1S \rightarrow 3^3D$ and

$1^1S \rightarrow 4^3D$: Experimental cross sections of Moustafa Moussa et al.(1969).

$2^3S \rightarrow 2^1P$, $2^3S \rightarrow 2^1S$ and $2^1S \rightarrow 2^3P$: Theoretical cross sections of Burk et al. (1969).

The fitting parameters α , β and ϕ of the above transitions are given in Table 2-4.

We calculated the rate coefficient for other forbidden transitions with change in spin between $n \leq 8$, using the expression given by Summers (1977). He deduced this expression from symmetrized classical binary encounter theory (Burgess, 1964a,b; Vriens 1966; Burgess and Percival 1968). Transitions with change in spin occur via the exchange part in which the incident electron is captured and the bound escapes. In such collisions, the binary encounter between the incident and the target electrons must be energetic, since, for exchange an energy greater than that of the ionization energy must be transferred between the two electrons. Consequently classical theory is likely to be a reasonable approximation for such a collision. The rate coefficient for an energy transfer in the range ε_1 to ε_2 is given by

$$q(\varepsilon_1 \rightarrow \varepsilon_2) = 8\sqrt{\pi}\alpha c a_0^2 \left(\frac{I_H}{kT_e}\right)^{3/2} \begin{cases} e^{-\frac{\varepsilon_2}{kT_e}} p(\varepsilon_2) - e^{-\frac{\varepsilon_1}{kT_e}} p(\varepsilon_1) & \text{for } \varepsilon_1, \varepsilon_2 > 0 \\ e^{-\frac{\varepsilon_2}{kT_e}} p(\varepsilon_2) - p(\varepsilon_1) & \text{for } \varepsilon_1 < 0, \varepsilon_2 > 0 \\ p(\varepsilon_2) - p(\varepsilon_1) & \text{for } \varepsilon_1, \varepsilon_2 < 0 \end{cases} \quad (2-39)$$

where

$$p(\varepsilon) = \begin{cases} \left(\frac{u}{|\varepsilon|} + 1\right) EEI\left(\frac{u+|\varepsilon|}{kT_e}\right) - \left(\frac{u}{|\varepsilon|} - 1\right) EEI\left(\frac{u}{kT_e}\right) - \frac{kT_e}{u} & \text{for } \varepsilon \neq 0 \\ \left(2 + \frac{u}{kT_e}\right) EEI\left(\frac{u}{kT_e}\right) - \left(1 + \frac{kT_e}{u}\right) & \text{for } \varepsilon = 0 \end{cases} \quad (2-40)$$

In these formula $EEI(x) = e^x E_1(x)$, where $E_1(x)$ is the exponential integral. Summers defined the classical energy band specified by ε_1 and ε_2 as

$$\varepsilon_2 - \varepsilon_1 = zI_H \left(\frac{1}{(n'^* - 1/2)^2} - \frac{1}{(n'^* + 1/2)^2} \right) \quad (2-41)$$

where I_H is the ionization of hydrogen, z is the initial charge number of ion, and n'^* is the effective principal quantum numbers.

Using these formula into different spin systems is a matter of some uncertainty (Burgess, 1964b). Summers (1977) introduced an approximate way to correct for the change in spin, he considered that the fractions of the finally bound electron leaving the spin system unchanged or changed will be proportional to the overlap of the final state wave function with LS coupled eigenstates, assuming no phase correlation. Thus, Summers obtained the following expression

$$C_{n'\ell',n\ell} = \frac{5}{12} \frac{\omega_{n\ell}}{\omega_p} \left| \eta_{n\ell}^{n'\ell'} \right|^2 q(\varepsilon_1 \rightarrow \varepsilon_2) \quad \text{for } s \neq s' \quad (2-42)$$

where

$$\left| \eta_{n\ell}^{n'\ell'} \right|^2 = \frac{\int_0^\infty \frac{|P_{n'\ell'} P_{n\ell}|^2}{r^2} dr}{\left\{ \sum_{\ell''} (2\ell'' + 1) \int_0^\infty \frac{|P_{n'\ell'} P_{n\ell''}|^2}{r^2} dr \right\}} \quad (2-43)$$

$(1/r)P_{n\ell}$ is the bound radial wave function, and ω_p is the statistical weight of the parent ion. Hydrogenic wave function are used in evaluating $\eta_{n\ell}^{n'\ell'}$.

The rate coefficients for de-excitation of a bound electron from state $n\ell$ to $n'\ell'$ by electron impact are calculated from the principle of detailed balance (Drawin, 1963)

$$C_{n\ell, n'\ell'} = \frac{\omega_{n'\ell'}}{\omega_{n\ell}} e^{E_{n'\ell', n\ell}/kT_e} C_{n'\ell', n\ell} \quad (2-44)$$

where $E_{n'\ell', n\ell}$ is the energy separation of levels $n'\ell'$ and $n\ell$, $\omega_{n'\ell'}$ and $\omega_{n\ell}$ are the statistical weights of the states $n'\ell'$ and $n\ell$, respectively.

(d) Ionization and three-body recombination rate coefficients.

The rate coefficient of the ionization by electron impact is obtained by integrating the cross section over the free electron velocity distribution, $f(v)$:

$$S_{n\ell} = \int_v \sigma_{n\ell}(v) v f(v) dv. \quad (2-45)$$

Using Equation (2-11), we obtain

$$S_{n\ell} = 2\sqrt{\frac{2}{\pi m}} \frac{I_{n\ell}^2}{(kT_e)^{3/2}} \int_1^\infty \sigma_{n\ell}(U) U e^{-\frac{I_{n\ell}}{kT_e} U} dU, \quad (2-46)$$

where $I_{n\ell}$ is the ionization potential, and the other symbols have their usual meaning.

Experimental cross section data are available only for 1^1S (Rapp et al., 1965) and 2^3S (Dixon et al., 1976) levels, and the theoretical cross sections for 2^1S (Ton-That et al., 1977). These were fitted to the semi-empirical formula (Drawin, 1967):

$$\sigma_{n\ell}(U) = 2.66\pi a_0^2 \alpha \frac{\xi}{E_{n\ell}^2} \frac{U-1}{U^2} \ln(1.25\beta U), \quad (2-47)$$

The numerical value of ξ for ionization from the ground state is given by Drawin (1967), for $n > 1$, $\xi = 1$, α and β are fitting parameters, and the other symbols have their

usual meaning. The cross sections for other levels were calculated using this formula with $\alpha = 1$, and β determined from the following expression (Drawin, 1967)

$$\beta_s = 1 + \frac{z_{eff} - 1}{z_{eff} + 2} \quad (2-48)$$

z_{eff} denotes the effective charge number of the nucleus acting on the electron.

The rate for three-body recombination of a free electron into state $n\ell$ of an atom or ion is obtained from the principle of detailed balance

$$\alpha_{n\ell} = \frac{h^3}{(2\pi mkT_e)^{3/2}} \frac{\omega_{n\ell}}{2u_i} e^{I_{n\ell}/kT_e} S_{n\ell} \quad (2-49)$$

where $I_{n\ell}$ is the ionization potential, u_i is the partition function of the ion before recombination, and $\omega_{n\ell}$ is the statistical weight of state $n\ell$.

(c) Radiative recombination.

The radiative recombination rate coefficient is obtained from the photoionization cross section by applying the principle of detailed balancing. The rate coefficient is then given by

$$\beta_{n\ell} = \frac{1}{c^2} \sqrt{\frac{2}{\pi}} (mkT_e)^{-3/2} \frac{\omega_{n\ell}}{\omega_i} e^{I_{n\ell}/kT_e} \int_{I_{n\ell}}^{\infty} (h\nu)^2 \sigma_{n\ell}(\nu) e^{-\frac{h\nu}{kT_e}} d(h\nu) \quad (2-50)$$

where ω_i is the statistical weight of the parent ion, and the other symbols have their usual meaning. Using threshold energy units, Equation (2-50) becomes

$$\beta_{n\ell} = \frac{1}{c^2} \sqrt{\frac{2}{\pi}} (mkT_e)^{-3/2} \frac{\omega_{n\ell}}{\omega_i} e^{I_{n\ell}/kT_e} I_{n\ell}^3 \int_1^{\infty} U^2 \sigma_{n\ell}(U) e^{-\frac{I_{n\ell}}{kT_e} U} d(U) \quad (2-51)$$

The tables by Marr and West (1976) give the recommended experimental photoionization cross sections from the ground state, and the theoretical cross sections of Jacobs(1973)

have been used for the levels 2^1S , 2^3S , 2^1P and 2^3P . These cross sections were fitted to a semi-empirical formula suggested by Millette and Varshni (1980),

$$a_{n\ell}(U) = \frac{C}{U^p} \left[1 + \frac{a_1}{U} + \frac{a_2}{U^2} + \dots + \frac{a_m}{U^m} \right], \quad (2-52)$$

where C and a_k , $k = 1, \dots, m$ are fitting parameters given in Table 2-5, and U is the energy of the incident photon in threshold unit.

Hydrogenic approximation was adopted to calculate the photoionization cross sections for other levels; the cross section being given by

$$a_{n\ell}(\nu) = 2.815 \times 10^{29} \frac{g_{II}(n, \nu)}{n^5 \nu^3} \quad (2-53)$$

where $g_{II}(n, \nu)$ is the Gaunt-factor, it can be approximated by the expression (Seaton, 1959)

$$g_{II}(n, \nu) = 1 + \frac{0.1728(U_n - 1)}{n^{2/3}(U_n + 1)^{2/3}} - \frac{0.0496(U_n^2 + \frac{4}{3}U_n + 1)}{(U_n + 1)^{4/3}} + \dots \quad (2-54)$$

where U_n is the threshold energy of the state $n\ell$.

TABLE 2-4. Fit parameters for the cross sections of the forbidden transitions (Eq. 2-38) with change in spin of He I.

Transition	α	β	ϕ
$1s^2 \ ^1S \rightarrow 1s2s \ ^3S$	1.190	0.65×10^{-2}	1.00
$1s^2 \ ^1S \rightarrow 1s3s \ ^3S$	0.82	0.67×10^{-2}	1.00
$1s^2 \ ^1S \rightarrow 1s4s \ ^3S$	0.740	0.30×10^{-2}	0.80
$1s^2 \ ^1S \rightarrow 1s5s \ ^3S$	0.60	0.40×10^{-2}	1.00
$1s^2 \ ^1S \rightarrow 1s2p \ ^3P$	0.440	-0.120×10^{-2}	0.77
$1s^2 \ ^1S \rightarrow 1s3p \ ^3P$	1.17	0.260×10^{-2}	1.00
$1s^2 \ ^1S \rightarrow 1s4p \ ^3P$	1.100	0.460×10^{-2}	1.00
$1s^2 \ ^1S \rightarrow 1s5p \ ^3P$	1.13	0.460×10^{-2}	1.00
$1s^2 \ ^1S \rightarrow 1s3d \ ^3D$	0.15	0.530×10^{-2}	1.00
$1s^2 \ ^1S \rightarrow 1s4d \ ^3D$	0.14	0.40×10^{-2}	1.00
$1s2s \ ^1S \rightarrow 1s2p \ ^3P$	0.03	0.0	1.00
$1s2s \ ^3S \rightarrow 1s2p \ ^1P$	0.024	0.0	0.98
$1s2s \ ^3S \rightarrow 1s2s \ ^1S$	0.10	0.0	1.00

TABLE 2-5. Fit parameters for the photoionization cross sections (Eq. 2-52) of He I.

State	p	m	C	a_1	a_2	a_3	a_4
$1s^2 \ ^1S$	0.0	4	0.0386	-35.88	366.44	-205.89	69.64
$1s2s \ ^1S$	0.5	1	-0.99	-9.91			
$1s2s \ ^3S$	2.0	1	12.26	-0.58			
$1s2p \ ^1P$	1.0	2	0.14	-20.68	119.91		
$1s2s \ ^3P$	0.5	2	0.13	-18.19	122.99		

D) Results and Discussion

The initial density of helium atoms before expansion was taken to be $1 \times 10^{14} \text{ cm}^{-3}$. Calculations were carried out for the population densities of 62 levels of He I for a grid of n_e and T_e values.

Population inversion of varying degrees was found to occur for a great many transitions, including several between $n = 4$ and $n = 3$, for appropriate values of n_e and T_e . However, most of them either fall in the infra-red region or else the population inversion is not very large. Two transitions which show large population inversion and which fall in the visible region are $3^1\text{S} \rightarrow 2^1\text{P}^o(\lambda 7281)$, and $3^1\text{D} \rightarrow 2^1\text{P}^o(\lambda 6678)$. To show the pattern of the results, we also include the next member of these two serieses, $4^1\text{S} \rightarrow 2^1\text{P}^o(\lambda 5047)$, and $4^1\text{D} \rightarrow 2^1\text{P}^o(\lambda 4922)$. We present the results for these four transitions. The population inversion is often measured in terms of P , where P is given by

$$P = N_k/\omega_k - N_i/\omega_i, \quad (2-55)$$

where N_i and N_k are the atomic populations of the lower and upper levels, and ω_i and ω_k are the respective statistical weights. P is sometime called the 'overpopulation density' (Oda and Furukane, 1983). P is related to the fractional gain per unit distance, α , at the centre of a Doppler-broadened line by the following expression (cf. Willett, 1974)

$$\alpha = \left(\frac{\ln 2}{\pi} \right)^{1/2} \left[\frac{\omega_k A_{ki}}{4\pi} \right] \frac{P \lambda_o^2}{\Delta\nu}, \quad (2-56)$$

where λ_o is the centre wavelength of the transition, and $\Delta\nu$ is the linewidth. α describes the intensity of a plane wave at λ_o according to

$$I = I_o e^{\alpha l}, \quad (2-57)$$

where l is the length over which gain occurs.

In Figures 2-1 to 2-4 we show the variation of P with n_e for some typical values of T_e for the four transitions under consideration. From such plots, contours of equal P on a n_e, T_e diagram were made and the results are shown in Figures 2-5 to 2-8. It will be noticed that in all the four cases, strong population inversion occurs only in a small region. The magnitude of maximum population inversion for $\lambda 5048$ and $\lambda 4922$ is seen to be much smaller than that for $\lambda 7281$ and $\lambda 6678$. Thus the latter two lines are the most promising lines for undergoing laser action by the rapid cooling through expansion mechanism. Further it will be noticed (Figures 2-5 and 2-7) that there is a considerable overlap in the regions of maximum population inversion for the two lines. If we assume $\Delta\nu$ to be the same for both the transitions, the gain factor α is proportional to $\omega_k A_{ki} P \lambda_o^2$. For a point common to the maximum population inversion regions for the two lines, we have $P(6678) \simeq 3 \times 10^5 \text{ cm}^{-3}$ and $P(7281) \simeq 1 \times 10^6 \text{ cm}^{-3}$. With these values we find that $\alpha(6678)/\alpha(7281) \simeq 4.4$. Thus, though $P(6678)$ is less than $P(7281)$, the $\lambda 6678$ line would be much stronger than $\lambda 7281$. It is of some interest to note (Figures 2-6 and 2-8) that for $\lambda 5048$ and $\lambda 4921$ also there is considerable overlap in the regions of maximum population inversion. Here we wish to emphasize that the calculations that we have presented are for a simple model and strong laser action, in lines other than $\lambda 6678$ and $\lambda 7281$ is feasible through other mechanisms, for instance, by interaction with an ambient gas (Gudzenko et al. 1974, 1975; Otsuka, 1980). We then turn our attention to the observational evidence concerning these four lines in the spectra of Wolf-Rayet and allied objects.

Emission bands at 4922 and 6678 Å have been known for many years (Plaskett, 1924; Payne, 1933) in Wolf-Rayet spectra. Swings (1942) observed the spectra of several Wolf-Rayet stars; he lists the wavelengths for two of these. Swings and Jose (1950) observed the spectra of seven Wolf-Rayet stars in the range $\lambda\lambda 6500 - 8800$. Smith (1955) observed

a large number of southern Wolf-Rayet stars, some in the range $\lambda 4000 - \lambda 6800$, and some in $\lambda 3600 - \lambda 6800$. He lists the wavelengths and intensities of lines for a few of these stars. The results of Swings (1942), Swings and Jose (1950), and Smith (1955) with respect to the four lines under consideration are summarized in Table 2-6.

Andrillat (1957) carried out an extensive investigation of the spectra of WR stars in the red and near infra-red regions. Her study covers the following categories of stars: four WC6 type, three WC7 type, one planetary nucleus of WC7 type, two planetary nuclei of WC8 type, eight WN5 type, six WN6 type, two WN7 type, and one WN8 type. He I $\lambda 6678$ is present in many of these, but $\lambda 7281$ appears to be absent.

For HD 192103, WC7, Underhill (1959) summarizes as follows: "The first three members of the 2^1P-n^1D series, $\lambda\lambda 6678, 4921$ and 4388 appear in emission. There is some evidence for the leading member of the 2^1P-n^1S series, $\lambda 5047$, in emission...". In HD 192163, WN6, Underhill (1959) found that $\lambda 6678, \lambda 4922$ and $\lambda 4388$ may be present weakly in emission.

For HD 191769, WN6, Underhill (1967) states: "The leading member, $\lambda 6678$, blends with He II $\lambda 6683$; $\lambda 4922$ may be present but the present spectra are inadequate here."

Cohen et al. (1975) have published the spectra of two WC9 stars in the range $\lambda\lambda 5650 - 7350$ and another two WC9 stars in the range $\lambda\lambda 5650 - 6770$. He I $\lambda 6678$ is of medium strength; $\lambda 7281$ appears to be quite weak.

Bromage and Nandy (1973) have obtained the spectrum of a WN5 star, Cyg OB2 No. WR2, in the wavelength range 5650 to 6850 Å. The micro-densitometer tracing shows a strong He I $\lambda 6678$, with a width of 1350 km s^{-1} .

From the foregoing summary, we find that there are three stars, HD 143414, HD 50896, and Cyg OB2 WR2, which show unusually strong $\lambda 6678$. The relative intensities of the four lines, that we are considering, amongst themselves and in relation to other He I

lines in other stars (for which data are summarized above) do not seem to show a strong departure from the laboratory values and we shall not consider these stars further. There is one possible complication in the strength of the $\lambda 6678$ line which we consider. He II $\lambda 6683$ line lies close to it and it might be thought that it may contribute to the intensity of the observed line. The line He II $\lambda 6683$ arises from $n = 13$ to $n = 5$ and its A_{ki} value is $1.464 \times 10^5 \text{ sec}^{-1}$ (for comparison, $A_{ki} = 1.438 \times 10^8 \text{ sec}^{-1}$ for $\lambda 4686$); thus this line is expected to be rather weak. Its contribution to the observed line can be estimated by looking at the intensity of other He II lines with comparable A_{ki} values. There is another line which arises from $n = 13$ and which falls in the visible region, He II $\lambda 4025.6$ ($n = 13$ to $n = 4$) and has $A_{ki} = 1.710 \times 10^5 \text{ sec}^{-1}$. Unfortunately this line also falls at the position of a He I line, $\lambda 4026.2$. However, by looking at the intensity of other He I lines, the observed intensity of the $\lambda 4026$ line can be appropriately apportioned between He I $\lambda 4026.2$ and He II $\lambda 4025.6$. Thus by scrutinizing the intensity of He I and He II lines, we find that the contribution of He II $\lambda 6683$ to the observed line in each of the three stars is quite small. We are thus led to conclude that very likely laser action is responsible for the unusual strength of He I $\lambda 6678$ in these three stars. The lines are broad which would indicate that the dominant mechanism for the population inversion is rapid cooling through expansion.

We note here that all the four lines, $\lambda\lambda 4921, 5048, 6678$ and 7281 are known to occur in novae and nova-like stars with good strength (Andrillat, 1964; Meinel *et al.*, 1975). Next we consider two other interesting objects, the emission lines in which are relatively narrow.

The spectrum of the remarkable emission line star CPD-56°8032 in the red and infrared has been described by Thackeray (1977). His Table II shows a remarkable thing : He I $\lambda 6678$ has an intensity of 9, while He I $\lambda 7281$ has an intensity of 10. This indicates evidence of population inversion in the transition responsible for $\lambda 7281$. For this reason we discuss this object in some detail. CPD-56°8032 was discovered by Bidelman *et al.* (1968).

Cowley and Hiltner (1969) have described the spectrum of this star as unique. They have identified lines on their Cerro Tololo spectra from 3712 to 4714 Å. The spectrum contains a continuum, strong, slightly broadened C II emission lines and fainter emission lines from ions such as He I, C III, O II, O III, Si III and Si IV, many of the latter group having P Cygni profiles. The blue hydrogen emission lines are sharp and extremely weak and [O II] is present. Webster and Glass (1974) have compared the object with M4-18, He 2-113 and V348 Sgr. Their discussion indicates that these four objects belong to a class, with low excitation surrounding nebulae, infra-red radiation from dust grains and characteristic spectra dominated by C II emission lines. They appear to form a cool extension to the carbon sequence of Wolf-Rayet stars, the ionization level in the stellar atmosphere is lower than in stars classified as WC9. The emission lines in CPD-56° 8032 are relatively narrow ($\sim 2\text{Å}$).

Downes (1984) has observed an emission line star, MWC 84 = KPD 0415+5552, which has strong He I emission lines. The tracing shows $\lambda 6678$ to be a strong line, much stronger than $\lambda 4921$ (by a factor of 15 or so). Approximate visual estimates (made from the tracing) of the relative intensities of He I lines in this star are given in following in the parenthesis: $\lambda 4388$ (0.2), $\lambda 4471$ (0.5), $\lambda 4713$ (0.5), $\lambda 4921$ (0.5), $\lambda 5015$ (1.5), $\lambda 5876$ (10), $\lambda 6678$ (10). The relative intensities of these lines in the laboratory are 3, 7, 4, 4, 6, 11, and 6 respectively (Moore, 1945). The relative strength of the line $\lambda 6678$ is seen to be much stronger in this star than in the laboratory, and it appears highly likely that this is due to population inversion. Downes's tracing extends only up to about 7000 Å. It would be of interest to investigate this star at longer wavelengths and to examine the behaviour of $\lambda 7281$.

As mentioned earlier the emission lines in these two objects are relatively narrow. The available evidence indicates that the expansion mechanism for cooling of the ejected plasma is not expected to be very effective, but rather it is the second mechanism referred to in

the Introduction which appears to be responsible for the laser action in the $\lambda 7281$ line in CPD-56°8032 and that in the line $\lambda 6678$ in MWC 84. Both experimental (Silfvast et al., 1979; Dixon and Elton, 1977; Dixon et al., 1978) and theoretical results (Wagli and Bohn, 1980) show that expansion of a plasma into an ambient gas can lead to population inversion.

TABLE 2-6. Relative intensities of the four lines in stars. A blank spot indicates that this region was not observed; 'abs.' stands for absent.

Star	Relative intensity			
	$\lambda 4922$	$\lambda 5048$	$\lambda 6678$	$\lambda 7281$
Swings(1942)				
HD 151932(WN7)	abs.	abs.		
HD 164270(WC8)	2	abs.		
Swings and Jose (1950)				
HD 184738(WC8)			3	present
HD 164270(WC8)			4	2
HD 168206(WC7)			abs.	abs.
HD 192103(WC7)			3	1?
HD 151932(WN6+)			3	
HD 192163(WN6)			8	2?
HD 193077(WN5)			2-3	
Smith(1955)				
HD 136488(WC8)	2	abs.	6	
HD 119078(WC7)	abs.	abs.	$W_\lambda = 20$	
HD 97152(WC7)	abs.	abs.	present	
HD 115473(WC6)	abs.	abs.	abs.	
HD 96548(WN8)	$W_\lambda = 6.3$	$W_\lambda = 2.5^a$	$W_\lambda \sim 12$	
HD 92740(WN7)	abs.	abs.	weak	
HD 143414(WN6)	?	abs.	$W_\lambda = 25^b$	
HD 50896(WN5+)	abs.	abs.	$W_\lambda = 21.2$	

^a blended with a N II line.

^b unusually strong as compared to other He I lines.

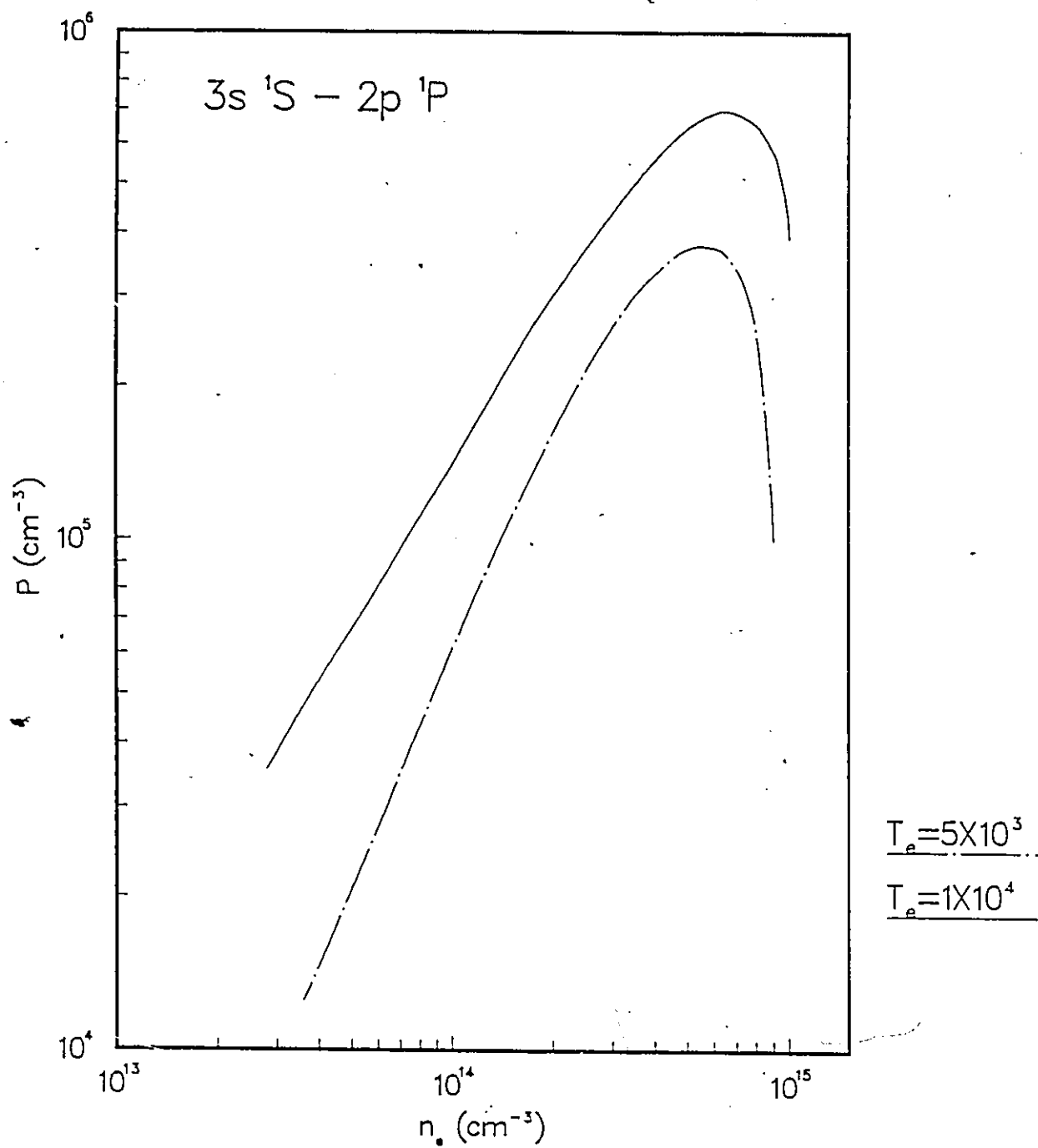


Figure 2-1. P as a function of n_e for $\lambda 7281$.

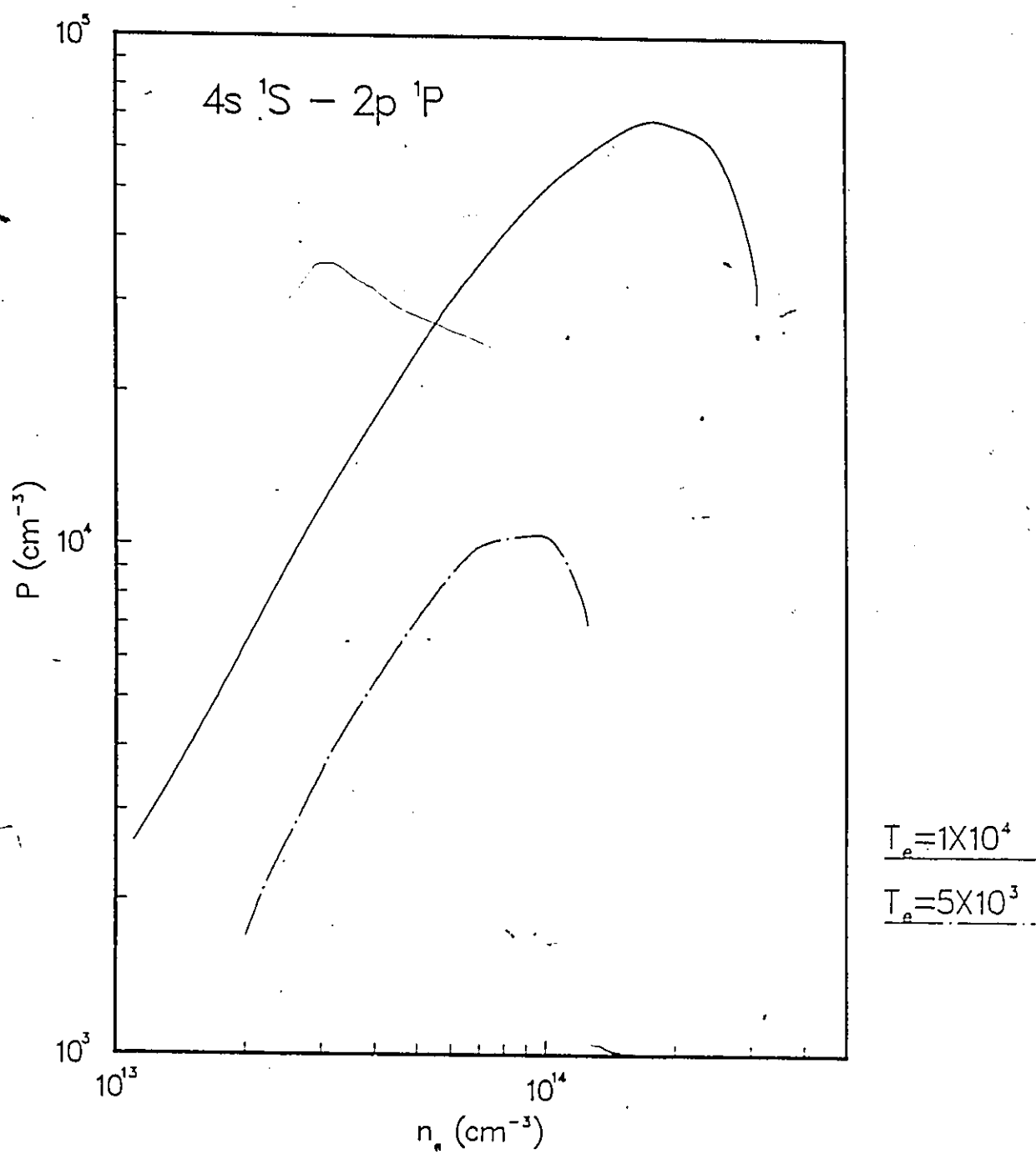


Figure 2-2. P as a function of n_e for $\lambda 5048$.

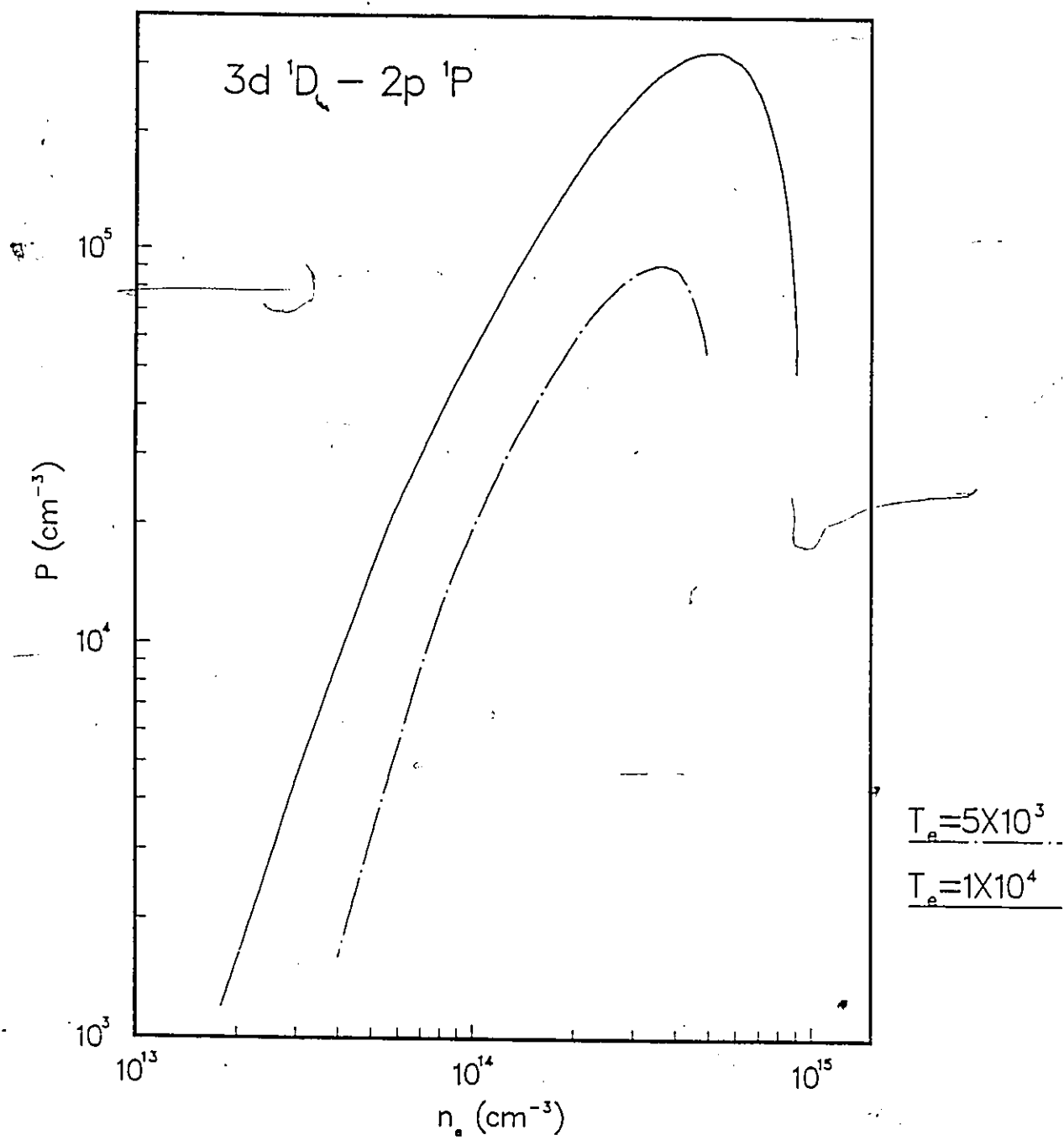


Figure 2-3. P as a function of n_e for $\lambda 6678$.

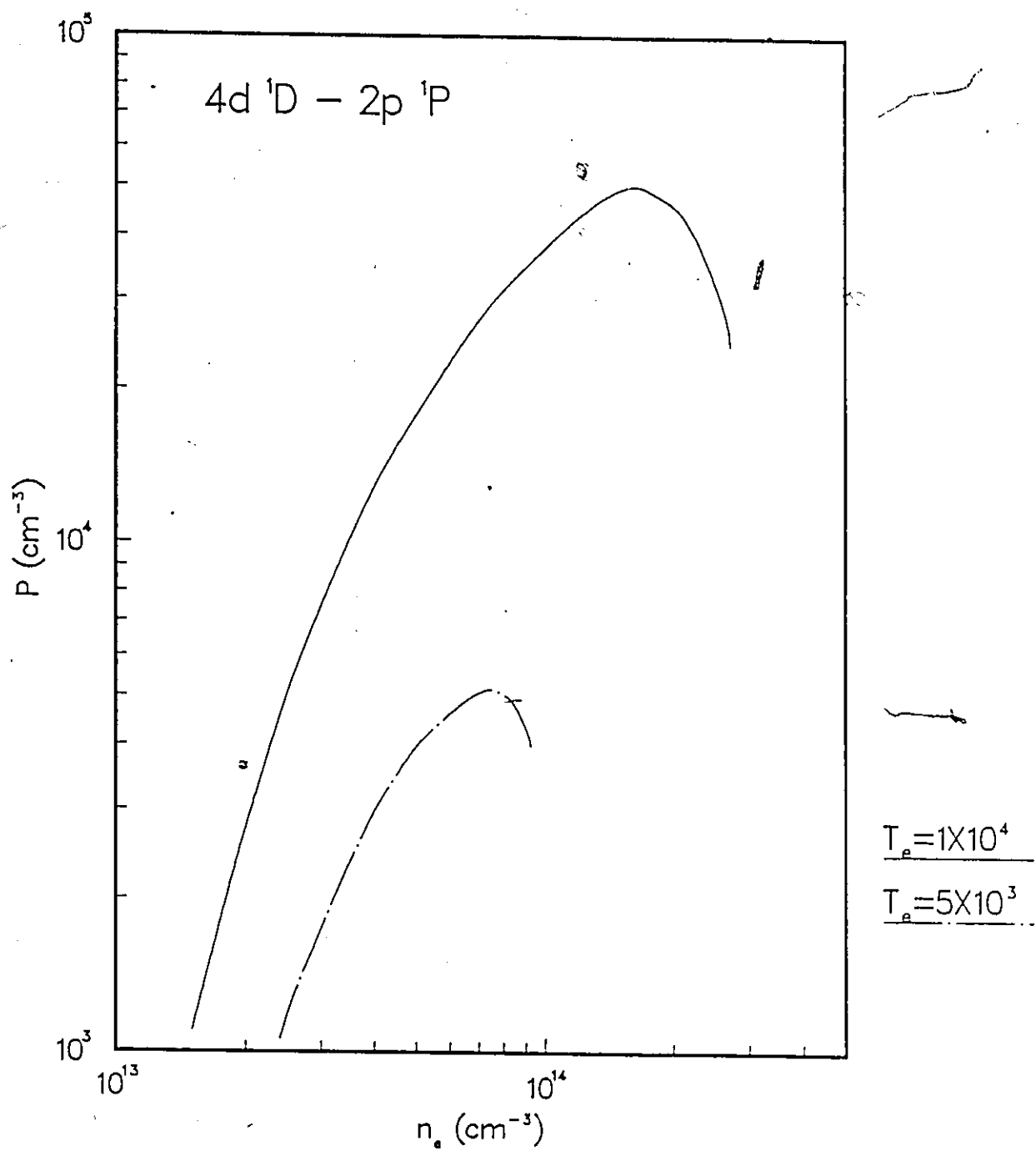


Figure 2-4. P as a function of n_e for $\lambda 4921$.

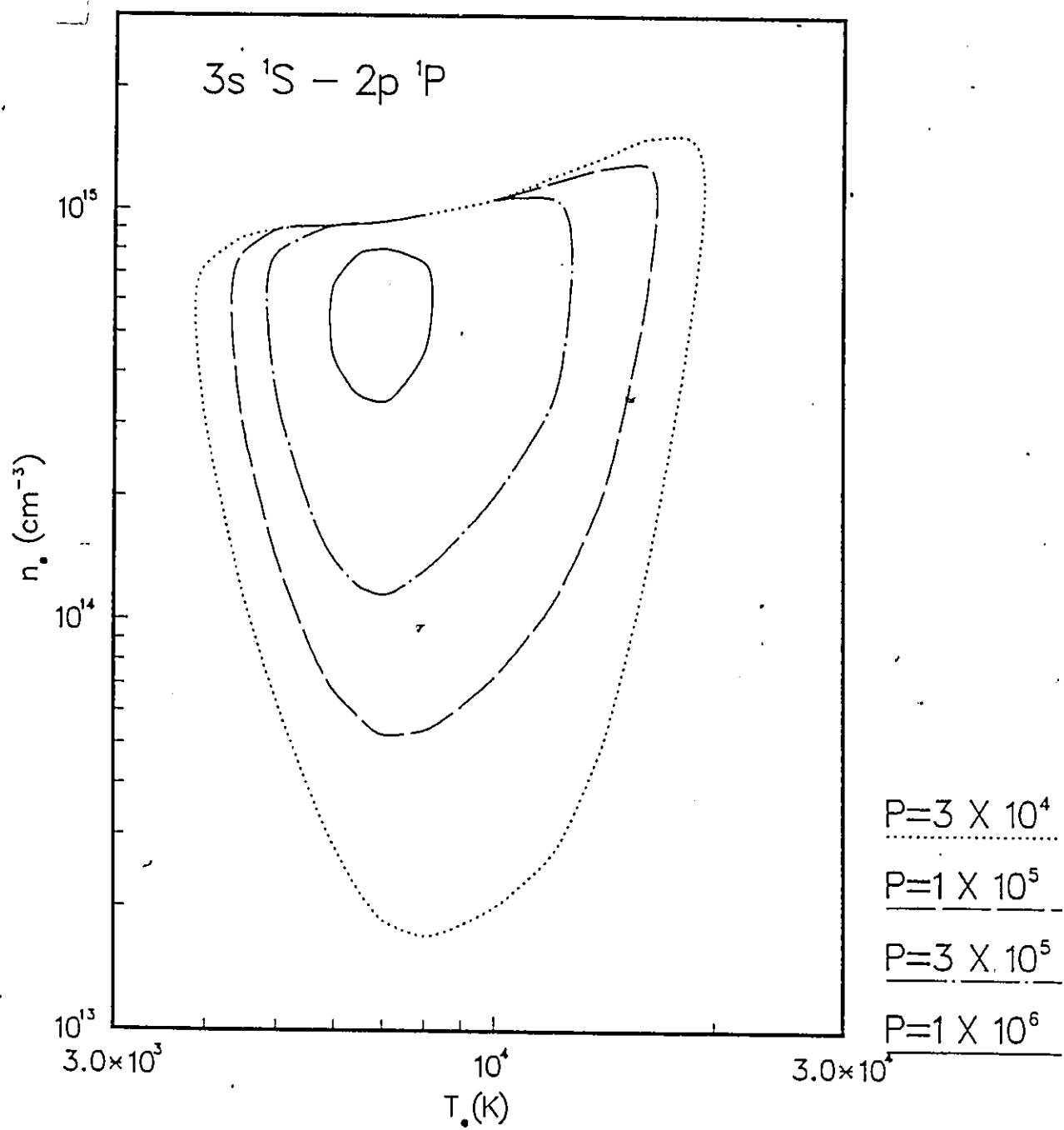


Figure 2-5. P as a function of n_e and T_e for $\lambda 7281$.

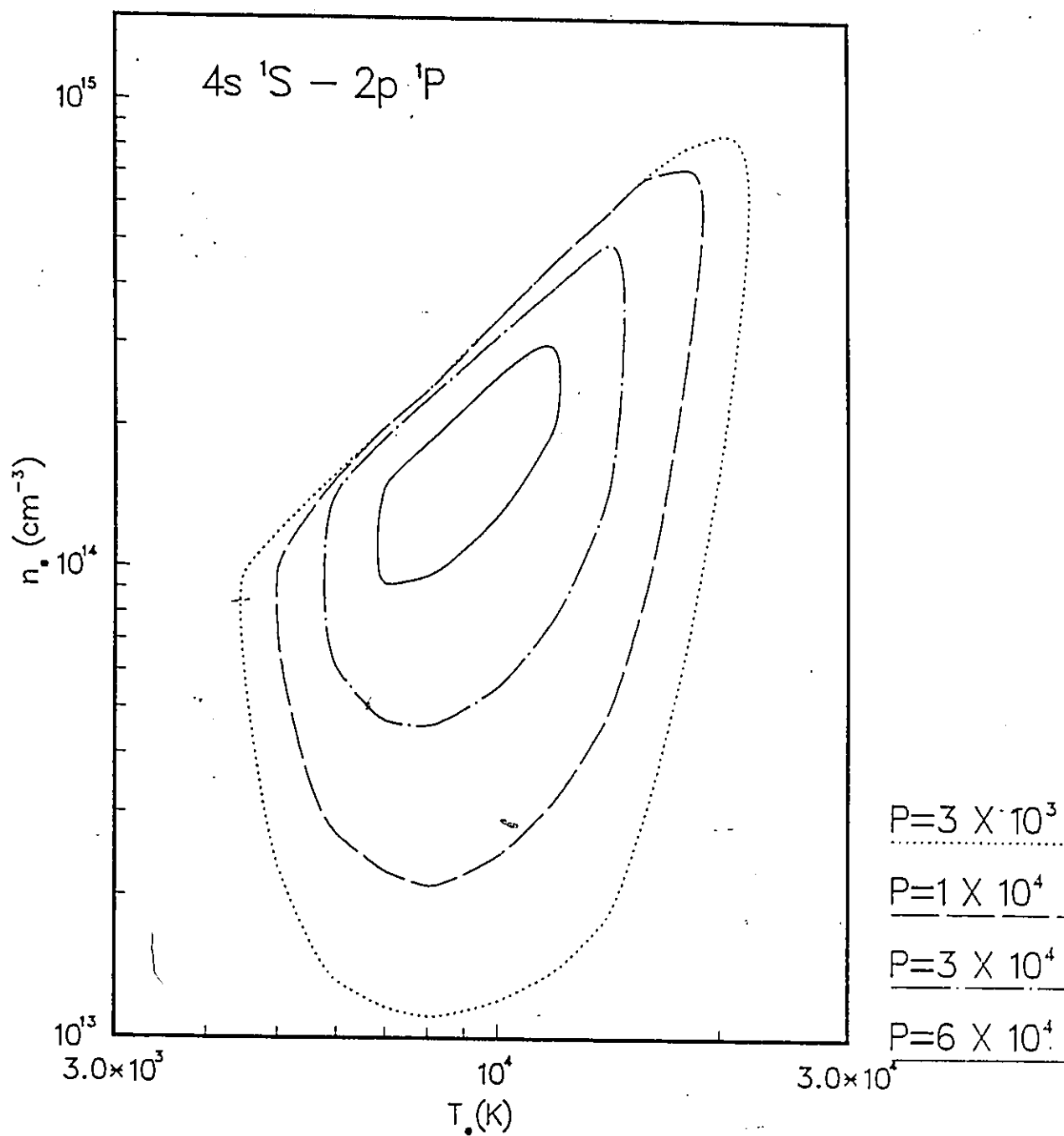


Figure 2-6. P as a function of n_e and T_e for $\lambda 5048$.

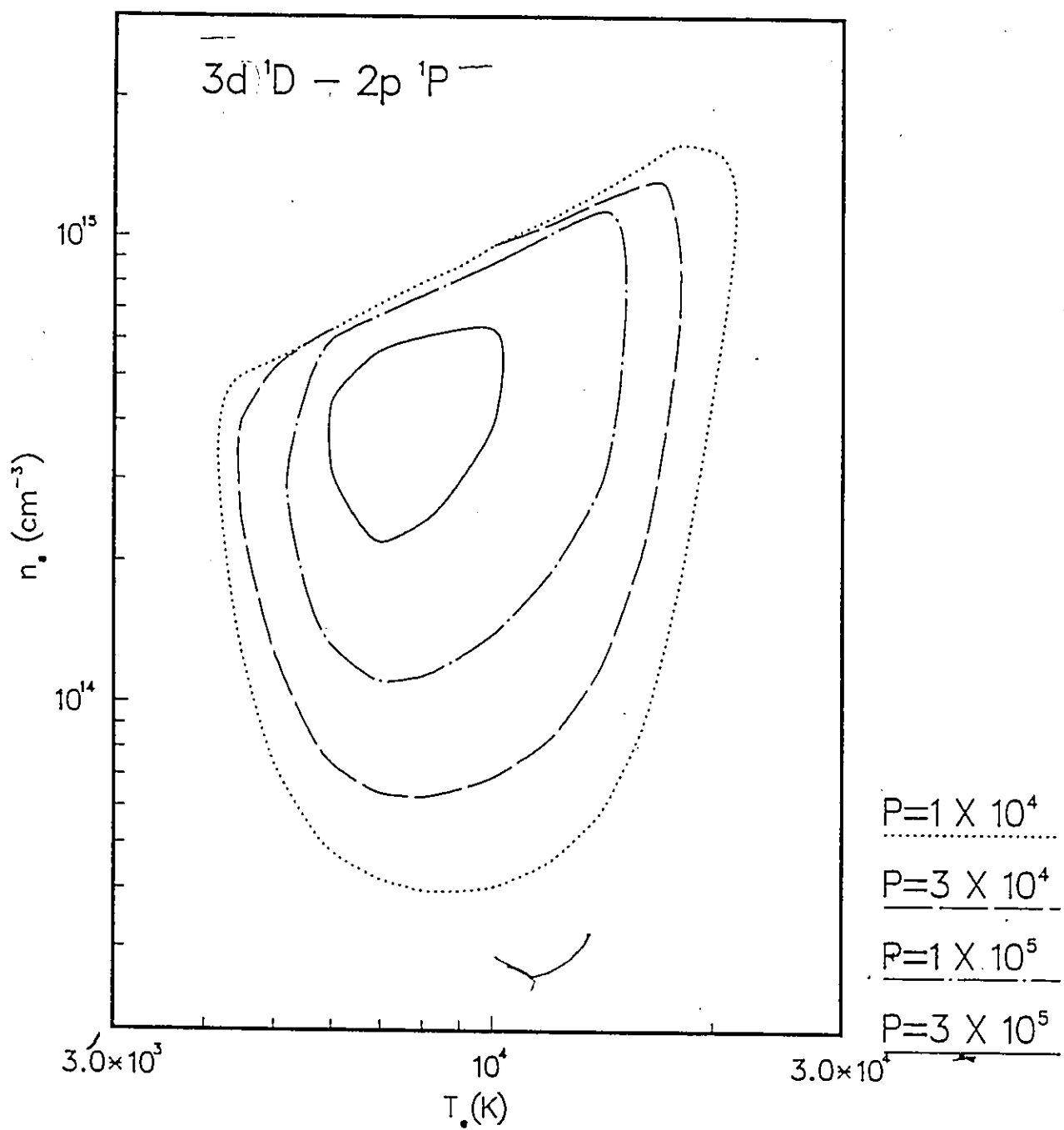


Figure 2-7. P as a function of n_e and T_e for $\lambda 6678$.

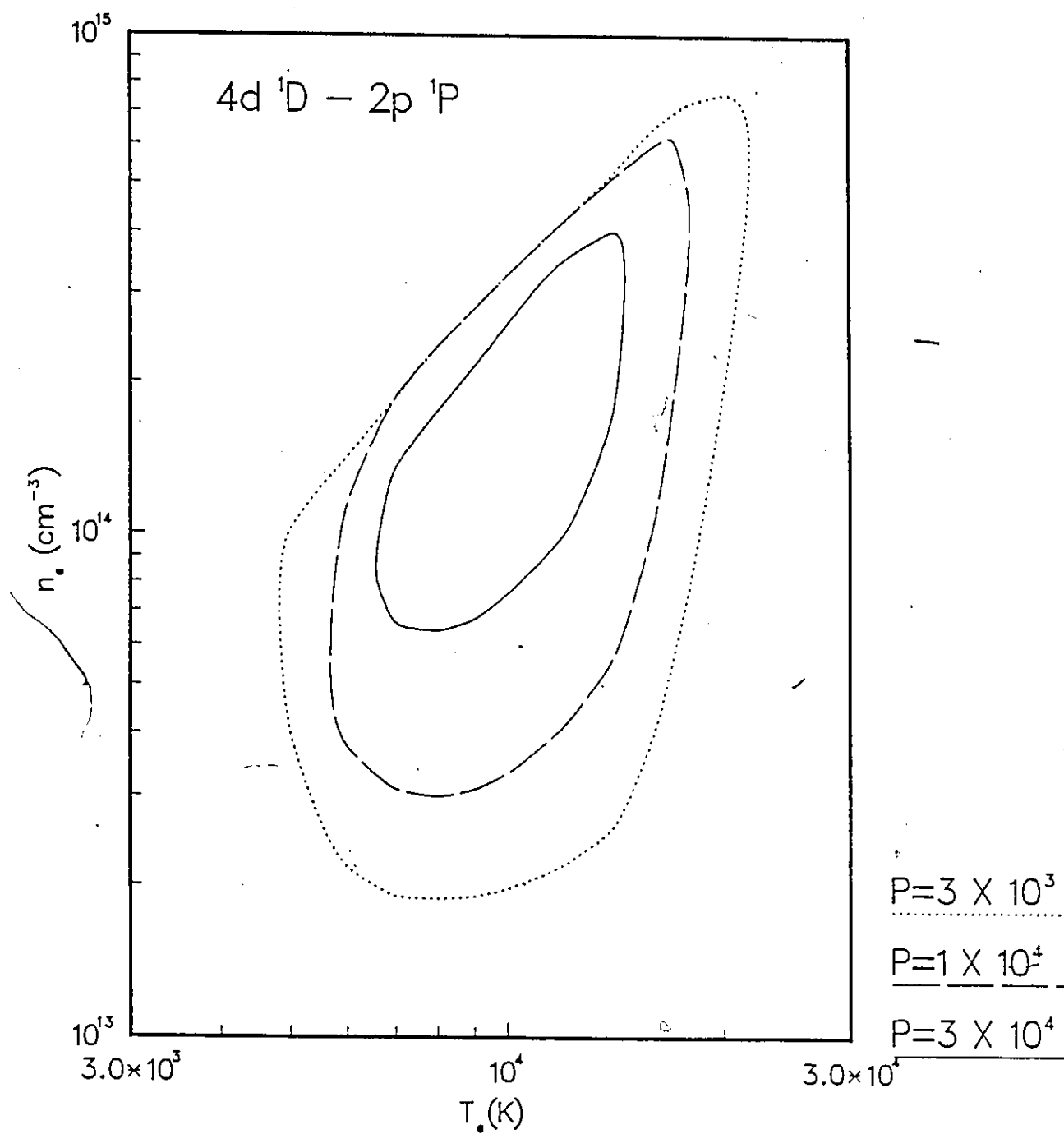


Figure 2-8. P as a function of n_e and T_e for $\lambda 4921$.

Chapter 3

Population Inversions in a Freely Expanding Helium Plasma.

A) Introduction

In this chapter we shall remove the assumption of a sudden cooling which was used in chapter 2. Instead we now adopt a more realistic picture and allow the plasma to expand in a finite time and we investigate in detail the evolution of the population densities of levels of He atoms.

There has been very little previous work on the evolution of population densities of He I levels with time. Limbaugh and Mason (1971) solved numerically the set of differential equations describing the time-dependent decay of a singly ionized optically thin monatomic gas for constant temperature-constant-pressure helium afterglows (no expansion). The initial condition was a Boltzmann distribution from the $2^3\hat{S}$ state throughout the higher states. Times for the plasma to reach the quasi-steady state (QSS) ranged from $t \approx 10^{-8}$ sec for high-density plasmas to $t \approx 10^{-4}$ sec for low-density plasmas.

B) Theoretical Model.

In general, to analyze the process of creating an inversion as a plasma expands, it is necessary to solve jointly the equations for the population relaxation, electron temperature and gas-dynamics.

We consider a spherically symmetric plasma consisting of neutral helium atoms, electrons, and helium ions of various charges (He^+ , He^{++}) expanding in a vacuum. The motion of these components can be specified by a common hydrodynamic velocity V which is approximately

$$V = \frac{1}{N} \left(\sum_{i=1}^{\infty} N_i V_i + \sum_m N^{+m} V_{+m} \right) \quad (3-1)$$

where V_i and V_{+m} are the mean macroscopic velocity of atom in level i and of ion of ionization stage m , respectively, and N is the total density of the heavy particles,

$$N = \sum_{i=1}^{\infty} N_i + \sum_m N^{+m}. \quad (3-2)$$

In writing Eqs. (3-1) and (3-2), we have made the usual assumption that all the ions are in the ground state. We now require equations for the components that describe the change of state of the plasma. If the rate of production per unit volume of particles of species a is Γ_a , these equation can be written in the form (Braginskii, 1965; Gudzenko *et al.*, 1970)

$$\frac{\partial N}{\partial t} + \text{div}(NV) = 0, \quad (3-3)$$

for He I

$$\frac{\partial N_i}{\partial t} + \text{div}(N_i V_i) = \Gamma_i, \quad (i = 1, 2, \dots, \infty) \quad (3-4)$$

for He⁺ and He⁺⁺

$$\frac{\partial N^{+m}}{\partial t} + \text{div}(N^{+m} V_m) = \Gamma_m, \quad (3-5)$$

and for electrons

$$\frac{\partial n_e}{\partial t} + \text{div}(n_e V_e) = - \sum_{i=1}^{\infty} \Gamma_i - n_e(N^{+2}\alpha^{+2} - N^{+1}S^{+1}), \quad (3-6)$$

where

$$\begin{aligned} \Gamma_i = & -n_e N_i S_i - n_e N_i \sum_{j \neq i}^{\infty} C_{ij} - N_i \sum_{j=1}^{i-1} A_{ij} \\ & + n_e \sum_{j \neq i}^{\infty} N_j C_{ji} + \sum_{j=i+1}^{\infty} N_j A_{ji} + \{\beta_i + \alpha_i n_e\} n_e N^{+m} \end{aligned} \quad (3-7)$$

and

$$\Gamma_{+m} = n_e [N^{+(m-1)} S^{+(m-1)} - N^{+m} (S^{+m} + \alpha^{+m}) + N^{+(m+1)} \alpha^{+(m+1)}] \quad (3-8)$$

the symbol S^{+m} denote the electron collisional rate coefficient for the process $N^{+m} \rightarrow N^{+(m+1)}$, and α^{+m} denote the total recombination rate coefficient for the process $N^{+m} \rightarrow N^{+(m-1)}$. We have here further assumed that the ionization stage m is coupled only to adjacent stages, $(m-1)$ and $(m+1)$, i.e., multiplet ionization and recombination processes are neglected.

From the momentum-transport equations (Braginskii, 1965; Gudzenko *et al.*, 1968; Golant *et al.*, 1977), the equations for the transport of internal energy, or the heat-balance can be written as (Gudzenko *et al.*, 1970)

$$\frac{3}{2} n_e \left(\frac{\partial T_e}{\partial t} + V_e \nabla T_e \right) + n_e T_e \operatorname{div} V_e + \operatorname{div} q_e = \frac{3}{2} T_e \sum_{i=1}^{\infty} \Gamma_i + Q_{inel} - Q_{\Delta T}, \quad (3-9)$$

$$\frac{3}{2} N \left(\frac{\partial T}{\partial t} + V \nabla T \right) + T \sum_a N_a \operatorname{div} V_a + \operatorname{div} q = Q_{\Delta T}, \quad (3-10)$$

where T is the temperature of the heavy particles (we assume that all the components of the plasma are at same temperature, $T_{He} = T_{He^+} = T_{He^{+2}} = T$, but the electron temperature can be different.), q_e and q are the heat fluxes carried by the electronic and heavy components, Q_{inel} denotes the rate of increase of the thermal energy due to the inelastic collisions and $Q_{\Delta T}$ denotes that due to the elastic collisions.

In order to simplify the problem, we have used the following assumption: the gas density decreases as a power-law function of the time, that the mean velocities of all components are the same, and that the velocity field is such that the densities and temperatures depend only on time (Gudzenko *et al.*, 1970). Thus, the system of partial differential

equations (3-3 to 3-10) can be converted to ordinary differential equations. We can then write

$$\frac{dN}{dt} + N \operatorname{div} V = 0 \quad (3-11)$$

$$\operatorname{div} V = -\frac{1}{N} \frac{dN}{dt} \quad (3-12).$$

The relaxation equations for the electronic level populations are:

$$\frac{dN_i}{dt} = \Gamma_i + \frac{N_i}{N} \frac{dN}{dt}, \quad (i = 1, 2, \dots, r) \quad (3-13)$$

For all the levels i located above r which is a sufficiently high lying level, the population density is assumed to be given by the Saha-Boltzmann equilibrium equation.

The rate of change of electron density n_e with time can be written as

$$\frac{dn_e}{dt} = -\sum_{i=1}^r \Gamma_i - n_e(N^{+2}\alpha^{+2} - N^{+1}S^{+1}) + \frac{n_e}{N} \frac{dN}{dt}, \quad (3-14)$$

and the time derivatives of the densities of He^+ and He^{+2} are

$$\frac{dN^{+1}}{dt} = \frac{N^{+1}}{N} \frac{dN}{dt} + \Gamma_{+1}, \quad (3-15)$$

$$\frac{dN^{+2}}{dt} = \frac{N^{+2}}{N} \frac{dN}{dt} + \Gamma_{+2}. \quad (3-16)$$

The heat-balance equations are

$$\frac{3}{2}n_e \frac{dT_e}{dt} = T_e \frac{n_e}{N} \frac{dN}{dt} + Q_{inel} - Q_{\Delta T} + \frac{3}{2}T_e \sum_i \Gamma_i \quad (3-17)$$

$$\frac{3}{2}N \frac{dT}{dt} = T \frac{dN}{dt} + Q_{\Delta T}. \quad (3-18)$$

In most treatments of the expansion of a plasma, usually the late, inertial stage of the expansion is considered when the rate of expansion is practically constant and the plasma density falls with the passage of time proportionally as $1/t^3$ (Kuznetsov and Raizer, 1965). Such an expression, however, cannot be used for the early stages for the expansion. The initial density at $t = 0$ clearly has to be finite. Hence we have used the following expression, the plasma density decreases with time in spherical expansion according to the relation

$$N(t) = N_0 \left(\frac{\beta}{t + \beta} \right)^3 \quad (3-19)$$

where β is a parameter. Expression (3-19) can be derived by assuming that the plasma is formed initially ($t = 0$) in a sphere of certain radius and then it expands with a constant velocity. Expression (3-19) goes smoothly to $N(t) \propto 1/t^3$ as t becomes large compared to β . Thus, for a given function of N , we can write

$$\frac{dN_i}{dt} = \Gamma_i - \frac{3}{t + \beta} N_i \quad (3-20)$$

$$\frac{dn_e}{dt} = - \sum_{i=1}^r \Gamma_i - n_e (N^{+2} \alpha^{+2} - N^{+1} S^{+1}) - \frac{3}{t + \beta} n_e, \quad (3-21)$$

$$\frac{dN^{+1}}{dt} = - \frac{3}{t + \beta} N^{+1} + \Gamma_{+1}, \quad (3-22)$$

$$\frac{dN^{+2}}{dt} = - \frac{3}{t + \beta} N^{+2} + \Gamma_{+2}. \quad (3-23)$$

and

$$\frac{dT_e}{dt} = - \frac{2}{t + \beta} T_e + \frac{T_e}{n_e} \left(\sum_{i=1}^r \Gamma_i \right) + \frac{2}{3} \frac{(Q_{incl} - Q_{\Delta T})}{n_e} \quad (3-24)$$

$$\frac{dT}{dt} = -\frac{2}{t + \beta} T + \frac{2}{3} \frac{Q_{\Delta T}}{N} \quad (3-25)$$

The energy transfer rate due to inelastic collisions, Q_{inel} , is expressed as

$$Q_{inel} = - \sum_{i=2}^r \sum_{j=1}^{i-1} (E_j - E_i) (C_{ji} N_j - C_{ij} N_i) - \sum_{i=1}^r E_i S_i N_i + n_e N^{+m} \sum_{i=1}^r E_i \alpha_i. \quad (3-26)$$

The first term on the R.H.S. of Eq. (3-26) denotes the net rate of the electron energy transfer due to excitation and de-excitation. The second and third terms represent the transfer rates of the electron energy due to ionization and three-body recombination, respectively.

Heat is evolved in the gas of heavy particles as a result of elastic collisions (Petschek and Byron, 1957; Bates and Kingston, 1964):

$$Q_{\Delta T} = 2m_e n_e (T_e - T) \sum_k \frac{\nu_{ek}}{M_k} \quad (3-27)$$

where m_e is the electron mass, and ν_{ek} is the frequency of the elastic collision between electrons and heavy particles (of mass M_k), which is estimated from

$$\nu_{ek} = \frac{4\pi N^k m_e}{3T_e} \int f(v) \sigma_{ek}(v) v^5 dv. \quad (3-28)$$

In the above equation $f(v)$ is the distribution function and σ_{ek} the cross section for the electron- k -species encounters, and N^k is the density of the k species. Using the Coulomb cross section for the electron-ion encounters, the electron-ion collision frequency is of the form (Bates and Kingston, 1964; Kruger and Mitchner, 1967)



$$\nu_{ei} = \frac{8}{3} \left(\frac{\pi}{m_e} \right)^{1/2} \frac{N_e^2 e^4}{(2T_e)^{3/2}} \ln \left[\frac{9T_e^3}{4\pi n_e e^6} \right]. \quad (3-29)$$

An effective scattering cross section for the electron-atom encounters is taken to be constant over the likely range of the electron temperature (Golant *et al.*, 1977). The electron-atom collision frequency is given by

$$\nu_{ea} = N_a \left(\frac{8T_e}{\pi m_e} \right)^{1/2} \sigma_{ea}, \quad (3-30)$$

where N_a is the density of atoms. For the case of the helium atom σ_{ea} is expressed as, for $T_e < 3$ eV (Nishida, 1975)

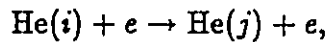
$$\sigma_{ea} = (0.946 \log T_e + 2.99) \times 10^{-16} \text{ cm}^2 \quad (T_e \text{ in K}). \quad (3-31)$$

At high energies, the cross section is a decreasing function of the energy. Thus for helium, in the region $3 \text{ eV} < T_e \leq 50 \text{ eV}$ it decreases approximately as $1/v$; in this case the collision frequency is velocity independent, and is given by (Golant *et al.*, 1977)

$$\nu_{ea} \approx 7 \times 10^{-8} N_a. \quad (3-32)$$

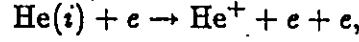
We note here that in writing the energy equation the following assumptions were made for the transfer of energy between electron and atom (ion) due to collisional and radiative processes:

- (1) In the excitation process



the kinetic energy of the excited atom does not change before and after the collision. All the energy correspond to the de-excitation process is regarded as the inverse reaction

in the excitation process. In the ionization process



the kinetic energy of the excited atom is transferred to the ion without loss. The corresponding energy reaction of the three-body recombination process is regarded as the inverse reaction of the ionization process.

- (2) The excitation or ionization energy is supplied by the electron in the collision between electron and atom.
- (3) The excess energy released in the inelastic radiative recombination process is carried off by the photon.

C) Numerical Calculations

As initial conditions of our numerical calculations, we assume that the helium plasma is in ionization equilibrium, and that the plasma parameters have been constant for a sufficiently long time. Under such conditions, steady state conditions will prevail and population densities of the levels will be given by the steady state solution (McWhirter and Hearn, 1963)

$$\begin{aligned} \dot{N}_i \equiv \frac{dN_i}{dt} = & -n_e N_i S_i - n_e N_i \sum_{j \neq i}^{\infty} C_{ij} - N_i \sum_{j=1}^{i-1} A_{ij} \\ & + n_e \sum_{j \neq i}^{\infty} N_j C_{ji} + \sum_{j=i+1}^{\infty} N_j A_{ji} + \{\beta_i + \alpha_i n_e\} n_e N^{+m} = 0, \end{aligned} \quad (3-33)$$

with $i = 1, 2, \dots, \infty$. Dividing Eq. (3-33) by N_i^E and using Eq. (2-2), the set of equations (3-33) becomes

$$- \left(n_e S_i + n_e \sum_{j \neq i}^{\infty} C_{ij} + \sum_{j=1}^{i-1} A_{ij} \right) \rho_i$$

$$+ \sum_{j=i+1}^{\infty} \left\{ C_{ij} n_e + \frac{Z_j}{Z_i} A_{ji} \right\} \rho_j + \frac{1}{Z_i} \{ \alpha_i n_e + \beta_i \} = 0. \quad (i = 1, 2, \dots, \infty) \quad (3-34)$$

As mentioned previously in section B of Chapter 2, there exists a high-lying quantum state r above which the discrete levels are in LTE. The population density of these levels is then given by

$$\rho_{i>r} = 1. \quad (3-35)$$

The infinite set of Eq. (3-34) then becomes

$$- \left(n_e S_i + n_e \sum_{j \neq i}^s C_{ij} + \sum_{j=1}^{i-1} A_{ij} \right) \rho_i + \sum_{j=i+1}^r \left\{ C_{ij} n_e + \frac{Z_j}{Z_i} A_{ji} \right\} \rho_j + \sum_{j>r}^s \left\{ C_{ij} n_e + \frac{Z_j}{Z_i} A_{ji} \right\} + \frac{1}{Z_i} \{ \alpha_i n_e + \beta_i \} = 0. \quad (i = 1, 2, 3, \dots, r) \quad (3-36)$$

Thus the population density of the levels can be obtained by solving these simultaneous equations. Then the plasma expands in a vacuum. We have made the calculations for the initial plasma parameters shown in Table 3-1 (8.617 eV $\equiv$ 100,000 K and 6.9 eV $\equiv$ 80,000 K).

For this calculation, singlet and triplet states were maintained separate through principal quantum number 5, except for the levels having the orbital angular momentum $\ell > 3$, which for the same n , were grouped together. All substate were summed together for each of the levels 6-10. The labelling of the various states, as used in this model, and the energies are given in Table 3-2. All the atomic data needed in these calculations are summarized in Chapter 2.

TABLE 3-1. Initial plasma parameters. Additional subscript 0 indicates initial value.

	T_{eo}	T_{ao}	N_o	β
a	8.617 eV	6.9 eV	$1 \times 10^{17} \text{ cm}^{-3}$	$1 \times 10^{-5} \text{ sec.}$
b	8.617	6.9	1×10^{15}	1×10^{-5}
c	8.617	6.9	1×10^{13}	1×10^{-5}
d	4.309	2.6	1×10^{17}	1×10^{-5}
e	4.309	2.6	1×10^{15}	1×10^{-5}
f	4.309	2.6	1×10^{13}	1×10^{-5}
g	8.617	6.9	1×10^{17}	1×10^{-7}
h	8.617	6.9	1×10^{15}	1×10^{-7}
i	4.309	2.6	1×10^{17}	1×10^{-7}

Unfortunately these calculations are very time consuming since the set of equations (3-20) required very small time step (smaller than the relaxation time of the excited state r). Thus, it would be desirable to use an assumption to reduce the number of equations in (3-20). In the present calculations, the number of levels included in the system of differential equations was reduced by using the following assumption: The quasi-steady state (QSS) assumption is made for the level $i > i^*$, the level i^* is determined from the condition (Gudzenko *et al.*, 1975),

$$n_e/N_i \gg 1 + 3\tau_{n_e}/t \quad (3-37)$$

where τ_{n_e} is the characteristic time for changes in free electron density, which is estimated from

TABLE 3-2. Energy levels of He I used in the model.

Level No. (i)	State	Energy $E_i(\text{cm}^{-1})$	g_i	Level No. (i)	State	Energy $E_i(\text{cm}^{-1})$	g_i
1	1^1S	0.0	1	20	5^3S	193347.09	3
2	2^3S	159856.07	3	21	5^1S	193663.63	1
3	2^1S	166277.55	1	22	5^3P	193800.80	9
4	2^3P	169086.94	9	23	5^3D	193917.24	15
5	2^1P	171135.00	3	24	5^1D	193918.39	5
6	3^3S	183236.89	3	25	5^3F	193921.18	21
7	3^1S	184864.55	1	26	5^1F	193921.19	7
8	3^3P	185564.68	9	27	$5^{1,3}\text{L}$	193922	36
9	3^3D	186101.65	15	28	5^1P	193942.57	3
10	3^1D	186105.07	5	29	6	195251	144
11	3^1P	186209.47	3	30	7	196070	196
12	4^3S	190298.21	3	31	8	196595	256
13	4^1S	190940.33	1	32	9	196955	324
14	4^3P	191217.13	9	33	10	197213	400
15	4^3D	191444.59	15	34	11	197403	484
16	4^1D	191446.56	5	35	12	197548	576
17	4^3F	191451.98	21	36	13	197661	676
18	4^1F	191451.99	7	37	14	197750	784
19	4^1P	191492.82	3	38	15	197822	900

$$\tau_{n_e} = \left| \frac{1}{n_e} \frac{dn_e}{dt} \right|^{-1} \quad (3-38)$$

Thus, the set of equations 3-20 will consist of i^* equations instead of r equations. The kinetics of the levels $i > i^*$ are coupled to the system of differential equations, Eqs.(3-20) to (3-25).

The applicability of this approximation can be examined, quantitatively, by comparing the decay time for the levels to return to QSS following a plasma perturbation and the expansion time. The level i return to its steady state value will take place in a time of order (McWhirter and Hearn, 1963)

$$\tau_i \sim \left\{ [S_i + \sum_{i \neq j} C_{ij}] n_e + \sum_{j < i} A_{ij} \right\}^{-1} \quad (3-39)$$

τ_i is the relaxation time of level i . The relaxation time for some levels, for electron density and electron temperature at different times during the expansion for case g are given in Table 3-3. It is apparent from this table that the characteristic relaxation time of the individual excited states is very small (compared to the expansion time) and less than the characteristic time for the changes in the free electron density. However, as the electron density and temperature drop the characteristic time of the metastable states become comparable to τ_{n_e} . Thus it is reasonable to assume that the plasma during the transient phase can be viewed as progressing from one QSS to next with the population densities for the levels adjusting themselves to the QSS distribution at the current conditions 'almost instantaneously'.

It is found from the numerical results of the cases considered, that only the ground state didn't satisfy the condition (3-37) at early time of the expansion, and continues to do so as the electron density drops. At a certain electron density the metastable states

start not obeying the condition. The use of this condition has reduced the computer time by more than 70%.

Integration of the equations was performed by using the Runge-Kutta-Gill method. The time step Δt was set to be one hundredth of the relaxation time for the population density of the level i^* . To see the effect of Δt on the numerical calculations, we repeated the calculations for some cases using Δt equal to one thousandth of the relaxation time for the level i^* , and found that the two results agree, reasonably well.

TABLE 3-3. Relaxation time in seconds.

t (sec)	T_e (eV)	τ_{n_s}	τ_1	τ_2	τ_3	τ_{10}	τ_{25}
1.0E-10	8.617	3.4E-8	2.7E-9	3.9E-12	2.18E-12	7.1E-13	1.6E-14
5.2E-9	8.054	3.5E-8	3.6E-9	4.3E-12	2.4E-12	7.8E-13	2.7E-14
7.3E-9	7.735	3.6E-8	4.4E-9	4.6E-12	2.5E-12	8.3E-13	3.8E-14
1.3E-8	7.02	3.7E-8	7.0E-9	5.4E-12	2.9E-12	9.5E-13	6.3E-14
2.0E-8	6.17	4.0E-8	1.3E-8	6.6E-12	3.5E-12	1.1E-12	7.4E-14
3.4E-8	5.00	4.4E-8	6.6E-8	9.5E-12	4.8E-12	1.8E-12	1.0E-13
4.6E-8	4.20	5.2E-8	1.4E-7	1.3E-11	6.2E-12	2.3E-12	1.3E-13
6.5E-8	3.30	5.5E-8	8.6E-7	1.9E-11	8.9E-12	3.4E-12	1.8E-13
8.2E-8	2.70	7.0E-8	4.7E-6	2.8E-11	1.2E-11	4.7E-12	2.4E-13
2.8E-7	0.603	1.2E-7	1.0E+7	9.6E-10	1.7E-10	5.1E-11	3.6E-12
4.7E-7	0.273	1.8E-7	9.5E+25	2.5E-8	1.2E-9	1.7E-10	1.9E-11
6.6E-7	0.166	2.4E-7	9.9E+59	7.4E-7	6.0E-9	3.9E-10	6.8E-11
8.5E-7	0.13	3.0E-7	∞	8.3E-5	1.6E-8	7.5E-10	1.6E-10

The quantity following E is the power of 10 by which the preceding number must be multiplied.

D) Results and Discussion

Figures 3-1 to 3-3 show the electron temperature T_e as a function of time t , in a plasma which expands in a vacuum. The electron temperature shows very little change for $t \ll \beta$, it starts decreasing at $t \sim \beta/5$ and decrease becomes quite rapid at $t \sim \beta$. The rate of decrease of T_e with t is seen to depend on the initial value of n_e . As the initial electron density is decreased, the rate of decrease of T_e with t becomes greater. This can be explained as follows: the three-body recombination is more important at high densities than at low densities, and it is well known that a portion of the energy freed in three-body recombination heats the electron gas (Kuznetsov and Raizer, 1965; Zel'dovich and Raizer, 1966). In all cases at first the rate of change of T_e with t , $|dT_e/dt|$, increases with time (called stage a), reaches a maximum, and then it decreases (called stage b). Fig. 3-4 shows the electron density as a function of time in the cases a, d, and g.

Population inversion was found to occur for a great many transitions in the infra-red and visible regions. Figs. 3-5 to 3-10 show the population densities for the levels 2^1P , 3^1S , 3^1D , and 4^1S (Fig. 3-10 includes 4^1D level also) as a function of time. Initially the population densities of these levels decrease with time until stage b is reached. In the stage b there is a rapid increase due to the increase in the recombination flux which is however followed by a rapid decrease due to reduction in the recombination flux and by reduction in the density of the plasma as it expands. We couldn't show the behaviour of the population densities beyond $t \sim 1 \times 10^{-4}$ s because of the electron temperature becoming lower than the limit of our computer program, the exponential factor in the rate coefficients becomes either very large or very small, but in some cases the population density shows a rapid decrease before the limiting T_e is reached, for example: see 3^1S in Fig. 3-5 and all the levels in Fig. 3-6, 3-8, and 3-9. The population density of the level 2^1P decreases more rapidly than other levels mainly because 2^1P has a shorter radiative

lifetime, and the electrons recombine with the upper levels much faster than the decay of 3^1S , 3^1D , and 4^1S (and 4^1D in Fig. 3-10) levels to 2^1P by emission. The population inversions in the lines $3^1S \rightarrow 2^1P$ ($\lambda 7281$), $3^1D \rightarrow 2^1P$ ($\lambda 6678$) and $4^1S \rightarrow 2^1P$ ($\lambda 5047$) begin at an early stage of the expansion, except in cases with high initial electron density, and reach maximum when the recombination flux increases (at the region where the population densities increase), and then decrease as the electron density and temperature become low. The degree of the population inversion between 2^1P and other levels vary with the initial conditions. From Fig. 3-5 and Fig. 3-7 we see, if T_{e0} increased with n_{e0} constant, the inverted population drops.

The population densities for the levels 2^1P , 4^1D , 5^1S , and 5^1D as a function of time are presented in Figs. 3-11 and 3-12. The population densities for these levels show similar behaviour to that described above. Large population inversions occur between 2^1P and other levels at the time where the recombination increases and also the degree of the population inversion depends on the initial conditions.

Fig. 3-13 shows the population densities of the levels 3^1P , 3^1D , 5^1D , and 5^1F as a function of time. The behaviour of the population densities for these levels are similar to those described above. Large population inversions in the lines $5^1F \rightarrow 3^1D$ ($\lambda 12790$) and $5^1D \rightarrow 3^1P$ ($\lambda 12968$) are obtained at the time where the rate of recombination is maximum.

The population densities versus time for the levels 3^3S , 3^3D , 4^3P , and 5^3P are presented in Fig. 3-14. The population density for the level 3^3S stays higher than that for the levels 4^3P and 5^3P till $t \approx 5 \times 10^{-5}$ s, and, after that, rapidly decreases while the population densities for the upper levels continue to increase due to the recombination flux. Finally, the population inversions in the transitions $4^3P \rightarrow 3^3S$, and $5^3P \rightarrow 3^3S$ appear after $t \approx 5 \times 10^{-5}$ s, and $t \approx 7 \times 10^{-5}$ s, respectively, and one expects a rapid decrease in the population inversions after a short time as the recombination flux starts to decrease due to the drop in

density. The population density for 3^3D drops faster than that for 3^3S . This is because the radiative lifetime of 3^3D level is shorter than that of 3^3S level. The population inversion in the line $4^3P \rightarrow 3^3D$ ($\lambda 19548$) appears after $t \approx 2 \times 10^{-5}$ s.

The population densities for the levels 3^3P , 4^3D , 5^3S , and 5^3D versus time are presented in Fig. 3-15. The population inversion in the line $4^3D \rightarrow 3^3P$ ($\lambda 17007$) appears at $t \approx 3 \times 10^{-5}$ s, and in transitions $5^3S \rightarrow 3^3P$, and $5^3D \rightarrow 3^3P$ it appears at $t \approx 8 \times 10^{-5}$ s.

In Fig. 3-16 we present the population densities as a function of time for the levels 2^3P , 3^3P , 4^3S , and 4^3D . The population density for the 3^3P level shows a behaviour similar to that for 3^3S in Fig. 3-14. It stays high till $t \approx 6 \times 10^{-7}$ s, and then starts to drop. At this time population inversions between 4^3S , 4^3D and 3^3P appear and reach maximum at $t \sim 2 \times 10^{-6}$ s.

The 2^3P level is much more populated than all other excited states (except the metastable states 2^1S and 2^3S), this is because the radiative decay of this level is small relative to other low-lying levels and it can radiate only to 2^3S . For this reason the behaviour of the population density for 2^3P is different than that for those described above. It is similar to the behaviour of the population density for the ground state and the metastable states 2^3S and 2^1S ; the population density shows rapid increase at early time of the expansion while the other levels shows drop in the population densities, and, after then make a sudden drop at the time where the recombination flux increases to maximum, at this time there is possible population inversion. Fig. 3-16 shows a population inversion between 4^3S and 2^3P states for a short time. In order to show the evolution of the population inversion clearly, we plot population inversion between 4^3S and 2^3P versus time in Fig. 3-17. It is clear that the population inversion takes place in a very short time and only when the speed of the expansion is very rapid with high initial electron temperature and density. Thus under these conditions there is a possible population inversion in the line $4^3S \rightarrow 2^3P$

($\lambda 4714$).

The variation of the inverted population with n_{e0} and T_{e0} showed that it depends very strongly on these parameters of the plasma. Thus, there is an optimum initial electron temperature and density at which the inverted population attains its maximum value. Therefore, from this result it is clear that the radiative and/or collisional depopulation of the lower working level can work efficiently, and used for lasing in large helium plasma volumes. In the astrophysical context, we can use this mechanism to explain, to some extent, the unusually strong emission lines in nova outbursts, in which a disturbance in the energy balance of the star leads to release of a large amount of energy and a shock wave is propagated from the central layers to the periphery. This shock wave separates from the star and emits a gas cloud into space.

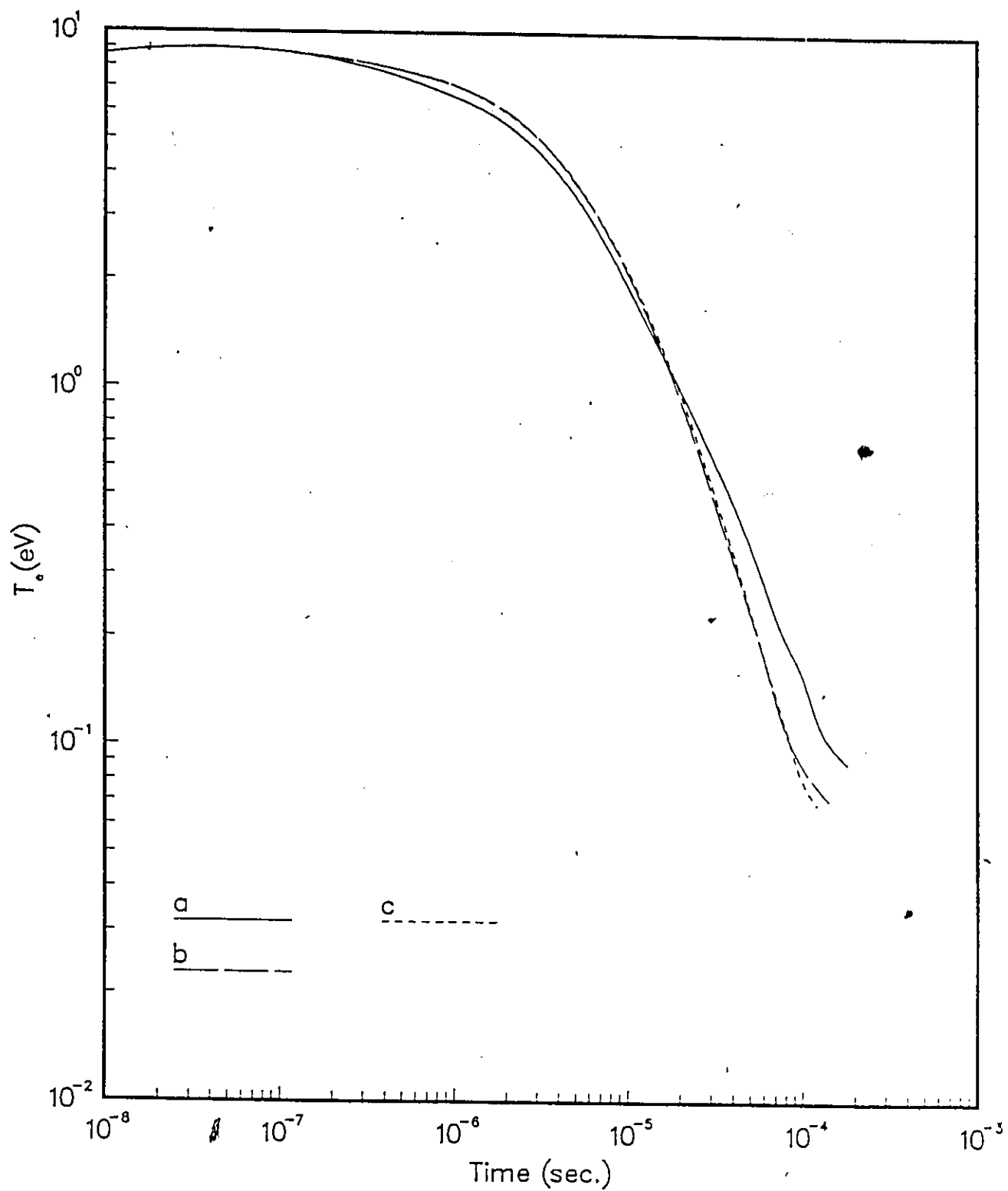


Fig. 3-1. Electron temperature vs. time for the cases a, b, c.

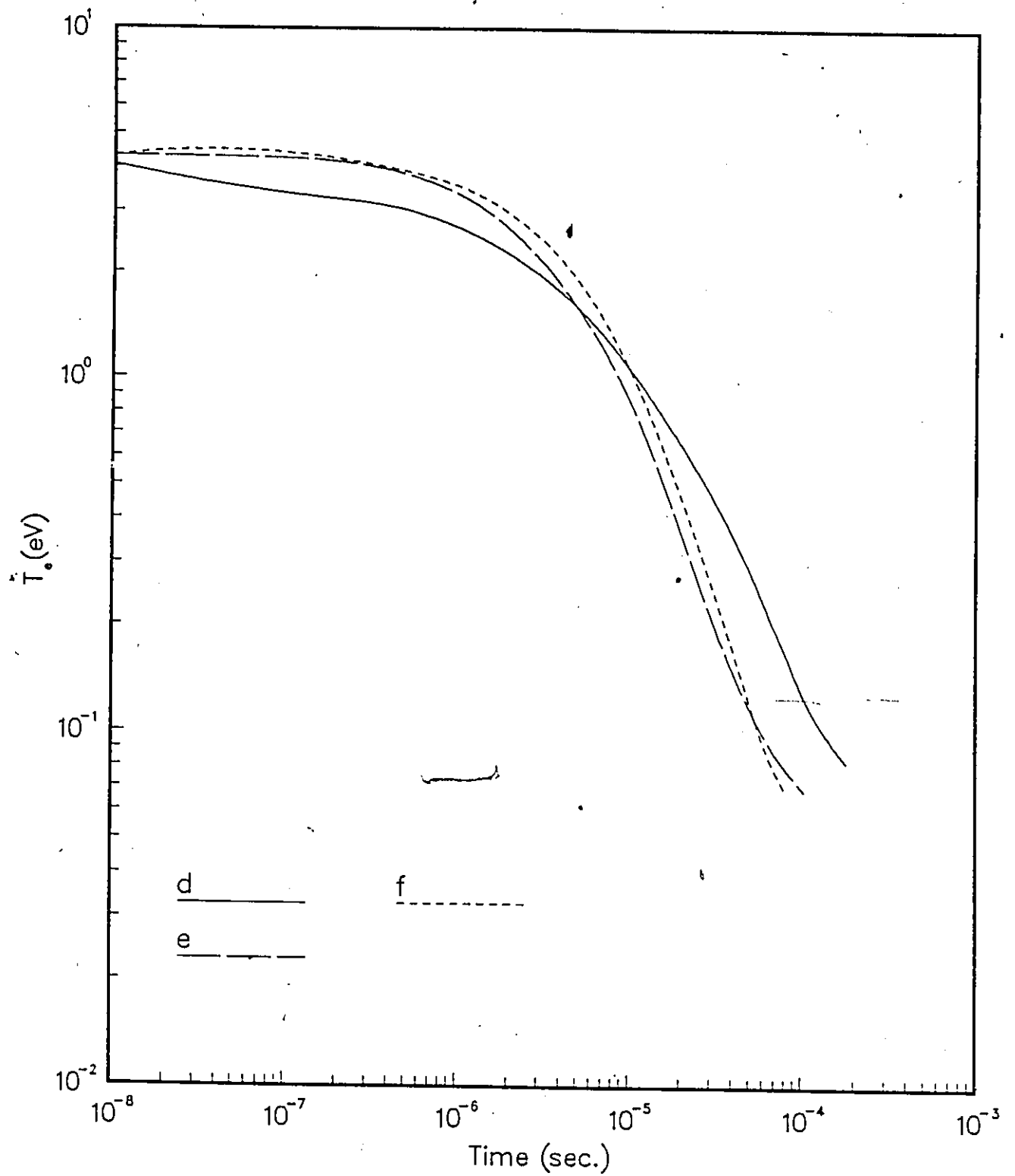


Fig. 3-2. Electron temperature vs. time for the cases d, e, f.

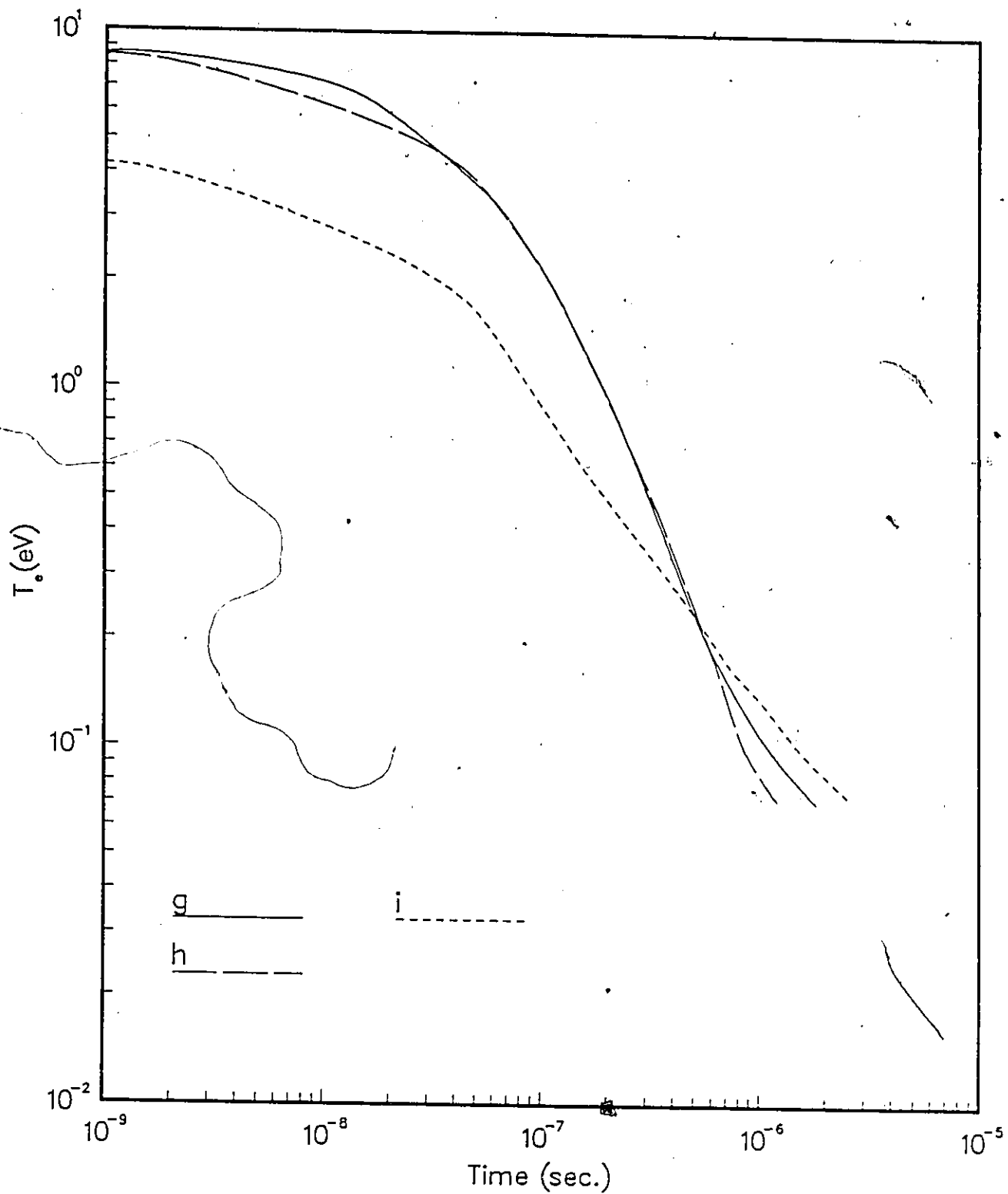


Fig. 3-3. Electron temperature vs. time for the cases g, h, i.

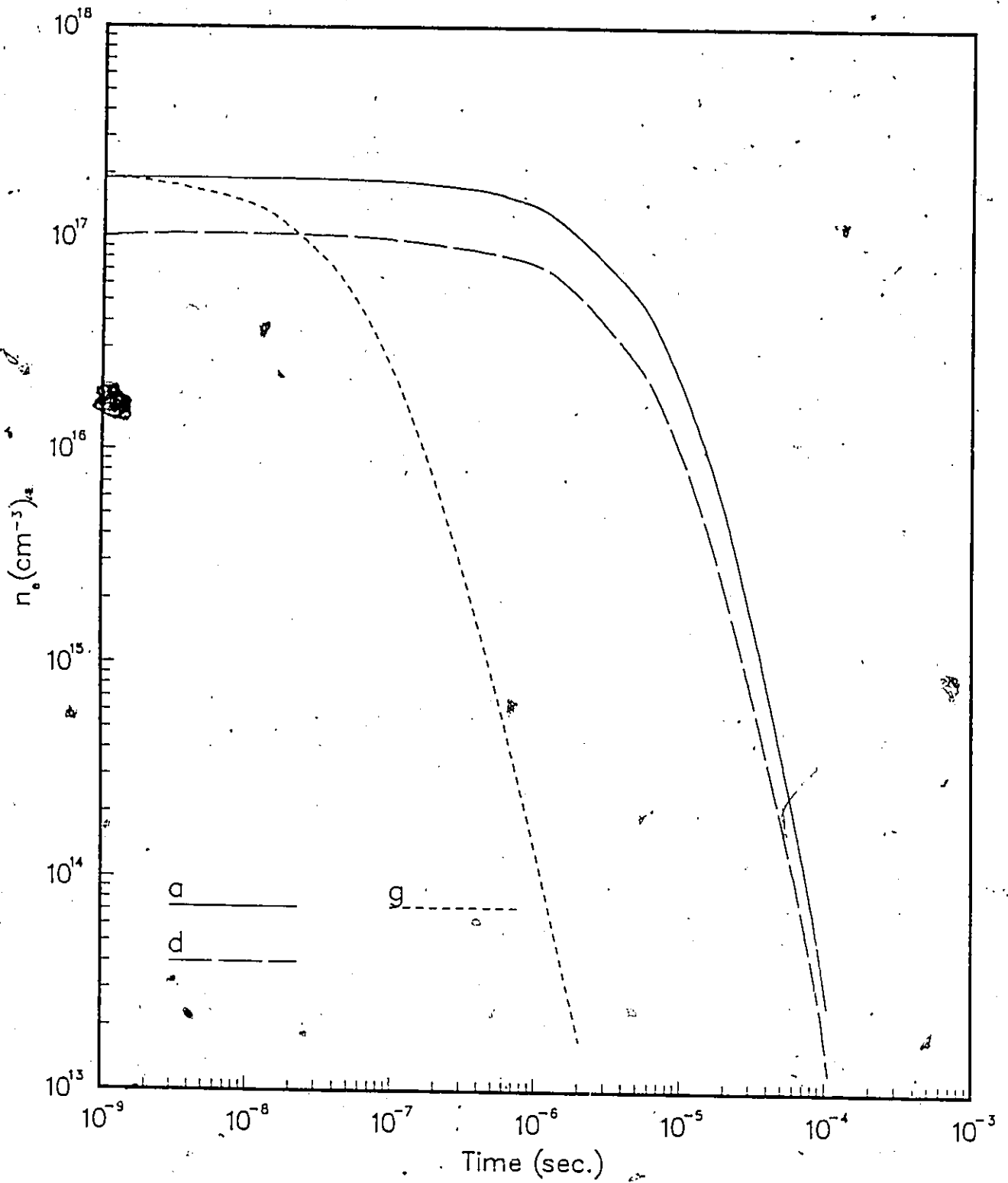


Fig. 3-4. Electron density vs. time for the cases a, d, g.

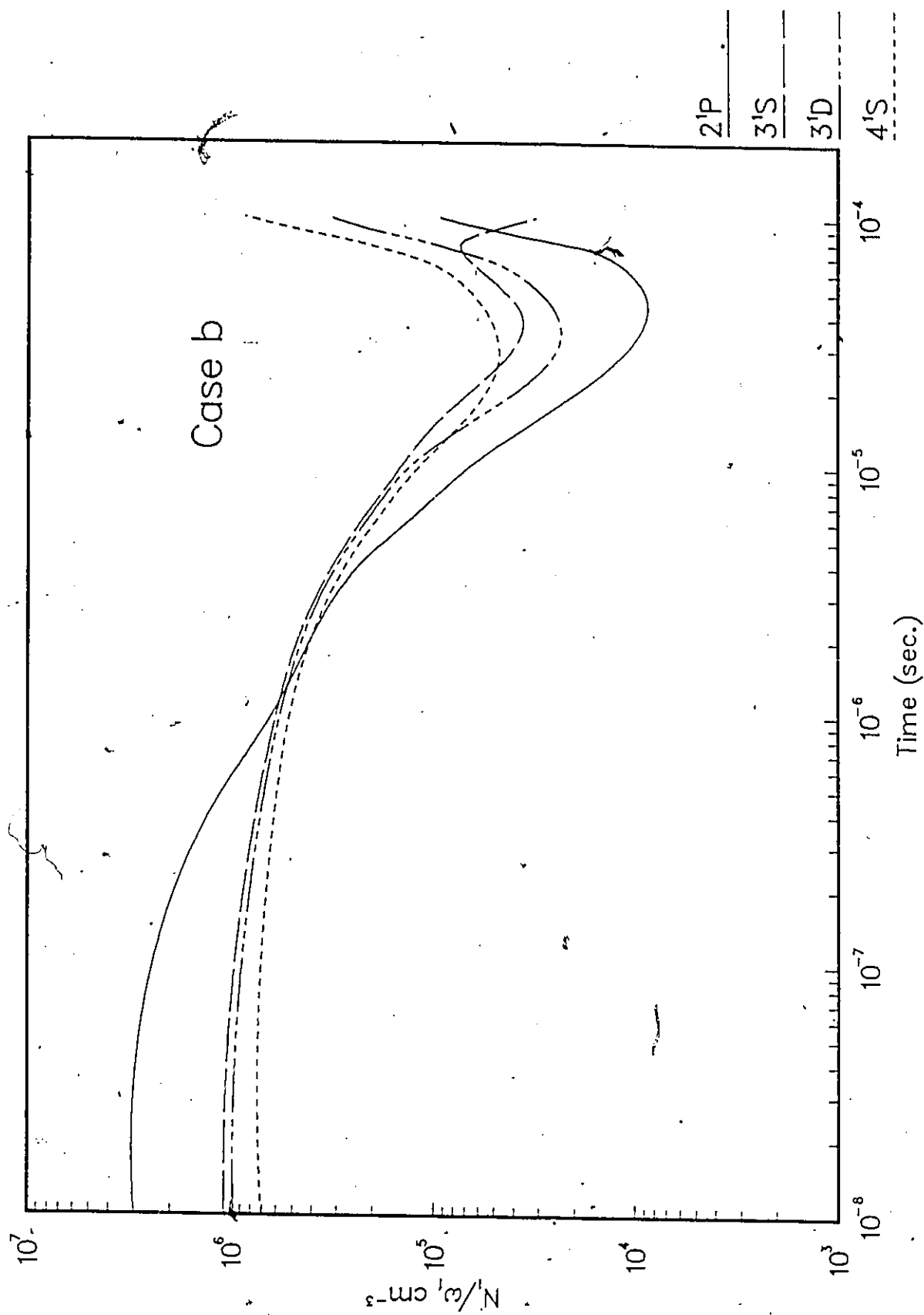


Fig. 3-5. Population densities vs. time for some levels in He I

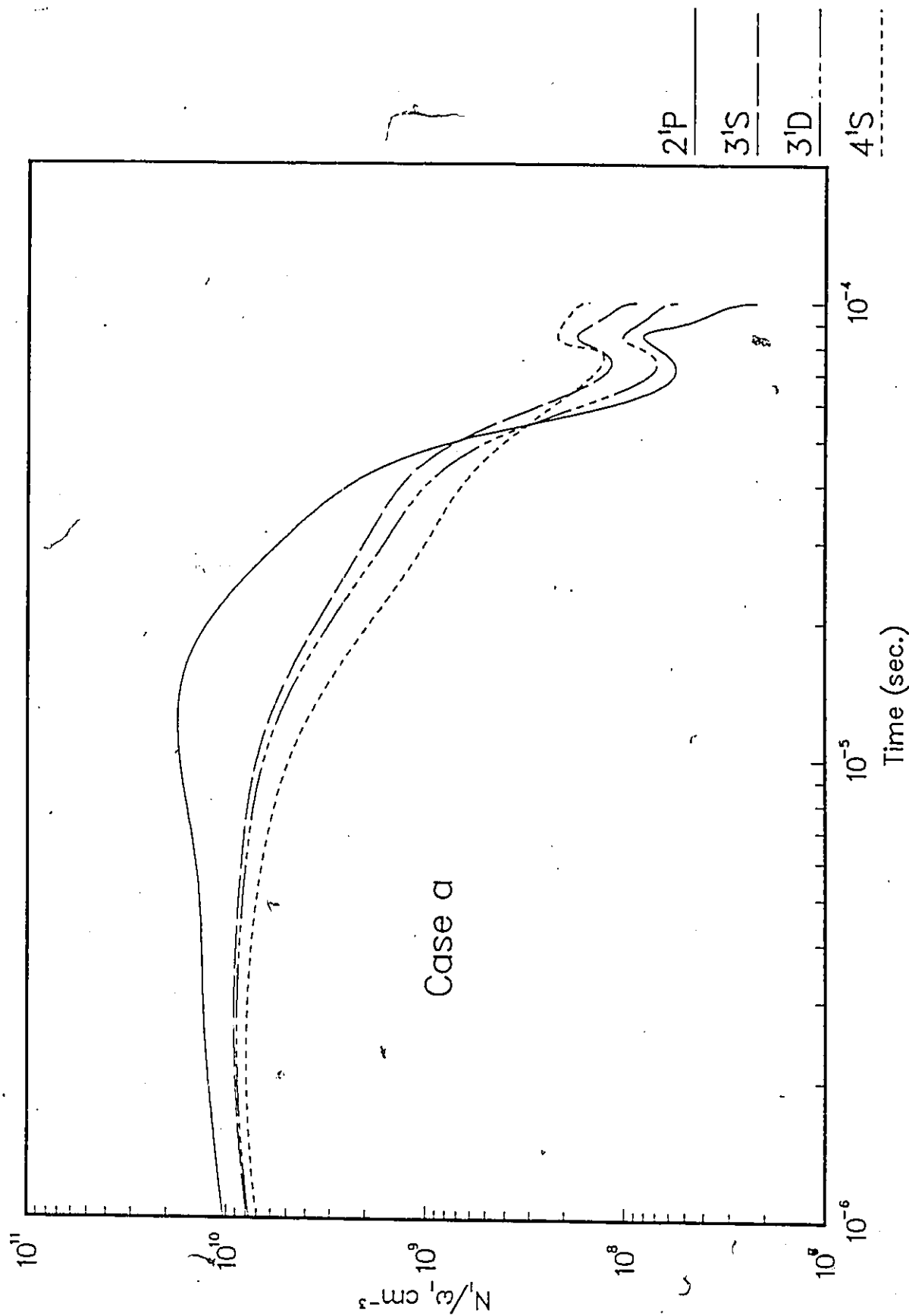


Fig. 3-6. Population densities vs. time for some levels in He I

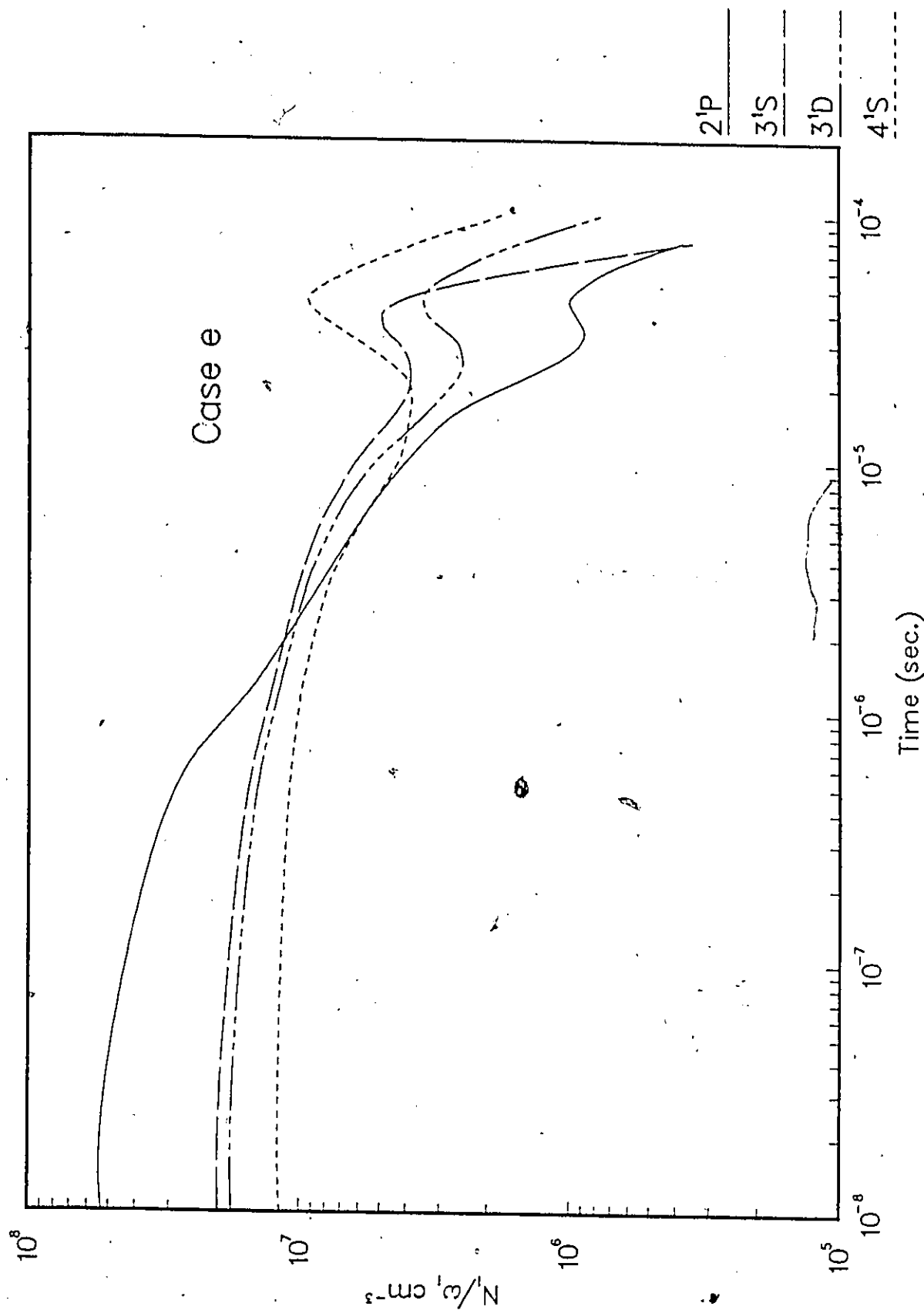


Fig. 3-7. Population densities vs. time for some levels in He I

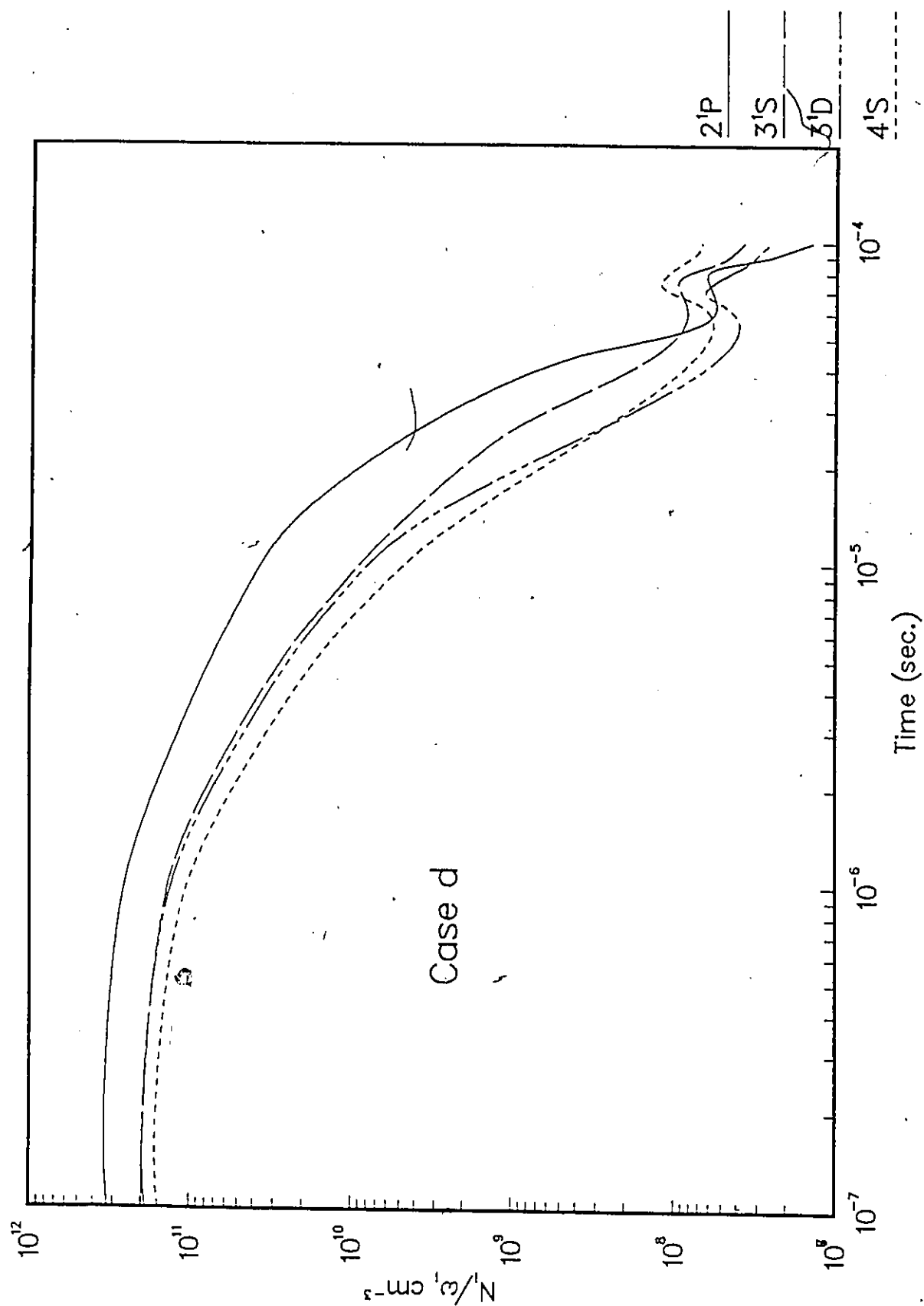


Fig. 3--8. Population densities vs. time for some levels in He I

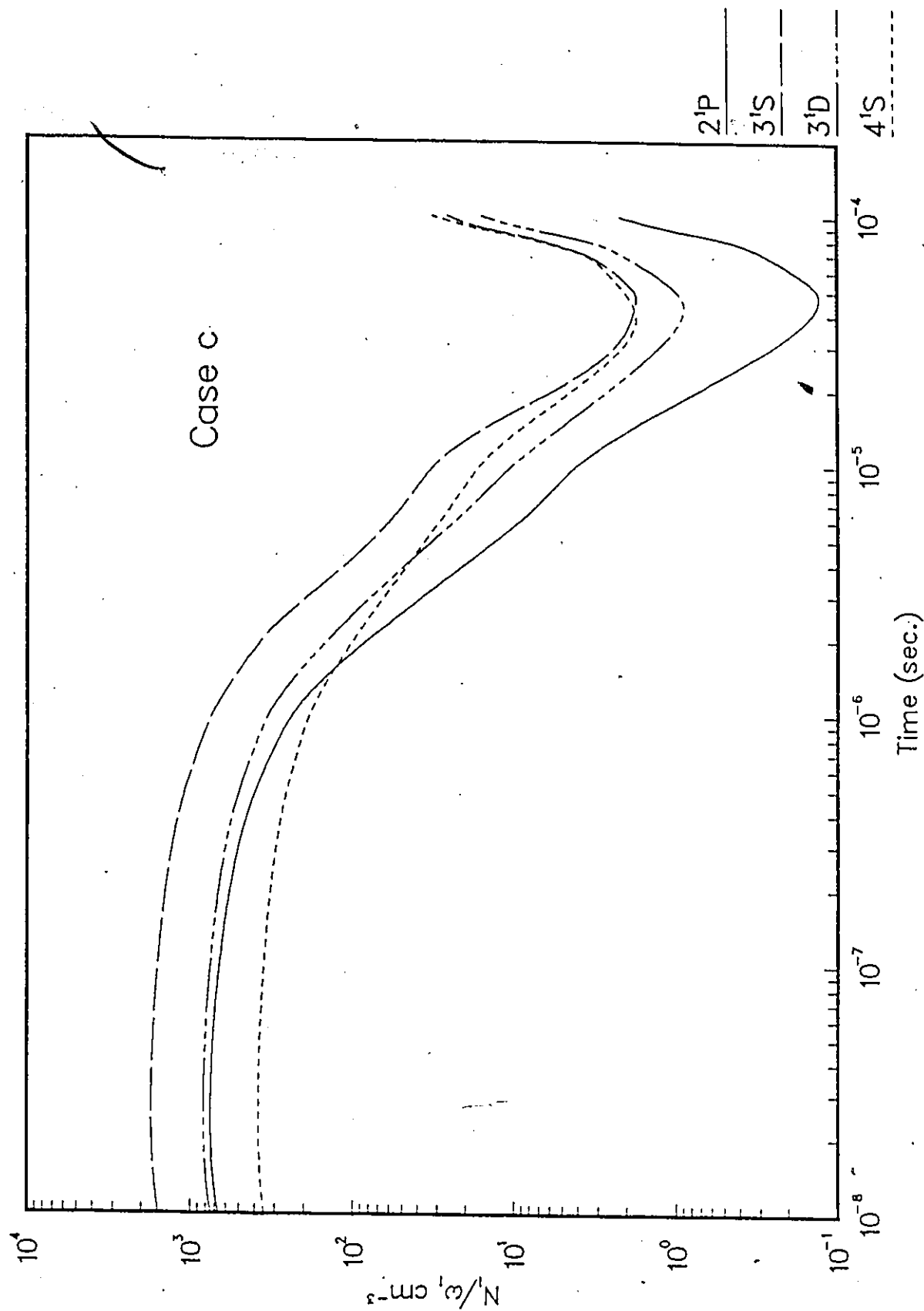


Fig. 3-9. Population densities vs. time for some levels in He I

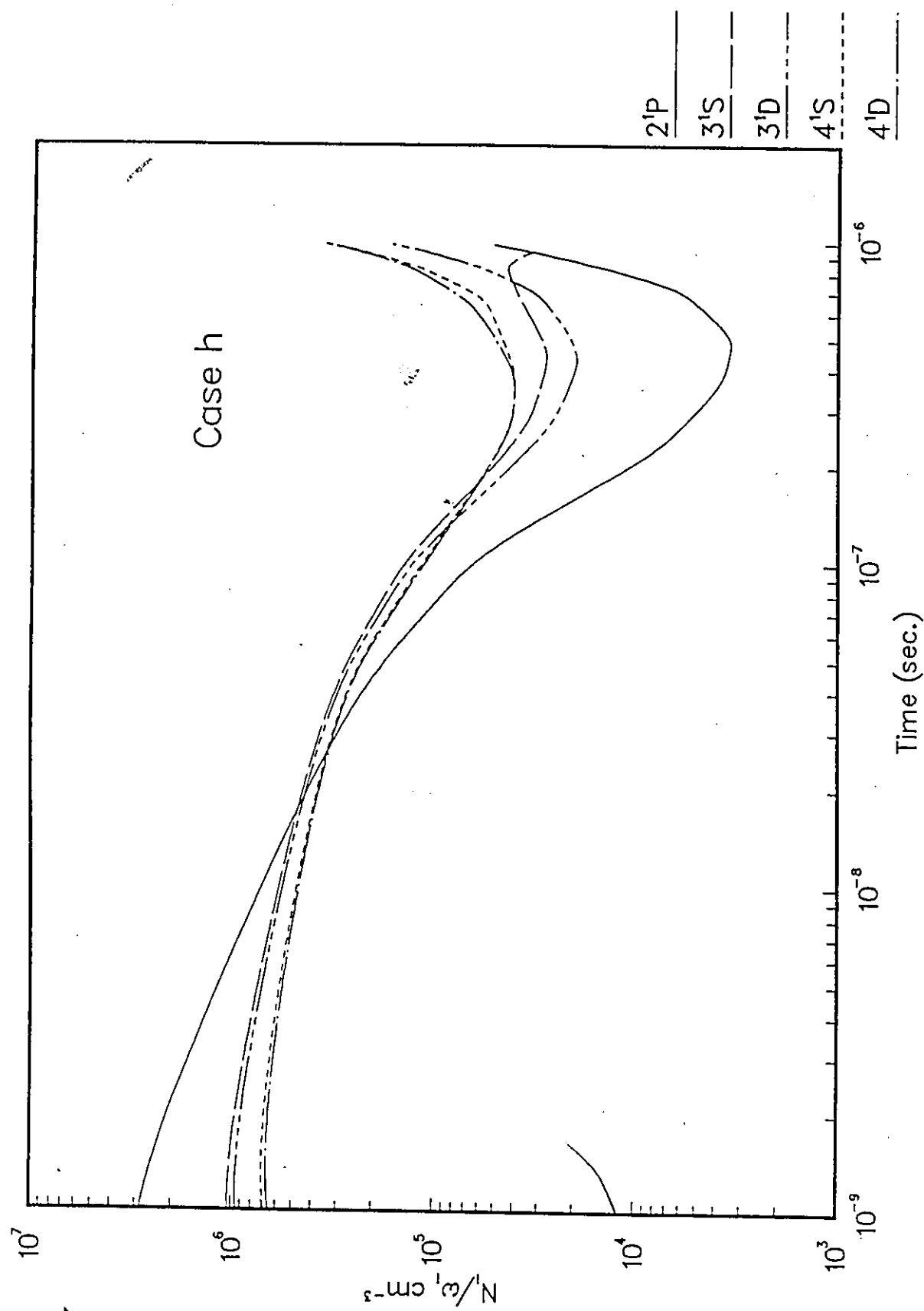


Fig. 3-10. Population densities vs. time for some levels in He I

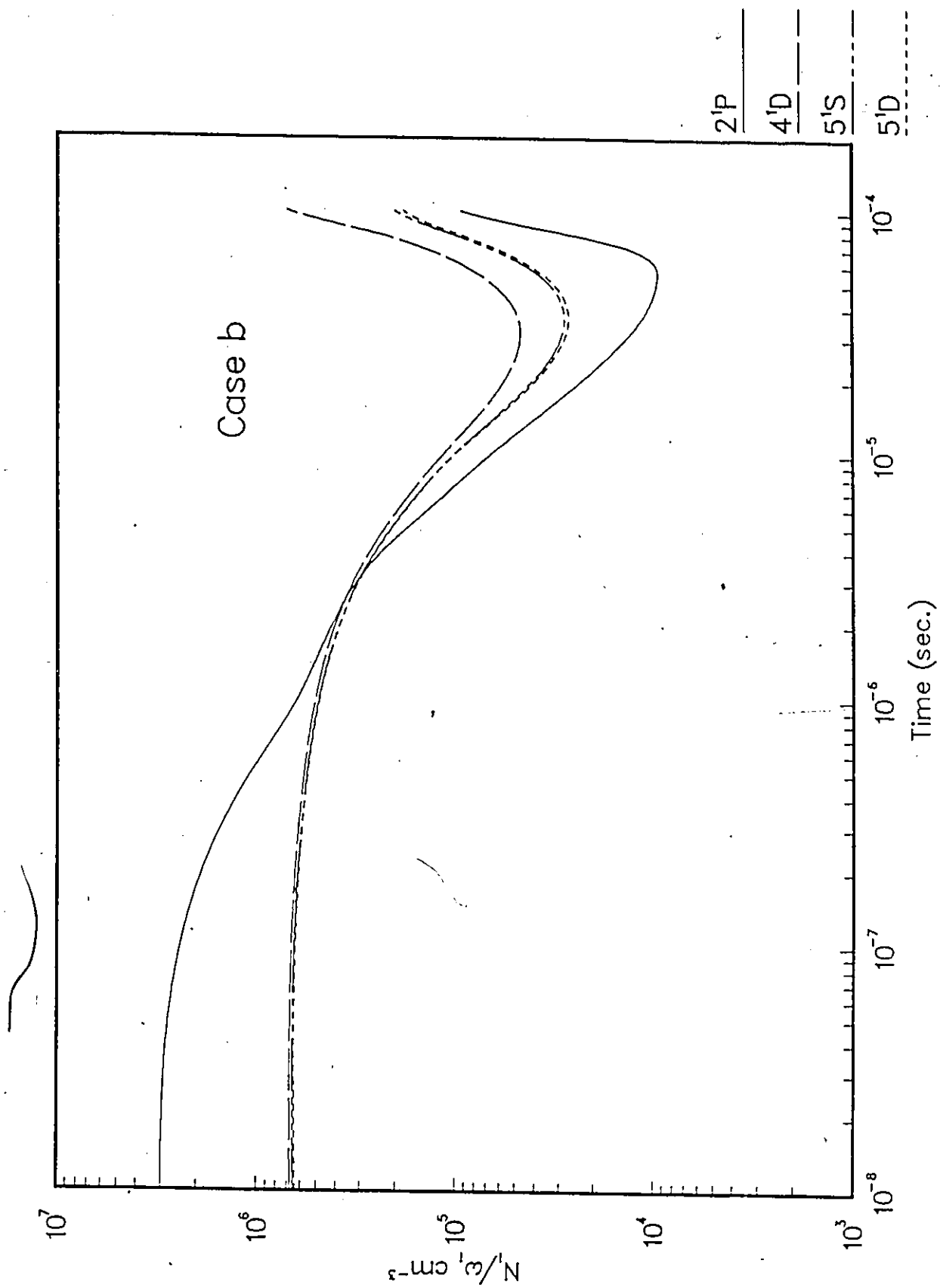


Fig. 3-11. Population densities vs. time for some levels in He I

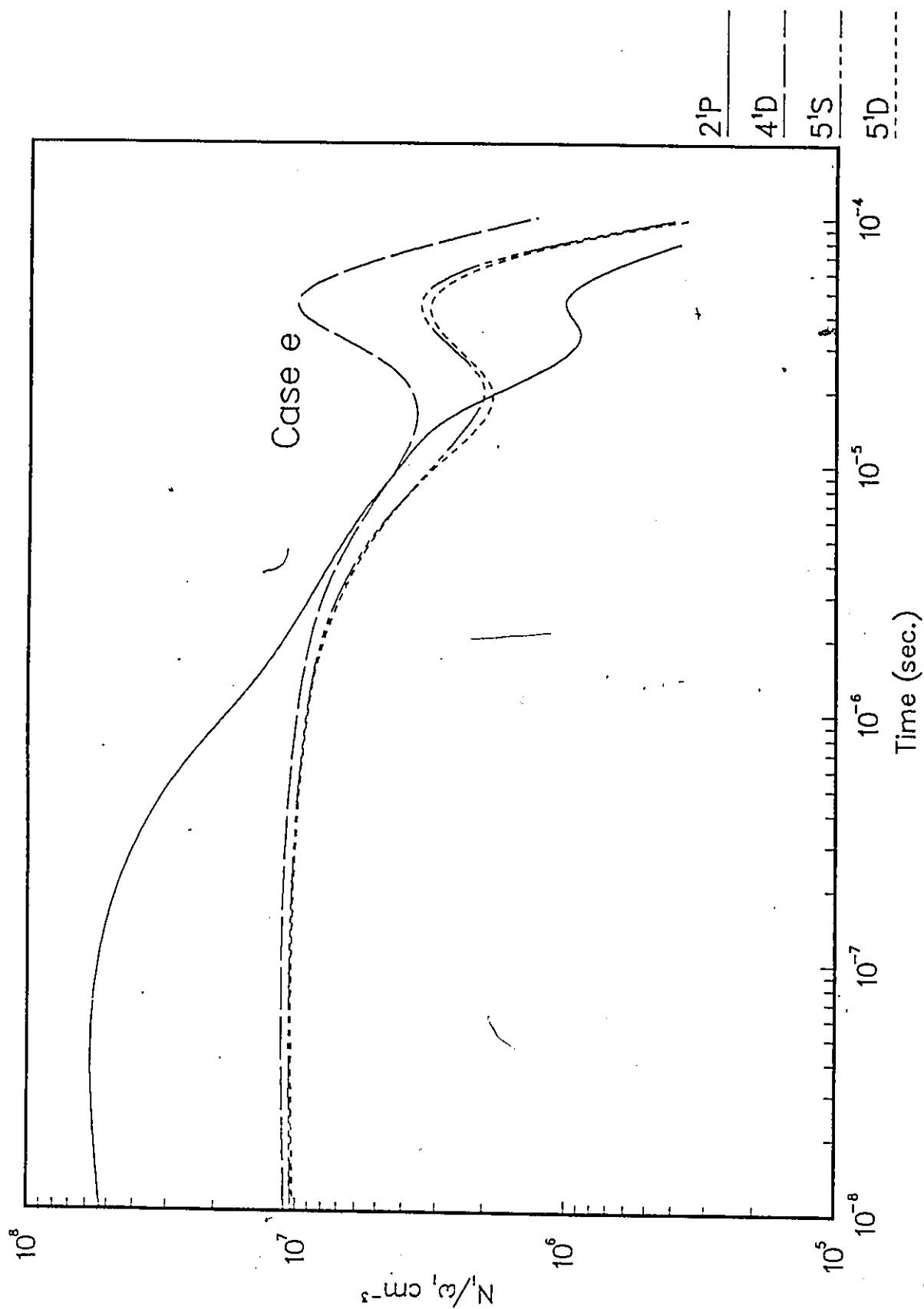


Fig. 3-12. Population densities vs. time for some levels in He I

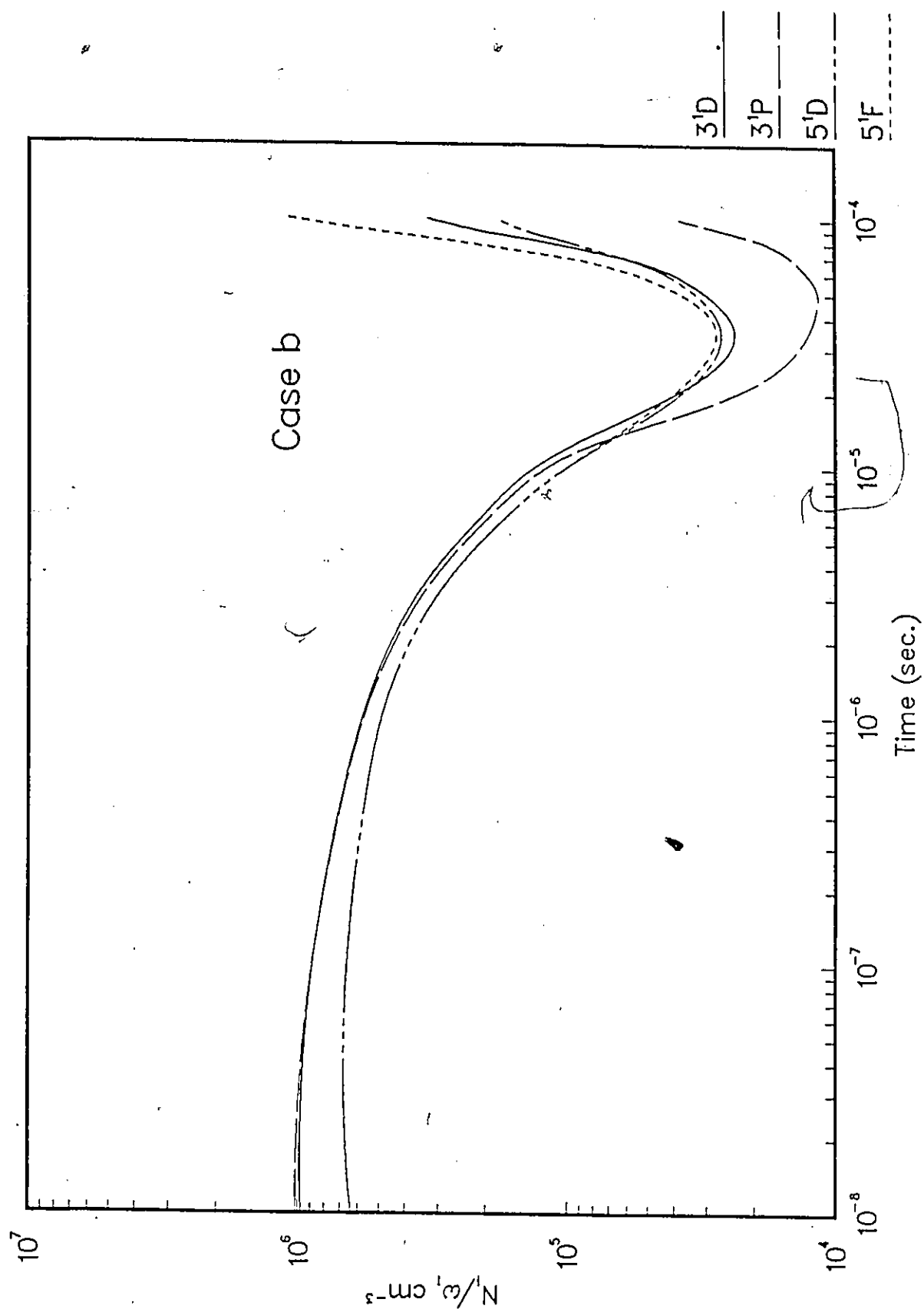


Fig. 3-13. Population densities vs. time for some levels in He I

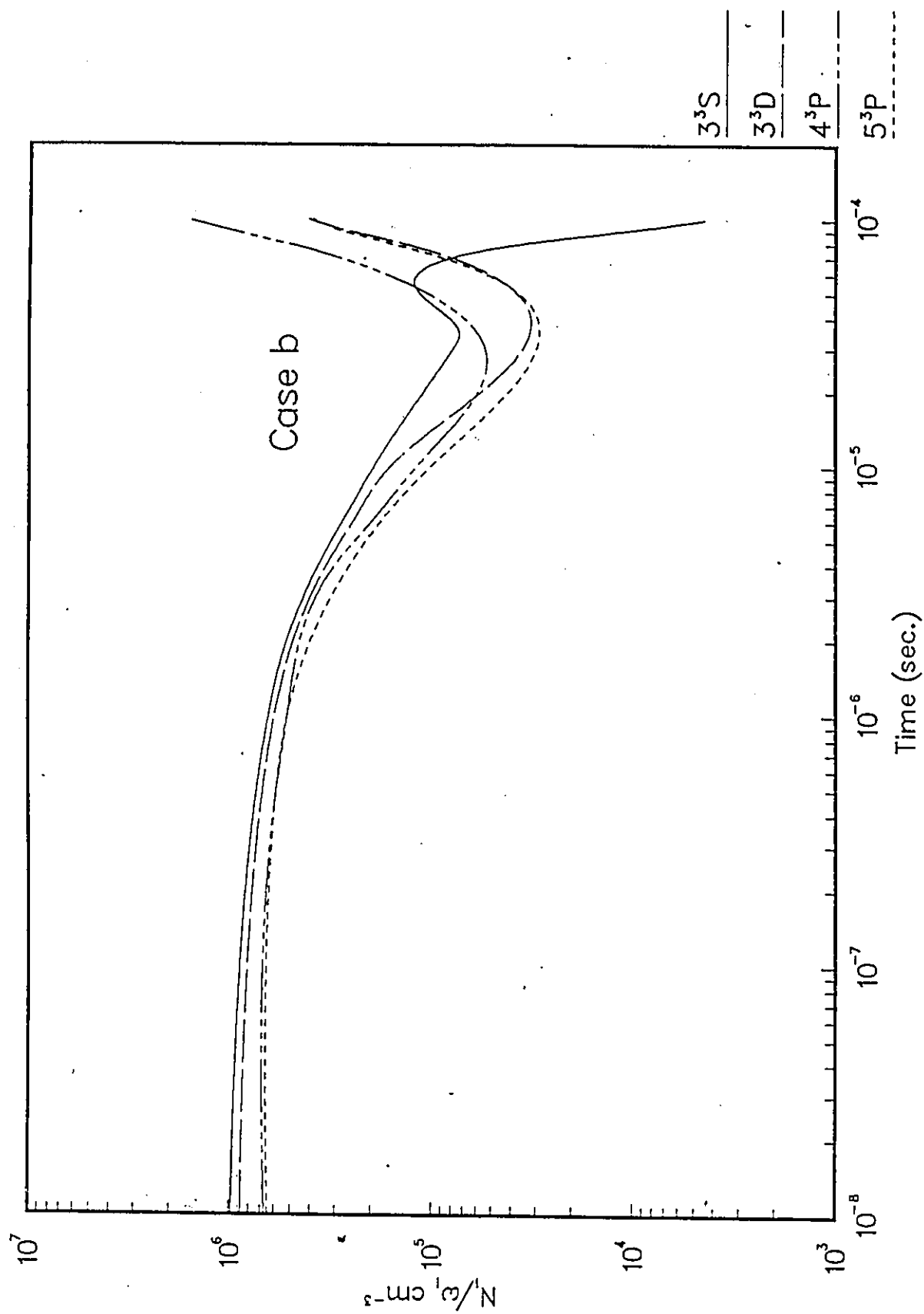


Fig. 3-14. Population densities vs. time for some levels in He I

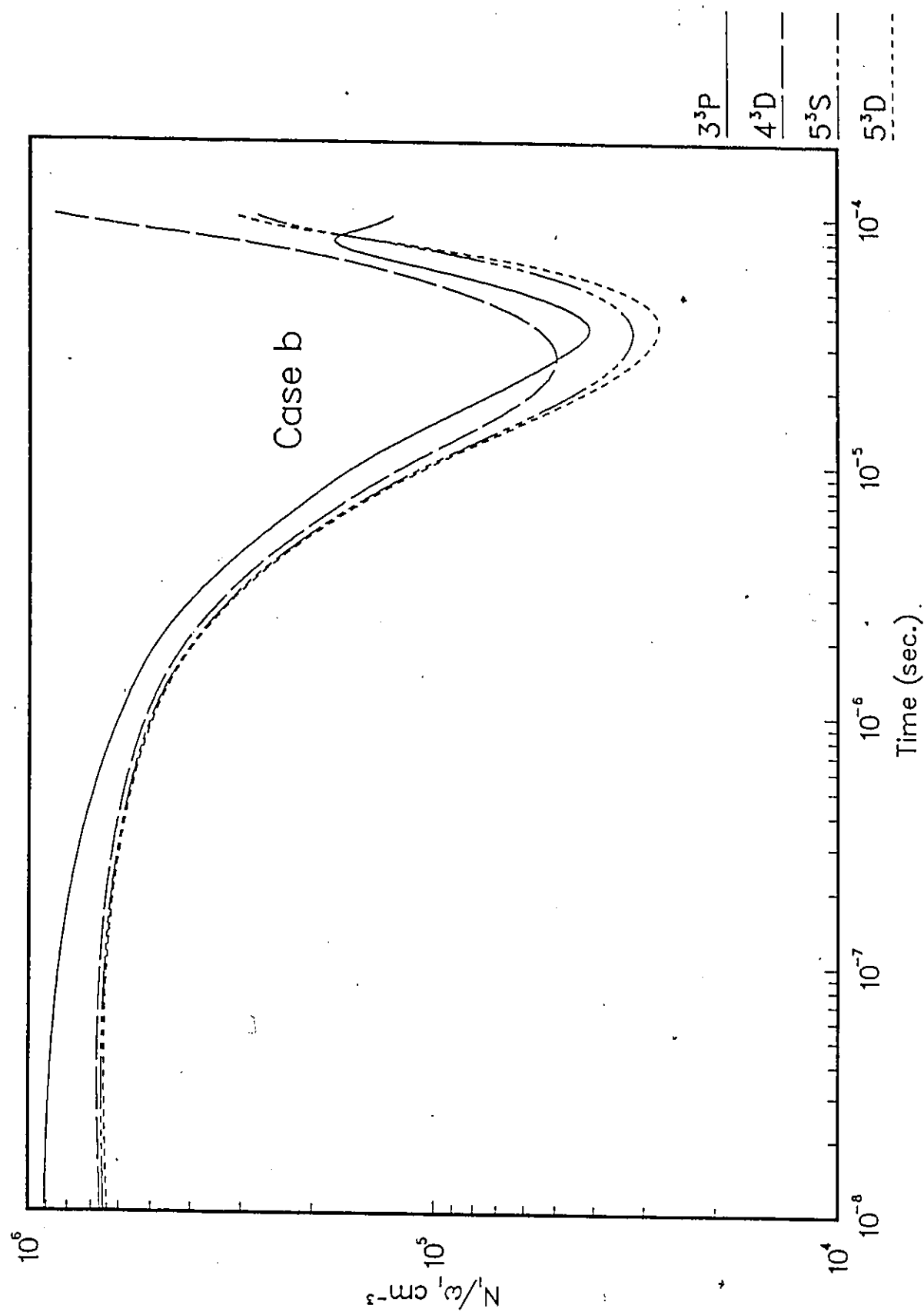


Fig. 3-15. Population densities vs. time for some levels in He I

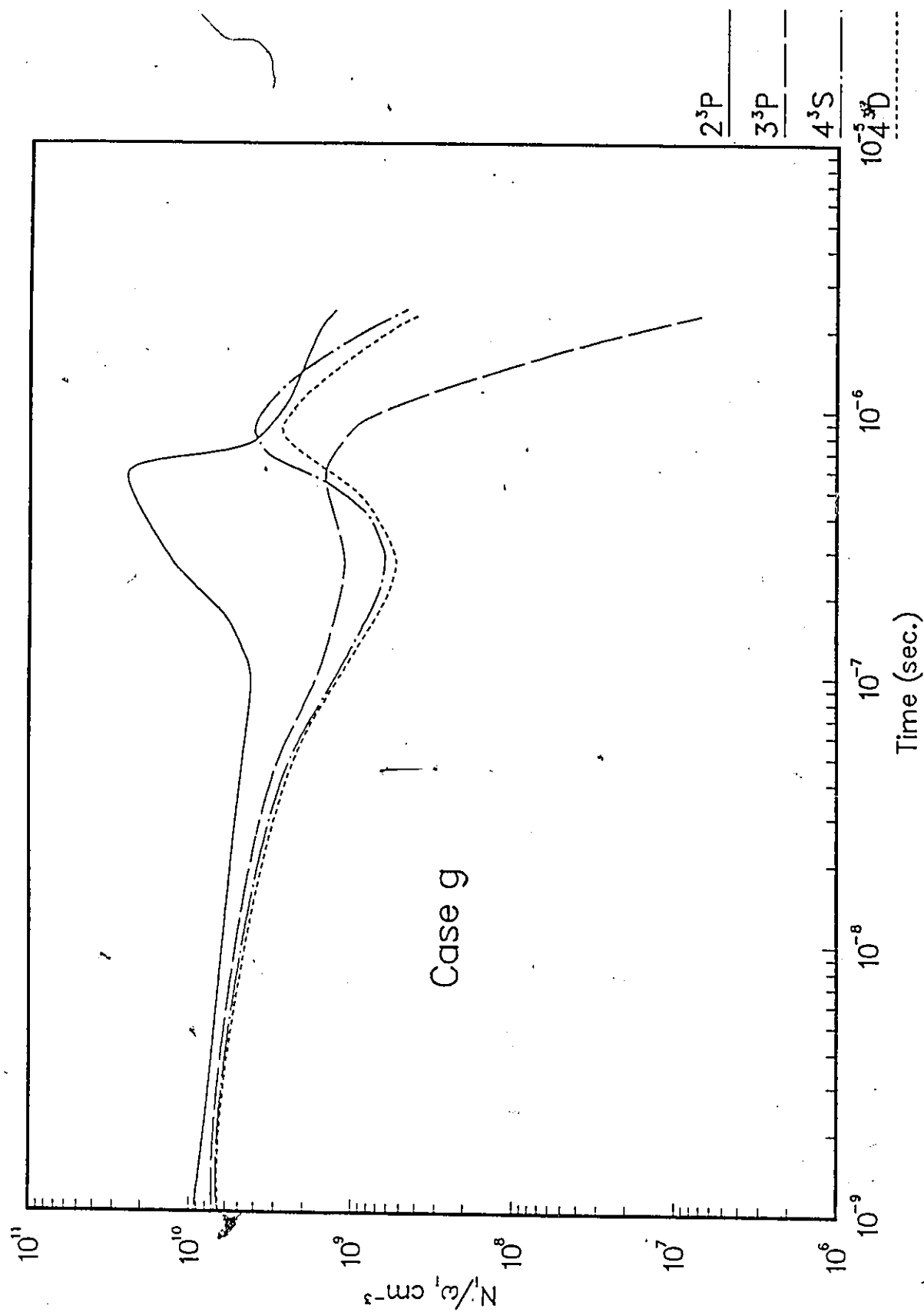


Fig. 3-16. Population densities vs. time for some levels in He I

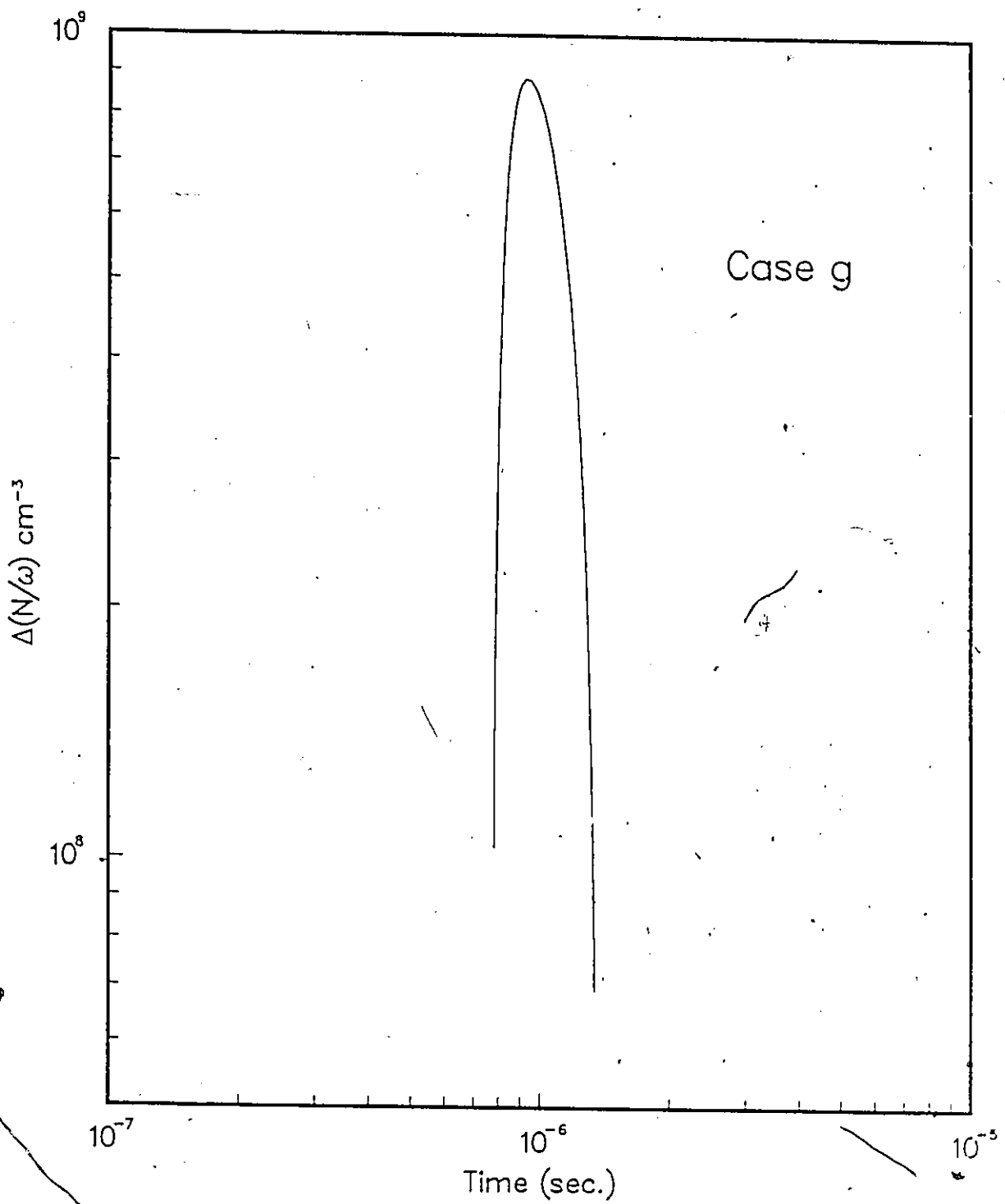


Fig. 3-17. Population inversion vs. time for $4^3\text{S}-2^3\text{P}$ line

Chapter 4

Oscillator strengths of C III lines.

A) Introduction.

There have been a number of previous theoretical calculations on the oscillator strength of C III transitions, both allowed and forbidden (Pfeennig *et al.*, 1965; Steele and Treffitz, 1966; Nussbaumer, 1972; Nicolaides *et al.*, 1973; Hummer and Norcross, 1974; Hibbert, 1974, 1976, 1979; Glass and Hibbert, 1978; Nussbaumer and Storey, 1978; Laughlin *et al.*, 1978; Glass, 1979, 1981, 1982; Zuplyauskis, 1980; Markiewicz *et al.*, 1981; Cowan *et al.*, 1982). It is generally considered that the best results are expected from configuration interaction wavefunctions. However, most of the calculations using such wavefunctions are confined to a few transitions between low lying levels, the largest number of transitions -24- have been calculated by Hummer and Norcross (1974). Glass (1981) has calculated the oscillator strengths of all the transitions between states having the principal quantum number $n = 4$ for the triplet system.

Accurate oscillator strength is needed also in calculating the cross sections. For electric dipole transitions, approximate collision cross sections can be obtained from the radiative transition probabilities by using the impact parameter method. Caution is, of course, necessary in those cases where the oscillator strength is very small due to cancellation effects; the dipole term may then no longer be the dominant contribution to the cross section. In this chapter we report the calculated values of oscillator strengths for all allowed transitions between the 40 lowest terms of C III ion, which is needed in this work.

B) Method of calculation.

The atomic structure model used in the present calculation is the one described by Burke *et al.* (1972). We used the general program CIV3 (Hibbert, 1975) to generate the

configuration- interaction (CI) wave functions. To summarize briefly, the radial functions used in the calculations were determined in an LS-coupled representation of the atomic states. The atomic state wave functions are represented by the CI expansion

$$\Psi(LS) = \sum_{i=1}^N a_i \Phi_i(\alpha_i LS) \quad (4-1)$$

where L and S are the total orbital and spin momenta, N is the total number of configurational wave functions, and α_i specifies the angular momentum coupling scheme of the i th configuration. Each configuration wave function is defined with respect to its subshells:

$$\Phi_i(\alpha_i LS) = \{ (1s)^{\lambda_1} (\alpha_1 S_1 L_1) (2s)^{\lambda_2} (\alpha_2 S_2 L_2) \cdots; \alpha SL \} \quad (4-2)$$

so that associated with each subshell, of occupancy λ_i , is a set of quantum numbers ($\alpha s \ell$) defining seniority, spin and orbital angular moments. The radial part of the orbital is written in Roothaan-form

$$P_{n\ell}(r) = \sum_{j=1}^k C_{jn\ell} r^{I_{jn\ell}} \exp(-\zeta_{jn\ell} r) \quad (4-3)$$

and $k \geq n - \ell$, so that the orthonormality condition

$$\int_0^\infty P_{n\ell}(r) P_{n'\ell'}(r) dr = \delta_{nn'} \quad \ell + 1 \leq n' \leq n \quad (4-4)$$

can be satisfied.

For $k = n - \ell$ the coefficients $\{C_{jn\ell}\}$ are uniquely determined by the orthonormality condition (4-4) for a given choice of $\{I_{jn\ell}, \zeta_{jn\ell}\}$. For $k > n - \ell$ some of the coefficients $\{C_{jn\ell}\}$ can be treated as variational parameters.

The eigenvalues of the Hamiltonian matrix with element $\langle \Phi_i | H | \Phi_i \rangle$, where H is the non-relativistic Hamiltonian operator, form upper bounds to the corresponding exact

energies, and the coefficient $\{a_i\}$ in (4-1) are given by the components of the associated eigenvectors. A different choice of $\{\zeta_{jnl}\}$ would lead to different eigenvalues. Because of the upper bound property, it is possible to treat an eigenvalue as a function to be minimized with respect to the orbital exponent $\{\zeta_{jnl}\}$ (Hibbert, 1974). The value of $\{I_{jnl}\}$ have been taken to satisfy

$$I_{1nl} = \ell + 1$$

$$I_{j+1,nl} = I_{jnl} + 1, \quad j \geq 1. \quad (4-5)$$

If only one configuration is retained in the expansion (4-1), this process yields an approximate solution of Hartree-Fock (HF) equations and the corresponding orbitals will be the HF orbitals. If further configurations are retained in the expansion involving additional orbitals then usually these orbitals will be nonphysical. Such orbitals are usually referred to as pseudo-orbitals (Weiss, 1967, 1972; Burke and Robb, 1975) and are distinguished by putting a bar over them.

The 1s, 2s and 2p radial functions were taken as the HF function of the $1s^2 2s2p \ ^1P^o$ state (Tatewaki et al., 1971). The 3p radial function were taken from the $1s^2 2s3p \ ^3P^o$ state optimizing on the second lowest state $^3P^o$ eigenvalue of the two configurations wave function:

$$1s^2 2s2p, \quad 1s^2 2s3p \quad (4-6)$$

The 3s radial function were taken from $1s^2 2s3s \ ^1S$ state optimizing on the third lowest 1S eigenvalues of the four configurations wave function:

$$1s^2 2s^2, \quad 1s^2 \underline{2p^2}, \quad 1s^2 2s3s, \quad 1s^2 2p3p \quad (4-7)$$

From $1s^2 2s3d \ ^1D$ state optimizing on the second lowest 1D eigenvalue of the three configurations wave function:

$$1s^2 2p^2, \ 1s^2 2s3d, \ 1s^2 2p3p \quad (4-8)$$

we obtained the 3d function. The 4s and 4d functions were taken from $1s^2 2s4s \ ^1S$ and $1s^2 2s4d \ ^1D$ states optimizing on the fourth lowest 1S and third lowest 1D eigenvalues respectively of the configurations wave functions:

$$1s^2 2s^2, \ 1s^2 2p^2, \ 1s^2 2s3s, \ 1s^2 2s4s, \ 1s^2 2p3p \text{ and} \\ 1s^2 2p^2, \ 1s^2 2s3d, \ 1s^2 2s4d, \ 1s^2 2p3p. \quad (4-9)$$

The 4p radial function was taken from the $1s^2 2s4p \ ^3P^o$ state optimizing on the fourth lowest $^3P^o$ eigenvalue of the four configurations wave function:

$$1s^2 2s2p, \ 1s^2 2s3p, \ 1s^2 2p3s, \ 1s^2 2s4p \quad (4-10)$$

The 4f radial function was taken from the $1s^2 2s4f \ ^1F^o$ state optimizing on the lowest $^1F^o$ eigenvalue of the two configurations wave function:

$$1s^2 2s4f, \ 1s^2 2p3d \quad (4-11)$$

The 5s and 5d radial functions were taken from the $1s^2 2s5s \ ^1S$ and $1s^2 2s5d \ ^1D$ states optimizing on the fifth lowest 1S and 1D eigenvalues respectively of the configurations wave functions:

$$1s^2 2s^2, \ 1s^2 2p^2, \ 1s^2 2s3s, \ 1s^2 2s4s, \ 1s^2 2s5s, \ 1s^2 2p3p \text{ and} \\ 1s^2 2p^2, \ 1s^2 2s3d, \ 1s^2 2s4d, \ 1s^2 2p3p, \ 1s^2 2s5d. \quad (4-12)$$

From the $1s^2 2s5p \ ^3P^o$ state optimizing on the fifth lowest $^3P^o$ eigenvalue of the five configurations wave function:

$$1s^2 2s2p, \ 1s^2 2s3p, \ 1s^2 2p3s, \ 1s^2 2s4p, \ 1s^2 2s5p \quad (4-13)$$

we obtained the 5p radial function. The 5f radial function was taken from the $1s^2 2s5f \ ^1F^o$ state optimizing on the third lowest $^1F^o$ eigenvalue of the three configurations wave function:

$$1s^2 2s4f, \ 1s^2 2p3d, \ 1s^2 2s5f. \quad (4-14)$$

The 5g radial function was taken from the $1s^2 2s5g \ ^3G$ state. In Table 4-1 we present the orbital exponents used in the calculation. We calculate correlation orbital up to $n = 6$ level.

C) Results.

Using the radial functions determined in the previous section, CI wave functions (4-1) were determined by including, for each symmetry, all possible configurations formed from these orbitals with constraint that the 1s shell remain fully occupied and not more than one electron in the 4f, 5f, $6\bar{f}$, 5g, $6\bar{g}$ shells. These CI wave functions were used in evaluated energy levels, and oscillator strengths for all allowed transitions between the $2sn\ell$ ($n \leq 5, \ell \leq 4$) ; $2p^2$; $2p3\ell$ ($\ell \leq 2$) states.

a) Energy levels

The energy of the 40 lower states in the C III ion were calculated using the common set of orbital exponents given in Table 4-1, with the pseudo-orbitals $6\bar{s}$, $6\bar{p}$, $6\bar{d}$, $6\bar{f}$, $6\bar{g}$ optimized on the lower state (and on second lower state in some cases) of the series $1s^2 2\ell n\ell' \ ^{2S+1}L$, $n \leq 5$. For example, the orbital exponents of $6\bar{s}$, $6\bar{p}$, $6\bar{f}$, and $6\bar{g}$ were

optimized on the ground state and the orbital exponent of $6\bar{d}$ were optimized on $2p^2 \ ^1S$ state in calculating the energies of $1s^2 2s^2 \ ^1S$, $1s^2 2p^2 \ ^1S$, $1s^2 2s3s \ ^1S$, $1s^2 2s4s \ ^1S$, $1s^2 2s5s \ ^1S$ and $1s^2 2p3p \ ^1S$ states. The wave functions settled on consisted of following:

38 configurations for the $1s^2 2\ell n \ell' \ ^1S$ series,

34 configurations for the $1s^2 2\ell n \ell' \ ^1P^o$ series,

40 configurations for the $1s^2 2\ell n \ell' \ ^1D$ series,

25 configurations for the $1s^2 2\ell n \ell' \ ^1F^o$ series,

14 configurations for the $1s^2 2s5g \ ^1G$ state,

30 configurations for the $1s^2 2\ell n \ell' \ ^3S$ series,

34 configurations for the $1s^2 2\ell n \ell' \ ^3P^o$ series,

32 configurations for the $1s^2 2\ell n \ell' \ ^3D$ series,

25 configurations for the $1s^2 2\ell n \ell' \ ^3F^o$ series,

14 configurations for the $1s^2 2s5g \ ^3G$ state,

12 configurations for the $1s^2 2p^2 \ ^3P^e$ state,

where $n \leq 5$ and $0 \leq \ell \leq 1$. The energies and the dominant structure of the S, P, D, F and G singlet and triplet levels up to and including $n = 5$ along with the observed energy levels are summarized in Table 4-2, the complete wave functions are not given – only those configurations with weight coefficient greater than 0.05 for any state are listed. Agreement with the observed data (Moore, 1970; Bashkin and Stoner, 1975) is very good, within 1.5%.

b) Oscillator strengths

The length and velocity forms of the electric dipole oscillator strengths, for transitions between initial and final states with normalized wave functions Ψ_i and Ψ_f and energies E_i and E_f respectively, are given

$$f_l = \frac{2}{3} \frac{(E_f - E_i)}{(2L_i + 1)(2S_i + 1)} \sum | \langle \Phi_i | \sum_{p=1}^N r_p | \Psi_f \rangle |^2 \quad (4-15)$$

$$f_v = \frac{2}{3} \frac{(E_f - E_i)^{-1}}{(2L_i + 1)(2S_i + 1)} \sum | \langle \Phi_i | \sum_{p=1}^N \nabla_p | \Psi_f \rangle |^2 \quad (4-16)$$

where the inner summation is over the N electrons, and the outer summation is over the M_L, M_S degeneracies of each state.

Oscillator strengths for all allowed electric dipole transitions among the 40 lowest terms in C III were calculated. Both the length and velocity forms of the oscillator strength were used. The program CIV3 assumes that the two states of a transition use the same set of radial functions. Generally some of the 6ℓ functions were optimized on the energy of one of the states, while the remaining ones were optimized on the energy of the other state in the transition. For example, in the $1s^2 2sn\ell' {}^1S^e \rightarrow 1s^2 2\ell n\ell' {}^1P^o$ transitions, the $6\bar{s}$ function was optimized on the ground state and $6\bar{p}, 6\bar{d}, 6\bar{f}, 6\bar{g}$ were optimized on the lower state in the series $1s^2 2\ell n\ell' {}^1P^o$, that is $1s^2 2s2p {}^1P^o$. Similarly for the $1s^2 2p^2 {}^1S^e \rightarrow 1s^2 2\ell n\ell' {}^1P^o$ transitions, the $6\bar{s}, 6\bar{p}, 6\bar{d}$ were optimized on the lower state of the series $1s^2 2\ell n\ell' {}^1P^o$, which is $1s^2 2s2p {}^1P^o$. This balancing of the effect of correlation orbital is necessary for a reasonably good evaluation of the energy difference between the two states in a transition. The energies shown in Table 4-2 and the energies of the states involved in the transition calculated using the common correlation orbitals are in agreement to within a few units in the last digit. Generally, the calculated ΔE (the energy difference of the two states in a transition) and the experimental ΔE are in good agreement, except in such cases where the two states are very close to each other.

All configurations included in the energy calculations were also included in the oscillator strength calculations the result of which are given in Tables 4-3 to 4-9. Theoretical ΔE

values were used in the calculation of oscillator strengths. The transition wavelengths (Moore, 1970; Bashkin and Stoner, 1975) are also shown in the second column of Tables 3-4 to 4-9. Some of the results are compared with those of available CI calculations and of other approaches to *ab initio* multiconfiguration calculations and with available experimental data in Table 4-10.

Generally speaking, our results are in satisfactory agreement with those of previous CI calculations (Nussbaumer, 1972; Hummer and Norcross, 1974; Hibbert, 1974, 1976; Nussbaumer and Storey, 1978; Glass, 1979, 1981, 1982). Our results are quite close to those of Glass (1979). As Table 4-10 shows there are several transitions for which experimental values are available. The agreement between our values and these experimental values is quite reasonable.

Where there is disagreement between the length and velocity forms of the oscillator strength (f_l and f_v), it seems that this discrepancy partly comes from neglecting inner-shell correlation (the velocity value could change by up to 10% by including the inner-shell effects, Hibbert, 1974) and partly from the lack of convergence in the outer shells. Moreover, it was found that as more configurations were included in the calculation, the oscillator strength (particularly the length form) changed slightly mainly as a result of the change in the theoretical ΔE ; only in some cases the cumulative or cancellation effects were important enough, so that the changes become sometime very large, especially for small oscillator strengths.

TABLE 4-1. Radial orbital parameters.

Orbital	I_{jne}	S_{jne}	Orbital	I_{jne}	S_{jne}
1s	1	5.132	3p	2	1.922
	1	8.519		3	1.007
	2	2.012			
	2	4.738	4p	2	1.698
	2	1.571		3	0.995
2s				4	0.733
	1	5.132	5p	2	0.584
	1	8.519		3	0.977
	2	2.012		4	0.747
	2	4.738		5	0.559
	2	1.571			
3s	1	4.200	3d	3	1.079
	2	1.847	4d	3	1.000
	3	1.158		4	0.706
4s	1	4.826	5d	3	0.953
	2	0.798		4	0.760
	3	1.004		5	0.534
	4	0.904	4f	4	0.690
5s	1	4.328		4	0.732
	2	0.523	5f	5	0.561
	3	1.686			
	4	1.199	5g	5	0.603
	5	0.605			
2p	2	1.475			
	2	3.194			
	2	1.831			
	2	9.485			

TABLE 4-2. Energy levels and configuration interaction.

State	E (calc.) (eV)	E (expt.) (eV)	configuration interaction
$(1s^2) 2s^2 \ ^1S$	0.0	0.0	$-0.961(2s^2)+0.27(2p^2) +0.052(2s3s)$
$2s2p \ ^3P^o$	6.555	6.499	$0.996(2s2p)+0.05(2s3p)$
$2s2p \ ^1P^o$	12.879	12.691	$0.989(2s2p)-0.1(2p3d) +0.09(2p6d)$
$2p^2 \ ^3P$	17.179	17.049	$0.998(2p^2)$
$2p^2 \ ^1D$	18.149	18.087	$0.98(2p^2)-0.14(2s3d)-0.05(2s4d) +0.09(2s6d)$
$2p^2 \ ^1S$	22.982	22.631	$0.27(2s^2)+0.945(2p^2)+0.14(2s3s) +0.05(3d6d)$ $-0.05(6d^2)$
$2s3s \ ^3S$	29.602	29.536	$0.98(2s3s)+0.06(2s4s)+0.16(2p3p)$
$2s3s \ ^1S$	30.770	30.647	$-0.137(2p^2)+0.95(2s3s)-0.08(2s4s) +0.21(2p3p)$ $+0.05(2p4p)-0.11(3s^2)$
$2s3p \ ^1P^o$	32.109	32.105	$0.95(2s3p)+0.28(2p3s)+0.08(2p3d) -0.06(3s3p)$
$2s3p \ ^3P^o$	32.260	32.202	$0.98(2s3p)+0.07(2p3s)+0.1(2p3d) -0.09(3s3p)$ $-0.05(2s2p)$
$2s3d \ ^3D$	33.541	33.479	$-0.98(2s3d)-0.13(2p3p)+0.08(3s3d) +0.05(2p6f)$
$2s3d \ ^1D$	34.421	34.281	$0.12(2p^2)+0.97(2s3d)-0.11(2s4d) +0.09(2p3p)$ $-0.05(2s5d)-0.09(3s3d)-0.05(3p6p)$
$2p3s \ ^3P^o$	38.224	38.224	$0.07(2s3p)-0.98(2p3s)+0.12(2p3d) +0.09(3s3p)$
$2s4s \ ^3S$	38.419	38.370	$-0.09(2s3s)+0.97(2s4s)+0.19(2p3p) +0.08(2p4p)$ $-0.09(3s4s)$
$2p3s \ ^1P^o$	38.530	38.438	$0.22(2s3p)-0.73(2p3s)-0.62(2s4p) -0.11(2s5p)$ $-0.1(3s3p)+0.07(2s6p)$
$2s4s \ ^1S$	38.664	38.650	$-0.96(2s4s)+0.09(2s5s)-0.21(2p3p) +0.08(2p4p)$ $+0.09(3s4s)-0.05(4s^2)$
$2s4p \ ^3P^o$	39.453	39.404	$-0.98(2s4p)-0.12(2p3d) +0.09(3s4p)$
$2s4d \ ^3D$	39.898	39.855	$0.9(2s4d)+0.4(2p3p)+0.05(2s5d) -0.09(3s4d)$ $+0.06(2p4p)$

TABLE 4-2. (Continued)

State	E (calc.) (eV)	E (expt.) (eV)	configuration interaction
2s4f $^3F^\circ$	39.963	39.925	0.9(2s4f)-0.4(2p3d)-0.09(3s4f) +0.17(2s5f) +0.05(2s6f)
2s4f $^1F^\circ$	40.048	40.012	-0.95(2s4f)+0.25(2p3d)-0.16(2s5f) +0.09(3s4f)
2s4p $^1P^\circ$	40.148	39.975	-0.12(2s3p)+0.57(2p3s)-0.76(2s4p) +0.12(2s5p) -0.10(2p3d)-0.14(2p4s)+0.07(3s3p)+0.09(3s4p) +0.11(2s6p)
2p3p 3D	40.162	40.063	-0.12(2s3d)-0.42(2s4d) +0.895(2p3p)
2s4d 1D	40.217	40.199	0.07(2p ²)+0.1(2s3d)+0.98(2s4d) -0.09(2p4f)
2p3p 3S	40.704	40.579	0.14(2s3s)+0.19(2s4s)-0.15(2s5s) -0.95(2p3p) +0.06(2s6s)+0.05(2p6p)
2p3p 1D	41.434	41.303	-0.08(2s3d)+0.05(2s4d)+0.97(2p3p) -0.08(2s5d) +0.06(2s6d)-0.09(2p4p)-0.05(2p5p)+0.14(3p ²)
2p3d $^3F^\circ$	41.439	41.337	0.43(2s4f)+0.88(2p3d)+0.07(3p3d) -0.17(2s5f) -0.07(2s6f)-0.06(2p6d)
2s5s 1S	42.065	41.972	0.9(2s5s)-0.09(2s6s)+0.4(2p3p) -0.09(3s5s)
2s5s 3S	42.152	42.149	-0.06(2s4s)-0.98(2s5s)+0.07(2s6s) +0.15(2p3p) +0.09(3s5s)
2p3d $^3P^\circ$	42.336	42.171	-0.09(2s3p)+0.09(2p3s)-0.11(2s4p) +0.58(2s5p) +0.79(2p3d)+0.07(3p3d)-0.056(3s5p)
2p3d $^1F^\circ$	42.496	42.327	-0.3(2s4f)-0.72(2p3d)+0.61(2s5f) +0.06(2p4d) -0.09(3p3d)+0.09(2s6f)-0.05(3s5f)
2s5p $^1P^\circ$	42.565	42.561	-0.13(2p3s)+0.92(2s5p)+0.33(2p3d) -0.09(3s5p) +0.11(2p4s)
2s5p $^3P^\circ$	42.826	42.681	0.06(2s3p)-0.06(2p3s)+0.05(2s4p) +0.81(2s5p) -0.57(2p3d)-0.05(3p3d)-0.07(3s5p)+0.06(2p4s) 0.052(3p4d)

TABLE 4-2. (Continued)

State	E (calc.) (eV)	E (expt.) (eV)	configuration interaction
2s5d 3D	42.850	42.838	$0.06(2s4d) - 0.99(2s5d) - 0.095(3s5d)$
2p3p 1S	42.978	42.790	$0.16(2s3s) + 0.15(2s4s) + 0.44(2s5s) + 0.23(2s6s)$ $- 0.77(2p3p) + 0.24(2p4p) + 0.11(2p5p) - 0.11(3p^2)$
2s5g 3G	42.980	42.972	$- 0.99(2s5g) + 0.1(3s5g) + 0.05(2p4f)$
2s5d 1D	42.996	42.982	$- 0.08(2p3p) - 0.99(2s5d) - 0.09(3s5d)$
2s5g 1G	43.182	42.972	$- 0.99(2s5g) + 0.10(3s5g) + 0.05(2p4f)$
2p3d $^1P^o$	43.345	42.990	$- 0.08(2s2p) + 0.09(2s3p) - 0.05(2p3s) + 0.08(2s4p)$ $+ 0.27(2s5p) - 0.92(2p3d) - 0.11(3p3d) + 0.16(2p4d)$ $+ 0.06(2p4s) + 0.08(2p5d) - 0.11(2p6d)$
2s5f $^3F^o$	43.069	43.044	$- 0.08(2s4f) + 0.23(2p3d) + 0.97(2s5f) - 0.09(3s5f)$
2s5f $^1F^o$	43.442	43.255	$- 0.6(2p3d) - 0.75(2s5f) + 0.11(2p4d) - 0.08(3p3d)$ $+ 0.09(2s6f) + 0.07(3s5f)$

TABLE 4-3. Absorption oscillator strengths for the transitions between $1s^2 2\ell n\ell' {}^1S$ and $1s^2 2\ell m\ell' {}^1P^o$ states ($n, m < 6$ and $0 \leq \ell \leq 1$).

Transition	λ (Å)	f_t	f_o
$(1s^2) 2s^2 {}^1S \rightarrow 2s2p {}^1P^o$	977.03	0.772	0.769
$\rightarrow 2s3p {}^1P^o$	386.20	0.222	0.223
$\rightarrow 2p3s {}^1P^o$	322.57	0.0425	0.040
$\rightarrow 2s4p {}^1P^o$	310.17	0.0320	0.0356
$\rightarrow 2s5p {}^1P^o$	291.33	0.0422	0.0436
$\rightarrow 2p3d {}^1P^o$	288.42	0.0064	0.0067
$2p^2 {}^1S \rightarrow 2s3p {}^1P^o$	1308.70	0.0272	0.0237
$\rightarrow 2p3s {}^1P^o$	784.39	0.1120	0.1190
$\rightarrow 2s4p {}^1P^o$	714.88	0.0686	0.0663
$\rightarrow 2s5p {}^1P^o$	622.13	0.0530	0.0546
$\rightarrow 2p3d {}^1P^o$	609.04	0.9300	0.8740
$2s3s {}^1S \rightarrow 2s3p {}^1P^o$	8500.32	0.3270	0.3720
$\rightarrow 2p3s {}^1P^o$	1591.44	0.6860	0.6210
$\rightarrow 2s4p {}^1P^o$	1329.19	0.0380	0.0480
$\rightarrow 2s5p {}^1P^o$	1040.72	0.0028	0.0013
$\rightarrow 2p3d {}^1P^o$	1004.60	0.0539	0.0442
$2s4s {}^1S \rightarrow 2s4p {}^1P^o$	9358.37	0.8410	0.8400
$\rightarrow 2s5p {}^1P^o$	3170.02	0.0950	0.0840
$\rightarrow 2p3d {}^1P^o$	2857.01	0.0142	0.0098
$2s5s {}^1S \rightarrow 2s5p {}^1P^o$	21081	1.1690	0.9700
$2s2p {}^1P^o \rightarrow 2p^2 {}^1S$	1247.40	0.1670	0.1770
$\rightarrow 2s3s {}^1S$	690.53	0.0208	0.0214
$\rightarrow 2s4s {}^1S$	477.62	0.0032	0.0033
$\rightarrow 2s5s {}^1S$	423.44	3.1E-4	3.3E-4

TABLE 4-3. (Continued)

Transition	λ (Å)	f_l	f_v
$2s2p\ ^1P^\circ \rightarrow 2p3p\ ^1S$	411.96	0.0051	0.0049
$2s3p\ ^1P^\circ \rightarrow 2s4s\ ^1S$	1894.90	0.1010	0.1013
$\rightarrow 2s5s\ ^1S$	1256.22	0.0211	0.0207
$2p3s\ ^1P^\circ \rightarrow 2s4s\ ^1S$	8065.90	0.0156	0.0072
$\rightarrow 2s5s\ ^1S$	3506.78	2.4E-3	4.5E-3
$\rightarrow 2p3p\ ^1S$	2849.10	0.0642	0.0850
$2s4p\ ^1P^\circ \rightarrow 2s5s\ ^1S$	6205.56	0.2530	0.2360
$\rightarrow 2p3p\ ^1S$	4407	9.8E-4	1.3E-3

TABLE 4-4. Absorption oscillator strengths for the transitions between $1s^2 2\ell n\ell' {}^3S$ and $1s^2 2\ell m\ell' {}^3P^o$ states ($n, m < 6$ and $0 \leq \ell \leq 1$).

Transition	λ (Å)	f_i	f_o
$(1s^2) 2s3s {}^3S \rightarrow 2s3p {}^3P^o$	4649	0.700	0.690
$\rightarrow 2p3s {}^3P^o$	1428	0.3210	0.3190
$\rightarrow 2s4p {}^3P^o$	1257	0.0630	0.0670
$\rightarrow 2p3d {}^3P^o$	1005	0.0168	0.0166
$\rightarrow 2s5p {}^3P^o$	943	0.0104	0.0116
$2s4s {}^3S \rightarrow 2s4p {}^3P^o$	11981	1.0530	1.0630
$\rightarrow 2p3d {}^3P^o$	3260	0.0303	0.0312
$\rightarrow 2s5p {}^3P^o$	2874	0.0471	0.0484
$2p3p {}^3S \rightarrow 2p3d {}^3P^o$	7788	0.4740	0.3800
$\rightarrow 2s5p {}^3P^o$	5898	0.0190	0.0280
$2s5s {}^3S \rightarrow 2p3d {}^3P^o$	5.49E5	0.1600	0.2100
$\rightarrow 2s5p {}^3P^o$	23256	1.1420	1.0310
$2s2p {}^3P^o \rightarrow 2s3s {}^3S$	538	0.0504	0.0525
$\rightarrow 2s4s {}^3S$	389	0.0112	0.0128
$\rightarrow 2p3p {}^3S$	364	0.0085	0.0086
$\rightarrow 2s5s {}^3S$	348.44	1.4E-3	1.6E-3
$2s3p {}^3P^o \rightarrow 2s4s {}^3S$	2010	0.1390	0.1370
$\rightarrow 2p3p {}^3S$	1480	0.0213	0.0194
$\rightarrow 2s5s {}^3S$	1247	0.0112	0.0110
$2p3s {}^3P^o \rightarrow 2s4s {}^3S$	85167	2.4E-4	1.7E-4
$\rightarrow 2p3p {}^3S$	5263	0.0678	0.0661
$\rightarrow 2s5s {}^3S$	3157	3.7E-3	4.1E-3
$2s4p {}^3P^o \rightarrow 2p3p {}^3S$	10550	0.0202	0.0138
$\rightarrow 2s5s {}^3S$	4517	0.1720	0.1640

TABLE 4-5. Absorption oscillator strengths for the transitions between $1s^2 2\ell n\ell' {}^1P^\circ$ and $1s^2 2\ell m\ell' {}^1D$ states ($n, m < 6$ and $0 \leq \ell \leq 1$).

Transition	λ (Å)	f_i	f_o
$(1s^2) 2s2p {}^1P^\circ \rightarrow 2P^2 {}^1D$	2296.90	0.178	0.179
$\rightarrow 2s3d {}^1D$	574.28	0.526	0.521
$\rightarrow 2s4d {}^1D$	450.70	0.169	0.169
$\rightarrow 2p3p {}^1D$	433.34	0.110	0.109
$\rightarrow 2s5d {}^1D$	409.30	0.0647	0.0618
$2s3p {}^1P^\circ \rightarrow 2s3d {}^1D$	5696.00	0.359	0.342
$\rightarrow 2s4d {}^1D$	1531.80	0.207	0.211
$\rightarrow 2p3p {}^1D$	1347.95	0.0294	0.0284
$\rightarrow 2s5d {}^1D$	1139.90	0.1142	0.1140
$2p3s {}^1P^\circ \rightarrow 2s4d {}^1D$	7037.25	0.463	0.470
$\rightarrow 2p3p {}^1D$	4325.70	0.414	0.408
$\rightarrow 2s5d {}^1D$	2727.56	1.7E-3	4.2E-3
$2s4p {}^1P^\circ \rightarrow 2s4d {}^1D$	1.033E5	0.0161	0.0208
$\rightarrow 2p3p {}^1D$	9331.01	0.0549	0.0818
$\rightarrow 2s5d {}^1D$	4122.05	0.478	0.530
$2s5p {}^1P^\circ \rightarrow 2s5d {}^1D$	29409	0.723	0.337
$2p^2 {}^1D \rightarrow 2s3p {}^1P^\circ$	884.53	0.0271	0.0271
$\rightarrow 2p3s {}^1P^\circ$	609.28	0.0508	0.0527
$\rightarrow 2s4p {}^1P^\circ$	566.48	0.0164	0.0190
$\rightarrow 2s5p {}^1P^\circ$	506.63	4.2E-4	2.7E-4
$2s3d {}^1D \rightarrow 2p3s {}^1P^\circ$	2982.20	0.0720	0.0782
$\rightarrow 2s4p {}^1P^\circ$	2177.00	0.0201	0.0114
$\rightarrow 2s5p {}^1P^\circ$	1497.56	0.0495	0.0228
$2s4d {}^1D \rightarrow 2s5p {}^1P^\circ$	5249.60	0.124	0.078
$2p3p {}^1D \rightarrow 2s5p {}^1P^\circ$	9859.41	0.0165	0.0066
$\rightarrow 2p3d {}^1P^\circ$	7353.96	0.027	0.012

TABLE 4-6. Absorption oscillator strengths for the transitions between $1s^2 2\ell n\ell' {}^3P^\circ$ and $1s^2 2\ell m\ell' {}^3D$ states ($n, m < 6$ and $0 \leq \ell \leq 1$).

Transition	λ (Å)	f_i	f_o
$(1s^2) 2s2p {}^3P^\circ \rightarrow 2s3d {}^3D$	460	0.559	0.555
$\rightarrow 2s4d {}^3D$	372	0.153	0.151
$\rightarrow 2p3p {}^3D$	369	5.5E-4	3.8E-4
$\rightarrow 2s5d {}^3D$	341	0.052	0.055
$2s3p {}^3P^\circ \rightarrow 2s3d {}^3D$	9710	0.192	0.203
$\rightarrow 2s4d {}^3D$	1621	0.550	0.540
$\rightarrow 2p3p {}^3D$	1577	0.0111	0.0105
$\rightarrow 2s5d {}^3D$	1167	0.108	0.114
$2p3s {}^3P^\circ \rightarrow 2s4d {}^3D$	7601	0.054	0.057
$\rightarrow 2p3p {}^3D$	6740	0.211	0.228
$\rightarrow 2s5d {}^3D$	2689	5.1E-4	1.4E-4
$2s4p {}^3P^\circ \rightarrow 2s4d {}^3D$	27495	0.256	0.265
$\rightarrow 2p3p {}^3D$	18811	0.115	0.106
$\rightarrow 2s5d {}^3D$	3609	0.319	0.319
$2p3d {}^3P^\circ \rightarrow 2s5d {}^3D$	18584	0.375	0.284
$2s5p {}^3P^\circ \rightarrow 2s5d {}^3D$	79177	0.113	0.126
$2s3d {}^3D \rightarrow 2p3s {}^3P^\circ$	2613	2.9E-3	3.1E-3
$\rightarrow 2s4p {}^3P^\circ$	2092	0.0452	0.0480
$\rightarrow 2p3d {}^3P^\circ$	1427	0.0596	0.0614
$\rightarrow 2s5p {}^3P^\circ$	1347	9.9E-3	6.7E-3
$2s4d {}^3D \rightarrow 2p3d {}^3P^\circ$	5349	0.0272	0.030
$\rightarrow 2s5p {}^3P^\circ$	4385	0.0348	0.0388
$2p3p {}^3D \rightarrow 2p3d {}^3P^\circ$	5880	0.0368	0.0270
$\rightarrow 2s5p {}^3P^\circ$	4759	5.8E-4	8.4E-4

TABLE 4-7. Absorption oscillator strengths for the transitions between $1s^2 2\ell n\ell' {}^1D$ and $1s^2 2\ell m\ell' {}^1F^\circ$ states ($n, m < 6$ and $0 \leq \ell \leq 1$).

Transition	λ (Å)	f_l	f_v
$(1s^2) 2p^2 {}^1D \rightarrow 2s4f {}^1F^\circ$	565.53	0.079	0.0794
$\rightarrow 2p3d {}^1F^\circ$	511.53	0.374	0.369
$\rightarrow 2s5f {}^1F^\circ$	492.65	0.206	0.199
$2s3d {}^1D \rightarrow 2s4f {}^1F^\circ$	2163.00	0.784	0.752
$\rightarrow 2p3d {}^1F^\circ$	1541.12	0.0516	0.0646
$\rightarrow 2s5f {}^1F^\circ$	1381.65	0.468	0.468
$2s4d {}^1D \rightarrow 2p3d {}^1F^\circ$	5826.42	0.568	0.497
$\rightarrow 2s5f {}^1F^\circ$	4056.06	0.403	0.396
$2p3p {}^1D \rightarrow 2p3d {}^1F^\circ$	12117	0.158	0.127
$\rightarrow 2s5f {}^1F^\circ$	6350.76	0.0571	0.0527
$2s5d {}^1D \rightarrow 2s5f {}^1F^\circ$	45420	0.375	0.060
$2s4f {}^1F^\circ \rightarrow 2p3p {}^1D$	9597.81	1.2E-3	1.4E-3
$\rightarrow 2s5d {}^1D$	4173.09	1.4E-3	2.0E-2

TABLE 4-8. Absorption oscillator strengths for the transitions between $1s^2 2\ell n\ell' {}^3D$ and $1s^2 2\ell m\ell' {}^3F^\circ$ states ($n, m < 6$ and $0 \leq \ell \leq 1$).

Transition	λ (Å)	f_l	f_v
$(1s^2) 2s3d {}^3D \rightarrow 2s4f {}^3F^\circ$	1923	0.596	0.576
$\rightarrow 2p3d {}^3F^\circ$	1577	0.249	0.254
$\rightarrow 2s5f {}^3F^\circ$	1296	0.253	0.253
$2s4d {}^3D \rightarrow 2s4f {}^3F^\circ$	1.648E5	0.022	0.087
$\rightarrow 2p3d {}^3F^\circ$	8346	0.391	0.401
$\rightarrow 2s5f {}^3F^\circ$	3887	0.385	0.368
$2s5d {}^3D \rightarrow 2s5f {}^3F^\circ$	60314	0.435	0.198
$2s4f {}^3F^\circ \rightarrow 2s5d {}^3D$	4257	4.3E-4	0.017
$2p3d {}^3F^\circ \rightarrow 2s5d {}^3D$	8276	0.091	0.030

TABLE 4-9. Absorption oscillator strengths for the transitions between $1s^2 2\ell n \ell' \ ^1\text{F}^\circ, \ ^1\text{G}$ states and $1s^2 2p^2 \ ^3\text{P}, \ 1s^2 2\ell m \ell' \ ^3\text{P}^\circ$ states ($n, m < 6$ and $0 \leq \ell \leq 1$).

Transition	λ (Å)	f_l	f_u
$(1s^2) \ 2s4f \ ^1\text{F}^\circ \rightarrow 2s5g \ ^1\text{G}$	4187.0	1.183	1.168
$2s4f \ ^3\text{F}^\circ \rightarrow 2s5g \ ^3\text{G}$	4069	1.048	1.042
$2p3d \ ^1\text{F}^\circ \rightarrow 2s5g \ ^1\text{G}$	19200	0.240	0.224
$2p3d \ ^3\text{F}^\circ \rightarrow 2s5g \ ^3\text{G}$	4069	0.326	0.291
$2s5g \ ^1\text{G} \rightarrow 2s5f \ ^1\text{F}^\circ$	43847	0.127	0.070
$2s5g \ ^3\text{G} \rightarrow 2s5f \ ^3\text{F}^\circ$	1.737E5	0.090	0.030
$2s2p \ ^3\text{P}^\circ \rightarrow 2p^2 \ ^3\text{P}$	1176	0.280	0.282
$2p^2 \ ^3\text{P} \rightarrow 2s3p \ ^3\text{P}^\circ$	818	2.2E-4	1.7E-3
$\rightarrow 2p3s \ ^3\text{P}^\circ$	585	0.135	0.135
$\rightarrow 2s4p \ ^3\text{P}^\circ$	555	4.3E-3	5.3E-3
$\rightarrow 2p3d \ ^3\text{P}^\circ$	493	0.096	0.0923
$\rightarrow 2s5p \ ^3\text{P}^\circ$	484	0.0134	0.0134

TABLE 4-10. Comparison of oscillator strengths with other calculations and with experimental values. The first line against each transition gives f_i and the second, f_o .

Transition	f^{a*}	f^b	f^c	f^d	f^e	f^f	f^g	$f(\text{exp})$
$2s^2 \ ^1S \rightarrow 2s2p \ ^1P^o$	0.777 0.784	1.114 0.542	0.709	0.760 0.780	0.756	0.776* 0.784*	0.768 0.850	0.65 ^h
$\rightarrow 2s3p \ ^1P^o$	0.222 0.223	0.1634 0.1826	0.230		0.211		0.220 0.217	0.203 ^h
$\rightarrow 2p3s \ ^1P^o$	0.0425 0.0400				0.038			
$2s2p \ ^3P^o \rightarrow 2p^2 \ ^3P$	0.280 0.282	0.2999 0.2255	0.297		0.271	0.276* 0.275*	0.276 0.301	0.28 ^h , 0.224 ⁿ
$\rightarrow 2s3s \ ^3S$	0.0504 0.0525	0.0395 0.0456	0.047		0.048	0.0525 0.0541	0.054 0.055	0.045 ^h
$\rightarrow 2s3d \ ^3D$	0.559 0.555	0.521 0.475	0.523		0.591	0.554 0.551	0.556 0.548	0.459 ^h
$2s2p \ ^1P^o \rightarrow 2p^2 \ ^1D$	0.178 0.179		0.207	0.165 0.155	0.182	0.184* 0.185*	0.188 0.245	0.18 ⁱ , 0.16 ^j , 0.14 ^k , 0.19 ^l
$\rightarrow 2p^2 \ ^1S$	0.167 0.177		0.230	0.173 0.163	0.176	0.166* 0.168*	0.172 0.171	0.13 ^m , 0.17 ⁿ
$\rightarrow 2s3s \ ^1S$	0.0208 0.0214		0.0155		0.0237		0.020 0.020	0.039 ^h
$\rightarrow 2s3d \ ^1D$	0.526 0.521	0.458 0.482	0.711		0.633		0.590 0.603	0.588 ^h
$2p^2 \ ^3P \rightarrow 2s3p \ ^3P^o$	2.2E-4 1.7E-4		7.8E-4		3.0E-4		1.3E-4 1.5E-4	
$2p^2 \ ^1D \rightarrow 2s3p \ ^1P^o$	0.0271 0.0271		0.0682		0.049		0.044 0.026	0.025 ^h
$2p^2 \ ^1S \rightarrow 2s3p \ ^1P^o$	0.0272 0.0237		0.0786		0.038		0.024 0.015	
$2s3s \ ^3S \rightarrow 2s3p \ ^3P^o$	0.700 0.690	0.814 0.719	0.730		0.724	0.717 0.728	0.712 0.710	0.72 ⁿ , 0.644 ^p
$2s3s \ ^1S \rightarrow 2s3p \ ^1P^o$	0.327 0.372		0.291		0.320		0.328 0.320	
$2s3p \ ^1P^o \rightarrow 2s3d \ ^1D$	0.359 0.342		0.345		0.328		0.325 0.235	
$2s3p \ ^3P^o \rightarrow 2s3d \ ^3D$	0.192 0.203	0.221 0.264	0.218		0.179	0.183 0.199	0.183 0.200	

*This work; ^bPfennig et al. (1965); ^cNussbaumer (1972); ^dNicolaides et al. (1973); ^eHummer and Norcross (1974); ^fHibbert (1974, 1976); ^gGlass (1979, 1981); ^hBuchet-Poulizac and Buchet (1973); ⁱCurnutte et al. (1968); ^jPinnigton and Lin (1969); ^kBergström et al. (1969); ^lPegg et al. (1970); ^mMartinson and Bickel (1970); ⁿPoulizac et al. (1971); ^pBromander (1971).

* The theoretical ΔE were used in calculating these oscillator strengths while in the others, experimental ΔE were used.

Chapter 5

Laser action in stellar envelopes. C III

A) Introduction

The C III ion is of considerable astrophysical importance. Emission lines due to C III are observed in spectra of Wolf-Rayet and Of stars. Especially in the Wolf-Rayet spectra, some C III emission lines occur with great intensity. The mechanism of the great intensity of some of these emission lines and of the variations thereof is not understood. The C III ion has the configuration $1s^2 2s^2$ and thus in some respects is similar to He I in that both systems have outer s^2 configuration.

In chapter 2 strong population inversions in some He I transitions, when helium plasma is rapidly cooled by expansion were reported. It was shown that laser action is feasible in the atmospheres of stars which are undergoing mass loss. It was thus of interest to carry out similar calculations concerning possible laser action in the emission lines of the C III ion. There are two C III lines, $\lambda 4650$ and $\lambda 5696$, which occur with great intensity in some Wolf-Rayet stars. The great intensity of the $\lambda 5696$ line has been a mystery for many years. Thus it was of interest to investigate if laser action is responsible for the intensity of this line. To the best of our knowledge, there has been no previous investigation on population inversion in C III in a recombining plasma.

The model that we adopt for investigating laser action in C III in stellar atmospheres is basically the same as the one used for He I in chapter 2. We consider what happens when a mass of the plasma in the photosphere of a star expands adiabatically. Under adiabatic expansion conditions, the density N and the temperature T_e of a gas are related by $T_e N^{1-\gamma} = \text{constant}$. But we use a different model for calculating the relative concentrations of C, C^+ , C^{+2} , ..., etc. at a particular electron density and electron temperature.

A number of ionization balance calculations have been carried out by different authors taking into account the following processes:

- (a) ionization by electron collision including autoionization;
- (b) radiative recombination;
- (c) dielectronic recombination;
- (d) collisional-radiative processes.

Authors who have carried out these calculations are Tucker and Gould (1966), Jordan (1969, 1970), Burgess and Summers (1969), Beigman et al. (1971), Summers (1972, 1974), Nussbaumer and Storey (1975), Jacobs et al. (1976). In the next section we will present the method used in calculating the relative concentration of the various stages of ionization of carbon, which similar to the calculation done by Jordan (1969). Our model is applicable to a density higher than the density considered in Jordan's calculation. The atomic data used in the CR model described in chapter 2 are summarized in sections B and C.

B) Ionization equilibrium

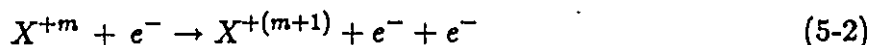
To calculate the relative concentrations of different carbon ions, a steady state model (House, 1964; Jordan, 1969; McWhirter, 1978) was used. The relative population of two successive stages of ionization of a monatomic non-LTE plasma is found by equating the rate of ionization from, and recombination to, a given stage of ionization. Thus in the steady state

$$\frac{N^{+(m+1)}}{N^{+m}} = \frac{S^{+m}}{\alpha_{tot}^{+m}} \quad (5-1)$$

where N^{+m} is the density of a m times charged atom (ion), S^{+m} is the total rate coefficient for ionization from m to $(m+1)$, and α_{tot}^{+m} is the total rate coefficient for recombination from $(m+1)$ to m . The model is based on the following assumptions: 1) Each stage of ionization

of element X consists of only a ground state and a continuum. 2) The monatomic plasma is optically thin. The relative concentration of ion with charge $+m$, N^{+m}/N , where N is the total number density of the element, is calculated from the values of $N^{+(m+1)}/N^{+m}$. The rate coefficients S^{+m} and α_{tot}^{+m} used in the calculation were obtained as follows.

(a) *Collisional ionization*



For neutral and singly ionized Carbon, collisional ionization rate was obtained from the formula given by Lotz (1968, 1969, 1970):

$$S = 6.7 \times 10^{-7} \sum_j \frac{a_j q_j}{(kT)^{3/2}} \left[\left(\frac{P_j}{kT} \right)^{-1} \int_{P_j/kT}^{\infty} \frac{e^{-x}}{x} dx - \frac{b_j e^{c_j}}{(P_j/kT) + c_j} \int_{\frac{P_j}{kT} + c_j}^{\infty} \frac{e^{-y}}{y} dy \right] \quad (5-3)$$

P_j is the binding energy of electrons in the j -th subshell, q_j is the number of equivalent electrons in the j -th subshell, a_j , b_j , and c_j are individual constants given by Lotz (1968). The values of the parameters P_j , q_j , a_j , b_j , and c_j used in the calculation of Equation (5-3) are listed in Table 5-1.

TABLE 5-1. The parameters used in Equation (5-3).

Species	Confi.	q_1	q_2	P_1	P_2	a_1	a_2	b_1	b_2	c_1	c_2
C I	2s ² 2p ²	2	2	11.26	16.59	3.5	4.0	0.7	0.7	0.4	0.5
C II	2s ² 2p	1	2	24.4	30.9	4.2	4.4	0.4	0.4	0.6	0.6

The ionization rate coefficients of the ground state for Carbon ions with $m \geq 2$ were calculated using the semi-empirical formula proposed by Burgess and Chidichimo (1983).

This allows for inner-shell excitation and autoionization effects. (In some cases autoionization can increase the total ionization rate by a substantial factor in certain ions, cf. Goldberg *et al.*, 1965). The procedure of including the autoionization effect was first suggested by Burgess *et al.* (1977). The formula is as follows:

$$S^{+m} = 2.1715 \times 10^{-8} C \sum_j \zeta_j \left(\frac{I_H}{I_j} \right)^{3/2} \left(\frac{I_j}{kT} \right)^{1/2} E_1(I_j/kT) w \quad (5-4)$$

where the summation is over shells (or subshells) j of the initial ion, ζ_j is the effective number of electrons in j , I_j is the effective ionization energy of j (this may differ from the true ionization energy because of auto-ionization effects), I_H is the ionization energy of hydrogen, $E_1(x)$ is the first exponential integral, and

$$w = [\ln(1 + kT/I_j)]^{\beta/(1+kT/I_j)} \quad (5-5)$$

with β given by

$$\beta = \frac{1}{4} \left\{ \left[\frac{100z + 91}{4z + 3} \right]^{1/2} - 5 \right\}. \quad (5-6)$$

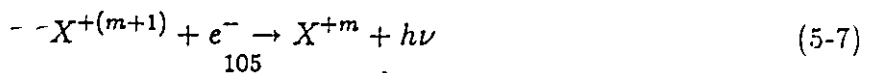
where z is the initial charge number of ion.

The factor w has a significant effect only for ions of low charge and for very small values of kT/I_j . Values of ζ_j , I_j and mean experimental values ($\bar{C}$) of C are given by Burgess *et al.* (1983).

(b) *Recombination*

Three recombination processes have been taken into account.

(i) Radiative recombination:



For temperature $T_e \leq 6 \times 10^5$ K, the radiative recombination rate via continuum has been calculated using the well known formula of Elwert (1952) given by

$$\alpha_{rad.c.}^{+m} = 5.16 \times 10^{-14} f_1 \left(\frac{I_H}{kT_e} \right)^{1/2} \frac{I_m}{I_H} n n_e G_1(I_m/kT) g \quad (5-8)$$

where

$$G_1(X) = X_m \exp(X_j) E_1(X_m), \quad (5-9)$$

n is the principal quantum number of ground state of lower stage of ionization, I_m is the ionization potential of ion of charge $+m$ in eV, I_H is the ionization potential of hydrogen, $E_1(x)$ is the first exponential integral, $f_1 = 0.8$, $g = 3$, and all other symbols have their usual meaning. For higher temperatures, the formula given by Burgess and Seaton (1964) was used:

$$\alpha_{rad.c.}^{+m} = 1.3 \times 10^{-9} (m+1)^2 I_m^{1/2} T_e^{-1} \quad (5-10)$$

where the symbols have the same meaning as before.

Radiative decay from bound levels above a certain level n_t (thermal limit) to those below is equivalent to recombination. The level n_t is given by Griem (1964)

$$n_t \approx 1.26 \times 10^2 Z^{(14/17)} n_e^{-(2/17)} \left[\frac{kT_e}{Z^2 I_H} \right]^{1/17} \exp \left[\frac{4Z^2 I_H}{17n_t^3 kT_e} \right], \quad (5-11)$$

where Z is the effective charge. Then, assuming that the level above n_t are hydrogenic, the rate for radiative recombination via bound levels can be calculated using the hydrogenic rate derived by Wilson (1967)

$$\alpha_{rad.b.l.}^{+m} = 1.2 \times 10^{-6} (m+1)^4 T_e^{-3/2} n_t^{-1} \exp(-X_t/kT_e), \quad (5-12)$$

where χ_t is the excitation energy (in eV) of the level n_t , and is given by

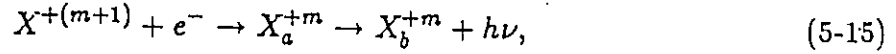
$$\chi_t^7 = 6 \times 10^{-28} \frac{I_m}{kT_e} n_e^2. \quad (5-13)$$

The total radiative recombination rate is

$$\alpha_{rad.}^{+m} = \alpha_{rad.c.}^{+m} + \alpha_{rad.b.l.}^{+m}. \quad (5-14)$$

where $\alpha_{rad.c.}^{+m}$ and $\alpha_{rad.b.l.}^{+m}$ are the radiative recombination via continuum and bound levels, respectively.

(ii) Dielectronic recombination:



where a and b represent an autoionizing state and a true bound state of the next lower ionization stage, respectively.

For temperature in the range 10^3 to 4×10^4 K the dielectronic recombination coefficients of C , C^+ , and C^{+2} are calculated using the formula given by Nussbaumer and Storey (1983, 1984):

$$\alpha_{diel.}^{+m} = 10^{-12} \left(\frac{a}{t} + b + ct + dt^2 \right) t^{-3/2} \exp(-f/t), \quad (5-16)$$

where

$$t = T_e[\text{K}]/10000 \text{ K}, \quad (5-17)$$

a , b , c , d , and f are fitting parameters.

For temperature greater than 6×10^4 K and for other Carbon ions, we used the expression given by Landini and Monsignori Fossi (1971)

$$\alpha_{diel}^{+m} = 2 \times 10^{-4} T_e^{-3/2} (m+2)^2 f_{1,0} \sqrt{W_1} \exp(-10.6 \times 10^3 \frac{W_1}{T_e}), \quad (5-18)$$

where W_1 is the excitation potential (in eV) of the first allowed level of the recombining ion, and

$$f_{1,0} = \sum_j f_j = n, \quad (5-19)$$

n being the number of electrons in the outer shell of the recombining ion.

iii) Three-body recombination:

It is the inverse of process (5-1). The rate coefficients are calculated from the condition of detailed balancing

$$\alpha_{three}^{+m} = \left(\frac{N^{+m}}{N^{+(m+1)}} \right) S^{+m} \quad (5-20)$$

where S^{+m} is the collisional ionization rate coefficient (Eq. 5-2), and $(N^{+m}/N^{+(m+1)})$ is given by the Saha-Boltzmann equation:

$$\frac{N^{+m}}{N^{+(m+1)}} = \left(\frac{h^2}{2\pi m_e k} \right)^{3/2} \frac{n_e}{T_e^{3/2}} \frac{U_m}{2U_{m+1}} \exp(I_m/kT_e), \quad (5-21)$$

U is the partition function, and all other symbols have their usual meaning.

The total recombination rate is given by

$$\alpha_{tot}^{+m} = \alpha_{rad}^{+m} + \alpha_{diel}^{+m} + \alpha_{three}^{+m}. \quad (5-22)$$

C) Atomic data

(a) *Energy levels.*

The energy levels needed in the calculation have been taken from Bashkin and Stoner (1975). All the levels in the configuration $1s^2 2sn\ell$ having principal quantum number $n \leq 5$, and the levels in the configuration $1s^2 2pn\ell$ having $n \leq 3$ are treated as individual levels except for the levels having orbital angular momentum $\ell \geq 2$ in the configuration $1s^2 2pn\ell$. These latter levels with same n are treated as a single level. The levels $n^{1,3}S$, $n^{1,3}P^o$, $n^{1,3}D$, ... in configuration $1s^2 2sn\ell$ with $n \geq 6$ are grouped together in one level. The levels with $n > 3$ in the configuration $1s^2 2pn\ell$ are not included in the calculation because most of these levels lie above the ionization limit (autoionization states). In the CR model calculation, the upper limits of the levels r and s considered are $n_r = 15$ and $n_s = 25$; the total number of levels whose population density is calculated is 49. The levels with $16 \leq n \leq 25$ are assumed to be in LTE. The labels, energies and weight factors for these levels are given in Table 5-2.

(b) *Transition probabilities.*

Spontaneous transition probabilities between resolved levels were calculated using Equation (2-9). For unresolved levels, we used Equation (2-10) in calculating the transition probabilities.

Oscillator strengths for all the allowed transitions between the states with $n \leq 5$ have been calculated using configuration interaction method, which is expected to give the best theoretical results. The method of calculating the oscillator strength and the results have been given in chapter 4. For transitions between resolved and unresolved states, and between unresolved states, Equation (2-11) was used to calculate the oscillator strength.

TABLE 5-2. Energy levels of C III used in the model.

Level No.(i)	State	Energy $E_i(\text{cm}^{-1})$	g_i	Level No.(i)	State	Energy $E_i(\text{cm}^{-1})$	g_i
1	2s ² ¹ S	0.0	1	31	2s5p ³ P	344236.29	9
2	2s2p ³ P	52390.75	9	32	2p3p ¹ S	345095.43	1
3	2s2p ¹ P	102352.04	3	33	2s5d ³ D	345496.72	15
4	2p ² ³ P	137454.40	9	34	2s5g ³ G	346579.00	27
5	2p ² ¹ D	145876.13	5	35	2s5g ¹ G	346579.00	90
6	2p ² ¹ S	182519.88	1	36	2s5d ¹ D	346658.34	5
7	2s3s ³ S	238213.00	3	37	2p3d ¹ P	346712.73	3
8	2s3s ¹ S	247170.26	1	38	2s5f ³ F	347154.00	21
9	2s3p ¹ P	258931.29	3	39	2s5f ¹ F	348860.00	7
10	2s3p ³ P	259711.22	9	40	6	358732	144
11	2s3d ³ D	270011.93	15	41	7	366027	196
12	2s3d ¹ D	276482.86	5	42	8	370778	256
13	2p3s ³ P	308248.91	9	43	9	374027	324
14	2s4s ³ S	309457.17	3	44	10	376350	400
15	2p3s ¹ P	310006.32	3	45	11	378068	484
16	2s4s ¹ S	311721.51	1	46	12	379382	576
17	2s4p ³ P	317796.51	9	47	13	380397	676
18	2p3p ¹ P	319720.35	3	48	14	381202	784
19	2s4d ³ D	321426.74	15	49	15	381851	900
20	2s4f ³ F	322012.00	21	50	16	382383	1024
21	2s4p ¹ P	322404.20	3	51	17	382824	1156
22	2s4f ¹ F	322702.00	9	52	18	383193	1296
23	2s4d ¹ D	324212.49	5	53	19	383505	1444
24	2p3p ³ S	327278.27	3	54	20	383772	1600
25	2p3p ³ P	329907.47	9	55	21	384002	1764
26	2p3L ^{1,3} L	332821	68	56	22	384201	1936
27	2s5s ¹ S	338514.33	1	57	23	384374	2116
28	2s5s ³ S	339934.72	3	58	24	384526	2304
29	2p3d ³ P	340127.53	9	59	25	384661	2500
30	2s5p ¹ P	343258.03	3				

The theoretical transition probabilities of Nussbaumer (1972) and Nussbaumer and Storey (1978) were adopted for the following optically forbidden transitions: $2s^2 \ ^1S \rightarrow 2s2p \ ^3P^o$, $2s2p \ ^3P^o \rightarrow 2p^2 \ ^1D$, $2s2p \ ^1P^o \rightarrow 2p^2 \ ^3P$, $2s^2 \ ^1S \rightarrow 2p^2 \ ^3P$, $2s^2 \ ^1S \rightarrow 2p^2 \ ^1D$, $2p^2 \ ^1D \rightarrow 2p^2 \ ^1S$.

(c) *Collisional excitation and de-excitation rate coefficients.*

The excitation rate coefficients for transition between bound levels were computed from the respective cross sections by integrating the cross section over Maxwellian energy distribution (Eq. 2-15). For most of the cross sections for low lying levels the best available theoretical data were fitted to semi-empirical formulas.

Equation (2-18) was fitted to the following allowed transitions:

$2s^2 \ ^1S \rightarrow 2s2p \ ^1P^o$, $2s2p \ ^1P^o \rightarrow 2p^2 \ ^1S$, and $2s2p \ ^1P^o \rightarrow 2p^2 \ ^1D$: Theoretical cross sections of Berrington *et al.* (1981, 1985).

$2s^2 \ ^1S \rightarrow 2s3p \ ^1P^o$, $2s^2 \ ^1S \rightarrow 2s4p \ ^1P^o$, and $2s^2 \ ^1S \rightarrow 2s5p \ ^1P^o$: Theoretical cross sections of Ganas and Green (1979).

The fitting parameters α , β , and ϕ for the above transitions are given in Table 5-3. For the allowed transition $2s2p \ ^3P^o \rightarrow 2p^2 \ ^3P$, the cross sections were calculated using the semi-empirical formula given by Merts *et al.* (1980):

$$\Omega(U) = C_0 + \frac{C_1}{U} + \frac{C_2}{U^2} + C_3 \ln U, \quad (5-23)$$

where $\Omega(U)$ is the collision strength, and is related to the cross section by

$$\Omega(U) = (2S + 1)(2L + 1)E\sigma(E), \quad (5-24)$$

C_0 , C_1 , C_2 , and C_3 are fitting parameters, and $U = E/E_{n'l,nt}$. The fitting parameters for this transition were taken from Merts *et al.* (1980).

TABLE 5-3. Fit parameters for the cross section (Eq. 2-18) of the allowed transitions of C III.

Transition	α	β	ϕ
$2s^2 \ ^1S \rightarrow 2s2p \ ^1P$	1.697	1.419	0.040
$2s^2 \ ^1S \rightarrow 2s3p \ ^1P$	0.770	0.962	0.10
$2s^2 \ ^1S \rightarrow 2s4p \ ^1P$	0.958	1.332	0.10
$2s^2 \ ^1S \rightarrow 2s5p \ ^1P$	1.164	3.766	0.10
$2s2p \ ^1P \rightarrow 2p^2 \ ^1S$	1.131	2.00	0.70
$2s2p \ ^1P \rightarrow 2p^2 \ ^1D$	2.140	3.50	1.00

TABLE 5-4. Fit parameters for the cross section (Eqs. 2-32 and 2-38) of the forbidden transitions of C III.

Transition	α	β	ϕ	k
$2s^2 \ ^1S \rightarrow 2p^2 \ ^1S$	3.2×10^{-2}	-0.74×10^{-2}	0.32	3
$2s^2 \ ^1S \rightarrow 2p^2 \ ^1D$	0.201	-5.52×10^{-2}	0.10	3
$2s^2 \ ^1S \rightarrow 2s4s \ ^1S$	0.886	1.27×10^{-2}	0.61	3
$2s^2 \ ^1S \rightarrow 2s5s \ ^1S$	1.48	-1.57×10^{-2}	0.62	3
$2s^2 \ ^1S \rightarrow 2s4d \ ^1D$	1.195	5.45×10^{-2}	0.77	3
$2s^2 \ ^1S \rightarrow 2s5d \ ^1D$	1.404	4.58×10^{-2}	0.64	3
$2p^2 \ ^1D \rightarrow 2p^2 \ ^1S$	0.021	0.210×10^{-2}	1.00	3
$2s^2 \ ^1S \rightarrow 2p^2 \ ^3P$	0.91×10^{-2}	0.12×10^{-2}	1.00	5
$2s^2 \ ^1S \rightarrow 2s2p \ ^3P$	0.480	0.82×10^{-2}	0.76	5
$2s2p \ ^3P^o \rightarrow 2p^2 \ ^1S$	0.017	0.05×10^{-2}	0.87	5
$2s2p \ ^3P^o \rightarrow 2p^2 \ ^1D$	0.149	1.04×10^{-2}	1.00	5
$2p^2 \ ^3P \rightarrow 2p^2 \ ^1S$	0.021	0.04×10^{-2}	1.00	5
$2p^2 \ ^3P \rightarrow 2p^2 \ ^1D$	0.055	0.00	1.00	5

For the remaining allowed transitions, the semi-classical IP method (Eqs. 2-20 and 2-27) was used for calculating the cross section of transitions with $\Delta n \leq 3$. For transitions with $\Delta n > 3$, we used Equation (2-31) for calculating the cross sections.

Equation (2-32) was fitted to the following cross sections for optically forbidden transitions without change in spin:

$2s^2 \ ^1S \rightarrow 2s4s \ ^1S$, $2s^2 \ ^1S \rightarrow 2s5s \ ^1S$, $2s^2 \ ^1S \rightarrow 2s4d \ ^1D$, and $2s^2 \ ^1S \rightarrow 2s5d \ ^1D$: Theoretical cross sections of Ganas and Green (1979).

$2s^2 \ ^1S \rightarrow 2p^2 \ ^1S$, $2p^2 \ ^1D \rightarrow 2p^2 \ ^1S$, and $2s^2 \ ^1S \rightarrow 2p^2 \ ^1D$: Theoretical cross sections of Berrington et al. (1981, 1985).

The parameters α , β , ϕ , and k are given in Table 5-4. The collision strengths of the transitions $2s^2 \ ^1S \rightarrow 2s3s \ ^1S$ and $2s^2 \ ^1S \rightarrow 2s3d \ ^1D$ were calculated using Equation (2-23) with the fitting parameters as given by Merts et al. (1980). For other optically forbidden transitions without change in spin between levels with $n \leq 5$, cross sections were calculated using Equation (2-33).

Equation (2-38) was fitted to the following cross sections of optically forbidden transition with change in spin:

$2s^2 \ ^1S \rightarrow 2s2p \ ^3P^o$, $2s^2 \ ^1S \rightarrow 2p^2 \ ^3P$, $2s2p \ ^3P^o \rightarrow 2p^2 \ ^1D$, $2s2p \ ^3P^o \rightarrow 2p^2 \ ^1S$, $2p^2 \ ^3P \rightarrow 2p^2 \ ^1D$, and $2p^2 \ ^3P \rightarrow 2p^2 \ ^1S$: Theoretical cross sections of Berrington et al. (1981, 1984).

The parameters α , β , ϕ , and k are given in Table 5-4. Equation (5-23) was used in calculating the collision strengths of the following transitions: $2s^2 \ ^1S \rightarrow 2s3s \ ^3S$, $2s^2 \ ^1S \rightarrow 2s3p \ ^3P^o$, $2s^2 \ ^1S \rightarrow 2s3d \ ^3D$, $2s2p \ ^3P^o \rightarrow 2s2p \ ^1P^o$, and $2s2p \ ^1P^o \rightarrow 2p^2 \ ^3P$. The parameters C_0 , C_1 , and C_2 are given by Merts et al. (1980), $C_3 = 0$ for forbidden transitions.

For other forbidden transitions with change in spin between $n \leq 5$, we have used Equation (2-42) to calculate the rate coefficients. The de-excitation rate coefficients are

obtained from the principle of detailed balance, Equation (2-44).

(d) *Ionization and three-body recombination rate coefficients.*

Equation (5-4) was used to calculate the ionization rate coefficient of the ground state $2s^2\ ^1S$. Burgess and Chidichimo (1983) have obtained the value of parameter $\bar{C}$ in the Equation (5-4) from the experimental data of Woodruff *et al.* (1978).

For the other resolved levels, Drawin formula (Eq. 2-47) was used to calculate the ionization cross section with $\alpha = 1$ and β determined from Equation (2-48), and the hydrogenic approximation was used for unresolved levels. The ionization rate coefficients for these levels were calculated using Equation (2-46). The three-body recombination rate coefficients are obtained from the principle of detailed balance (Eq. 2-49).

(e) *Radiative recombination.*

Hidalgo (1968) has computed photoionization cross sections for the lowest three C III levels $2s^2\ ^1S$, $2s2p\ ^3P^o$, and $2s2p\ ^1P^o$, and Sakhibullin and Willis (1978) have calculated the photoionization cross sections for the levels $2sns\ ^1,^3S$, $2snp\ ^1,^3P^o$, $2snd\ ^1,^3D$, $n \leq 9$, using the Quantum Defect Method. These cross sections were fitted to Equation (2-52), and the fitting parameters C , p , a_1 , $a_2, \dots, a_m$, are given in Table 5-5. Hydrogenic approximation was adopted to calculate the photoionization cross sections for other levels. The radiative recombination rate coefficient was obtained from Equation (2-51).

(f) *Dielectronic recombination.*

Nussbaumer and Storey (1984) have calculated the effective dielectronic recombination coefficients for selected lines and ground and metastable states of C III ion, and fitted to a convenient function of temperature in the range 10^3 to 6×10^4 K (Eq. 5-16).

TABLE 5-5. Fit parameters for the photoionization cross sections (Eq. 2-52) of C III.

State	p	m	C	a ₁	a ₂	a ₃	a ₄	a ₅	a ₆
2 ¹ S	0.5	3	-6.14E-2	-9.95	-24.21	13.43			
3 ¹ S	0.0	3	2.27E-3	-28.13	9.82E2	-2.42E2			
4 ¹ S	0.0	6	-3.83E-4	34.87	-7.0E3	64.26	1.64E3	1.18E3	-1.4E3
5 ¹ S	0.0	6	-6.70E-4	-11.15	-3.9E3	2.6E3	1.50E3	-3.55E3	1.6E3
3 ³ S	0.5	3	-4.07E-2	-17.60	-17.02	11.61			
4 ³ S	0.5	4	-1.73E-2	-34.43	-1.4E2	1.59E2	-58.99		
5 ³ S	0.0	4	-2.95E-4	-1.2E2	1.2E4	-6.4E3	1.91E3		
2 ¹ P	0.0	4	1.73E-3	-12.90	2.8E2	1.17E3	-2.9E2		
3 ¹ P	0.0	4	1.34E-2	-20.11	2.5E2	5.459	-37.10		
4 ¹ P	0.0	6	9.18E-3	-48.52	9.7E2	-7.2E2	4.74E2	-2.35E2	58.44
5 ¹ P	0.0	6	3.94E-3	-62.21	1.7E3	-1.2E3	2.11E3	-2.70E3	1.2E3
2 ³ P	0.0	4	8.10E-3	-4.701	1.14E2	1.8E2	-44.96		
3 ³ P	0.0	4	-6.93E-2	-5.29	-40.68	29.12	-28.16		
4 ³ P	0.0	5	5.23E-3	-38.9	5.76E2	9.4E2	-1.1E3	4.0E2	
5 ³ P	0.5	4	3.59E-3	-82.4	3.61E3	-3.29E3	1.42E3		
3 ¹ D	0.0	6	4.63E-6	1.6E3	-3.9E4	3.1E5	-2.8E5	1.3E6	-8.7E5
4 ¹ D	0.0	5	-1.12E-3	-42.33	7.03E2	-5.4E3	4.04E2	7.189E2	
5 ¹ D	0.0	6	-5.78E-4	-67.02	1.79E3	-2.24E4	7.5E3	7.7E3	-5.6E3
3 ³ D	0.0	5	3.44E-3	8.93	1.06E2	6.8E2	2.7E2	-1.3E2	
4 ³ D	0.0	6	-1.37E-3	-33.01	5.5E2	-5.4E3	1.50E3	6.12E3	-3.0E3
5 ³ D	0.0	4	-4.14E-3	-29.36	3.0E2	-3.9E3	2.13E3		

Since the range of temperature we are interested in falls within the applicable range of the equation proposed by Nussbaumer and Storey (1984), we used this equation to calculate the dielectronic recombination coefficients, and included them in the CR calculation by adding them to radiative recombination coefficients. Thus, β_n in Equation (2-6) will represent both processes:

$$\beta_n = \beta_n^{rad.} + \beta_n^{diel.}$$

The dielectronic recombination coefficients for the levels other than those calculated by Nussbaumer and Storey were set equal to zero. This will not cause an error because most of the remaining levels belong to the first series (configuration $1s^2 2sn\ell$), where the contributions from direct radiative recombination are more important than dielectronic recombination in the temperature range considered (Nussbaumer and Storey, 1983).

D) Results and discussion

The initial density of carbon atoms before expansion was taken to be $1 \times 10^{12} \text{ cm}^{-3}$, this very roughly represents the density of carbon in normal stellar atmospheres, calculations were carried out for population densities 59 levels of C III for a grid of n_e and T_e values. Before we come to the results we wish to make a cautionary remark. The results are based on the cross sections for various atomic processes, the overall accuracy of these cross sections for C III is less than those for He I. For many of the cross sections there are no experimental data and in several cases there may be large uncertainty in the theoretical cross sections. In view of this the results given below are less secure than those given in Chapter 2.

Most of our search for population inversions was concentrated towards transitions which give lines in the visible region. Appreciable population inversion was found for only two transitions: $2s3p \ ^3P^o \rightarrow 2s3s \ ^3S$ ($\lambda 4650$), and $2p3p \ ^3S \rightarrow 2p3s \ ^3P^o$ ($\lambda \lambda 5273, 5254, 5244$)

(weighted average is $\lambda 5263$). Overpopulation density, P has already been defined in chapter 2. In Figures 5-1 and 5-2, we show the variation of P with n_e for some typical values of T_e for the aforesaid two transitions. From such plots, contours of equal P on a n_e, T_e diagram were made and the results are shown in Figures 5-3 and 5-4. The peak value of P for $\lambda 4650$ is about $5 \times 10^5 \text{ cm}^{-3}$, and that for $\lambda 5263$, about $7 \times 10^4 \text{ cm}^{-3}$.

There are two C III lines in the visible region which appear strongly in Wolf-Rayet spectra (WC sequence). These are $\lambda 4650$ (Beals, 1930; Swings, 1942; Smith, 1955) and $\lambda 5696$ (Beals, 1934; Smith, 1955). As these two lines are sometimes unusually strong in WC spectra, the possibility arises that laser action may be responsible.

There is no definite data on the value of the electron density in Wolf-Rayet atmospheres. The best available estimate (Varshni, 1978) is $4 \times 10^{14} \text{ cm}^{-3}$ but it could be higher. Corresponding to this value of the electron density, the maximum value of P for $\lambda 4650$ is $\approx 5 \times 10^4 \text{ cm}^{-3}$ and that for $\lambda 5263$ is $\approx 5 \times 10^3 \text{ cm}^{-3}$ (both at $T_e \approx 15000 \text{ K}$). If we assume these values for P and $\Delta\lambda = 40 \text{ \AA}$, then the gain per unit length $\alpha(\lambda 4650) = 5.1 \times 10^{-10} \text{ cm}^{-1}$ and $\alpha(\lambda 5263) = 2.08 \times 10^{-11} \text{ cm}^{-1}$. Thus we find that under the above conditions, $\lambda 5263$ is expected to be quite weak in comparison with $\lambda 4650$. We may note here that under ordinary conditions (i.e. without laser action), the laboratory intensity of the $\lambda 4650$ line is much greater than that of $\lambda 5263$. In Wolf-Rayet spectra, a strong emission line is observed at $\lambda 4650$ but it is a blend of C III $\lambda 4649$ and C IV $\lambda 4650$ (which is a strong line in the C IV spectrum); $\lambda 5263$ has been detected (Swings, 1942) but it is quite weak. The available evidence on the two lines $\lambda 4650$ and $\lambda 5263$ from Wolf-Rayet spectra is consistent with both possibilities, i.e., presence or absence of laser action.

In Table 5-6 we show the relative intensities of the lines $\lambda 4650$ and $\lambda 5696$ in a few Wolf-Rayet stars. It will be noticed that while in the laboratory the $\lambda 5696$ line is weaker

than $\lambda 4650$, in some Wolf-Rayet stars the reverse is the case. We have noted earlier that in WR spectra $\lambda 4650$ is a blend of C III $\lambda 4649$ and C IV $\lambda 4650$, thus we expect that $\lambda 4650$ should be very much stronger than $\lambda 5696$. The unusual strength of $\lambda 5696$ indicates that some special excitation mechanism is at work.

In the simple model that we have investigated, we do not find any population inversion for $\lambda 5696$ in the QSS regime. If the expanding plasma interacts with a gas, it is possible that atom-atom interactions and charge-exchange processes may lead to laser action in this line.

TABLE 5-6. Equivalent widths (in arbitrary units) of $\lambda 4650$ and $\lambda 5696$ in a few Wolf-Rayet stars.

Star	Relative intensity	
	$\lambda 4650$	$\lambda 5696$
Beals(1934):		
HD 184738	8600	24875
HD 192103	34600	15220
HD 193793	18500	4359
Smith(1955)		
HD 164270(WC8)	87	160
HD 119078(WC7)	475	450
HD 115473(WC6)	>1300	65.5
Laboratory intensity	57	8

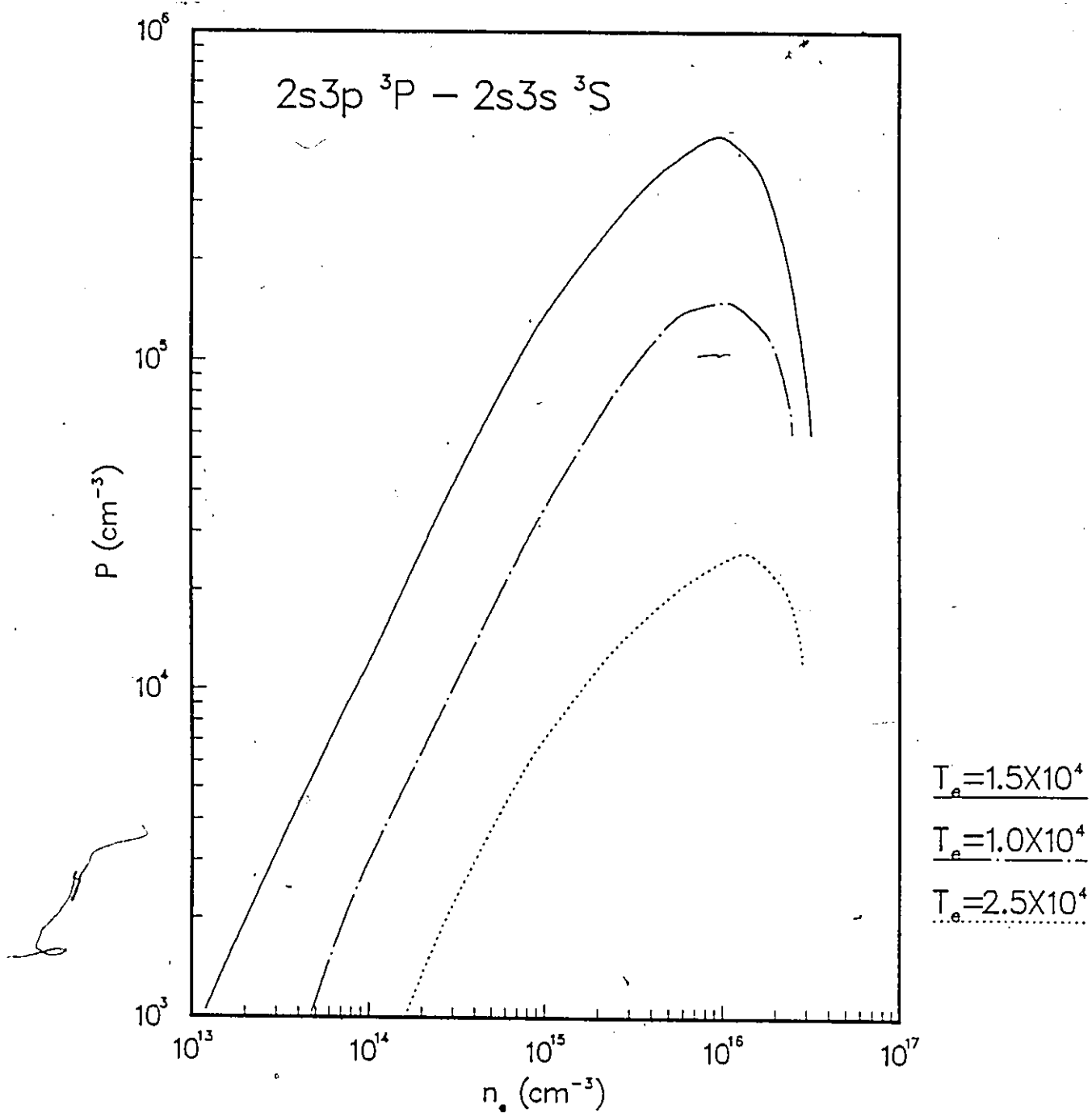


Figure 5-1. P as a function of n_e for $\lambda 4650$.

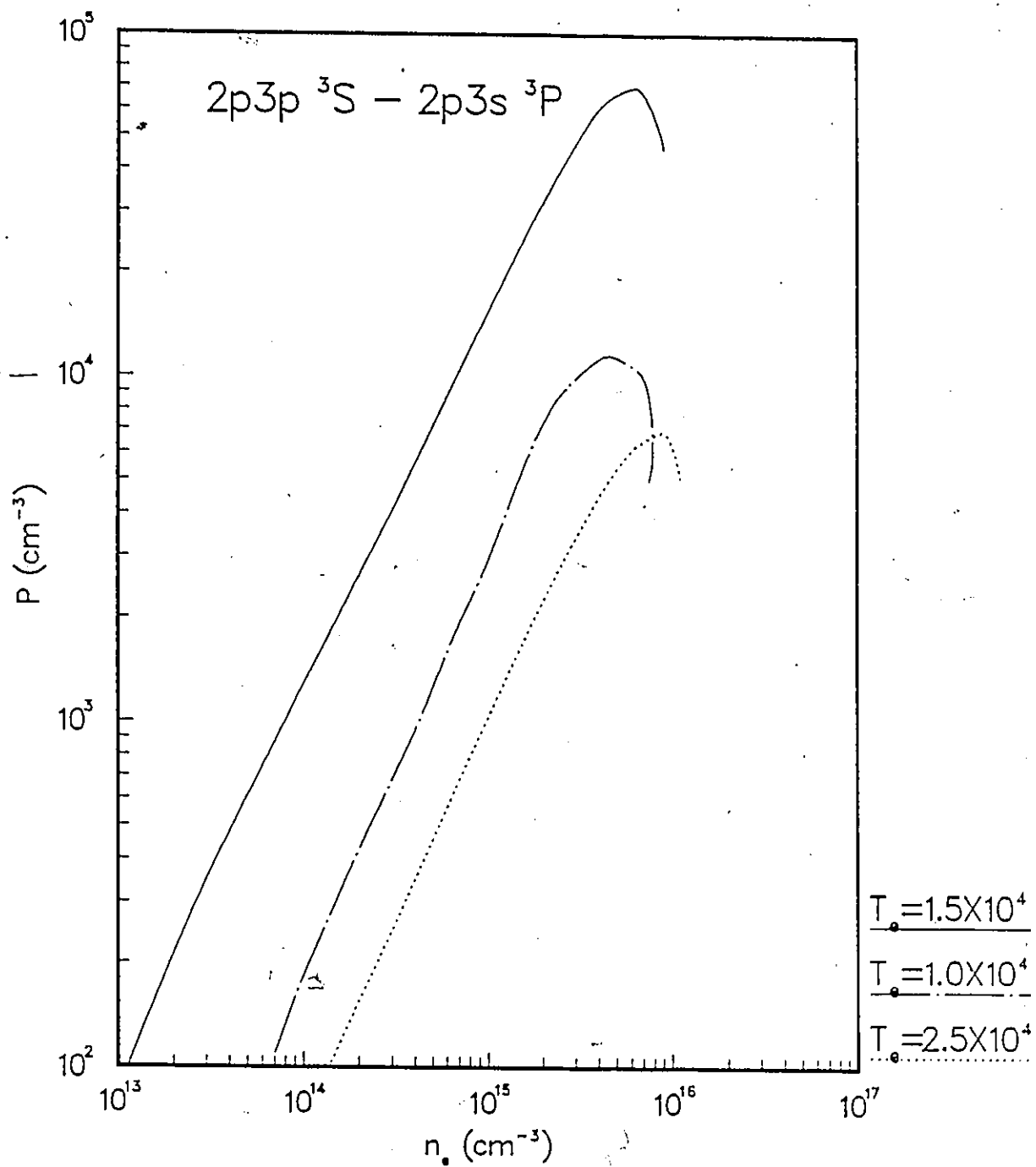


Figure 5-2. P as a function of n_e for $\lambda 5263$.

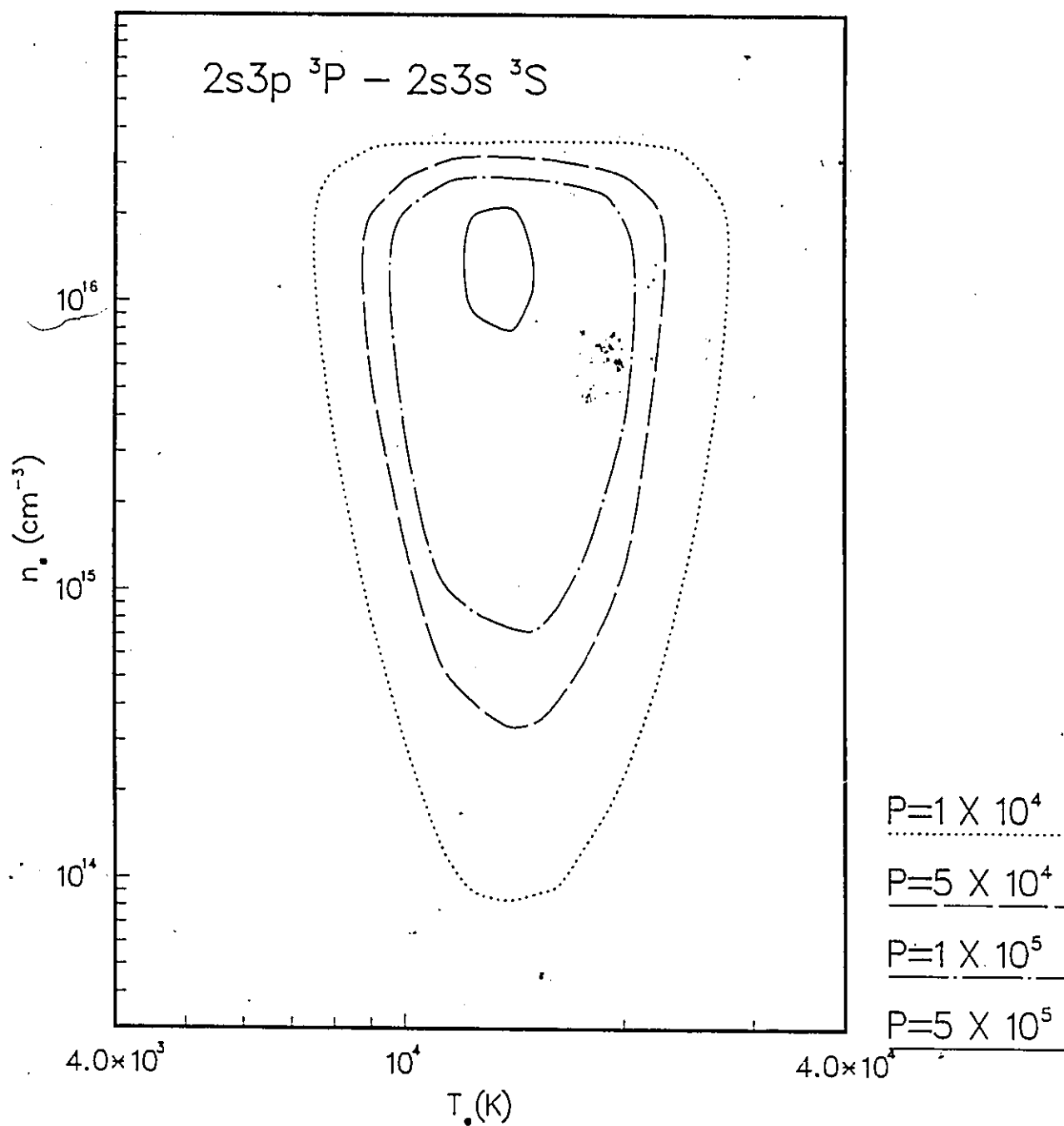


Figure 5-3. P as a function of n_e and T_e for $\lambda 4650$.

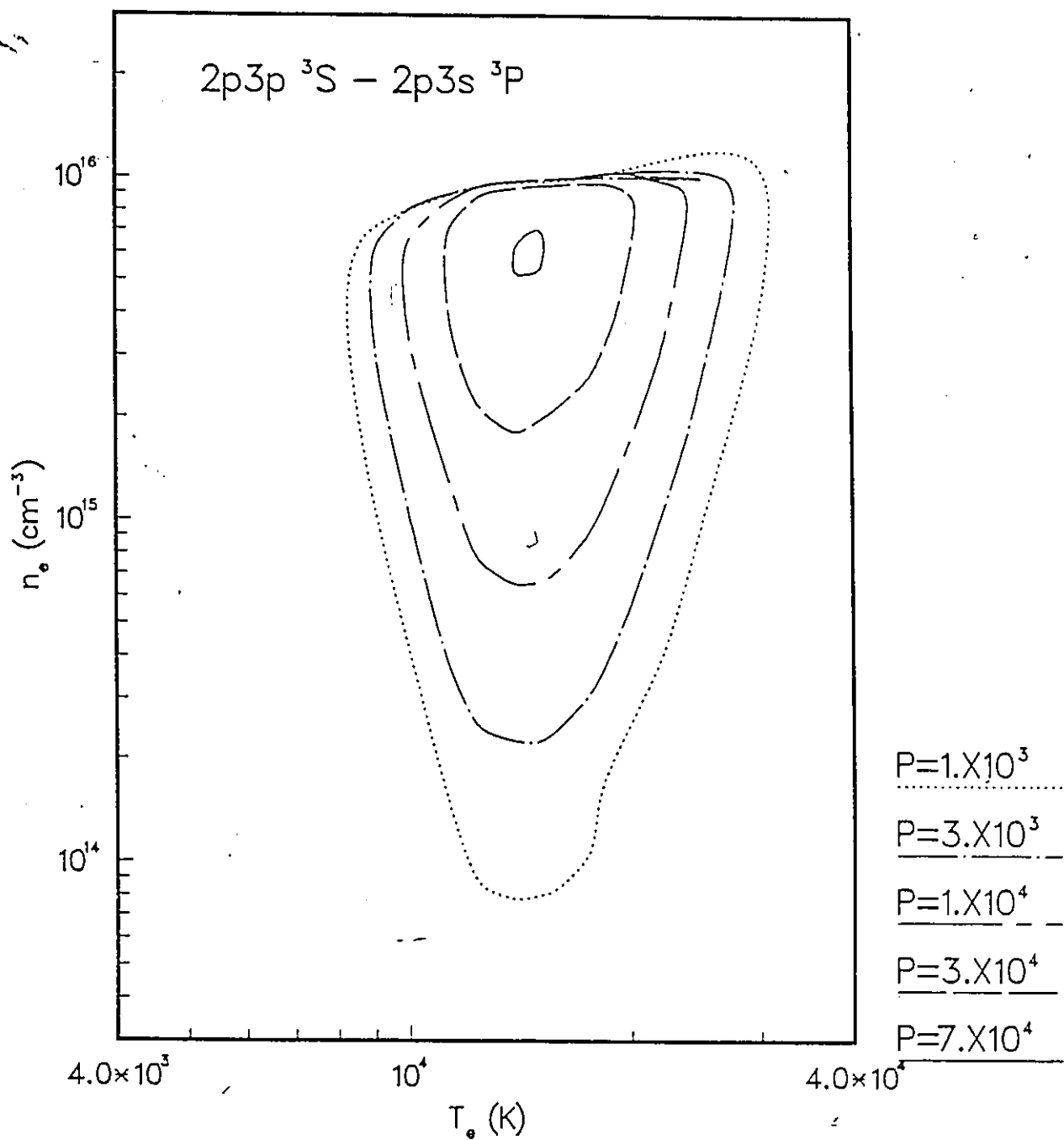


Figure 5-4. P as a function of n_e and T_e for $\lambda 5263$.

Chapter 6

Population Inversions in CIII in a Freely Expanding Carbon Plasma.

A) Introduction

In this chapter the behaviour of the population densities of the levels of C III ion in free expansion of carbon plasma are studied to pursue the possibility of using this plasma as a lasing medium. Population inversions in the transitions in the visible and ultraviolet region are reported. In addition, the possibility of using these results in explaining the observed intensity of the line $\lambda 2297$ in the spectra of nebular stage nova is pointed out.

B) Basic equations

The model calculation is similar to that described in chapter 3. We consider a spherically symmetric carbon plasma expanding in vacuum. Using the same assumptions as those in chapter 3, the relaxation equations for the electronic level populations of C III ion are given by

$$\frac{dN_i}{dt} = \Gamma_i - \frac{3}{t + \beta} N_i \quad (i = 1, 2, \dots, r), \quad (6-1)$$

and the rate of change of electron density in the uniformly expanding carbon plasma is given by

$$\frac{dn_e}{dt} = - \sum_{i=1}^r \Gamma_i - n_e (N^{+4} \alpha^{+4} + N^{+2} \alpha^{+2} + N^{+1} \alpha^{+1} - N^{+3} S^{+3} - N^{+1} S^{+1}) - \frac{3}{t + \beta} n_e. \quad (6-2)$$

The time derivatives of the densities of C^0 , C^{+1} , C^{+3} , C^{+4} are given by

$$\frac{dN^0}{dt} = - \frac{3}{t + \beta} N^0 + \Gamma_0, \quad (6-3)$$

$$\frac{dN^{+1}}{dt} = -\frac{3}{t+\beta}N^{+1} + \Gamma_{+1}, \quad (6-4)$$

$$\frac{dN^{+3}}{dt} = -\frac{3}{t+\beta}N^{+3} + \Gamma_{+3}, \quad (6-5)$$

$$\frac{dN^{+4}}{dt} = -\frac{3}{t+\beta}N^{+4} + \Gamma_{+4}, \quad (6-6)$$

where Γ_{+m} is given by

$$\Gamma_{+m} = n_e [N^{+(m-1)} S^{+(m-1)} - N^{+m} (S^{+m} + \alpha^{+m}) + N^{+(m+1)} \alpha^{+(m+1)}] \quad (6-7)$$

and the heat balance equations are

$$\frac{dT_e}{dt} = -\frac{2}{t+\beta}T_e + \frac{T_e}{n_e} \sum_{i=1}^r \Gamma_i + \frac{2}{3} \frac{(Q_{inel} - Q_{\Delta T})}{n_e} \quad (6-8)$$

$$\frac{dT}{dt} = -\frac{2}{t+\beta}T + \frac{2}{3} \frac{Q_{\Delta T}}{N} \quad (6-9)$$

The rate of increase of the thermal energy Q_{inel} of the electron, can be calculated from Eq. (3-26). The energy transfer rate due to elastic collisions, $Q_{\Delta T}$, is calculated using equation (3-27), and the collision frequency for electron-ion and ion-ion estimated from the following expressions (Golant, et al., 1977):

For electron-ion collisions

at $T_e < 10$ eV,

$$\nu_{ek} \approx \frac{4\pi e^4 N^k}{m_e^2 v^3} \left(23 + \frac{3}{2} \ln T_e - \frac{1}{2} \ln n_e \right) \quad (6-10)$$

at $T > 10$ eV,

$$\nu_{ek} \approx \frac{4\pi e^4 N^k}{m_e^2 v^3} \left(24 + \ln T_e - \frac{1}{2} \ln n_e \right) \quad (6-11)$$

where v is the relative velocity and N^k is the density of the k specie.

C) Numerical calculations

We assume that the carbon plasma is in ionization equilibrium whose electron and heavy particles temperature, electron density, and total heavy particles density are T_{e0} , T_{a0} , n_{e0} , and N_0 and then it is allowed to expand in a vacuum. At $t = 0$, the population densities for the electronic levels of C III ion were calculated using the steady state assumption,

$$\frac{dN_i}{dt} = 0 \quad (i = 1, 2, 3, \dots, r), \quad (6-12)$$

and we used the ionization equilibrium model described in section (B) of chapter 3 to calculate the initial relative concentrations of various stage of ionization of carbon at n_{e0} and T_{e0} . We have made the calculation for three sets of initial temperature and density which are summarized in Table 6-1.

TABLE 6-1. Initial plasma parameters.

	T_{e0}	T_{a0}	N_0	β
a	8.617 eV	6.9 eV	$1 \times 10^{15} \text{ cm}^{-3}$	$1 \times 10^{-5} \text{ sec.}$
b	8.617	6.9	1×10^{15}	1×10^{-7}
c	4.309	2.6	1×10^{15}	1×10^{-7}

The excitation model of the C III ion is the same as the one used in chapter 3. All the levels in the configuration $1s^2 2sn\ell$ having principal quantum number $n \leq 5$, and the

levels in the configuration $1s^2 2pn\ell$ having $n \leq 3$ are treated as individual levels except for the levels having orbital angular momentum $\ell \geq 2$ in the configuration $1s^2 2pn\ell$. These latter levels with same n are treated as a single level. The levels $n^1,^3S$, $n^1,^3P^o$, $n^1,^3D$, ... in configuration $1s^2 2sn\ell$ with $n \geq 6$ are grouped together in one level. The levels with $n > 3$ in the configuration $1s^2 2pn\ell$ are not included in the calculation because most of these levels lie above the ionization limit (autoionization states). The labelling of the various states and the energies are given in Table 3-2. All the rate coefficients needed in this calculation are described in section (C) of chapter 3.

Numerical results obtained from the set of differential equations (6-1) to (6-8) are given as a function of time. The quasi-steady state assumption is made for all levels satisfying the condition (3-37). In three cases studied in this chapter, we found that at early time of the expansion large number of levels in C III ion do not satisfy the condition (3-37) as the time approach β the number of such levels decrease and at $t \approx \beta$ only the ground state $2s^2 \ ^1S$ and the metastable state $2s2p \ ^3P^o$ do not satisfy condition (3-37). The relaxation time of some levels, the relaxation time of electron density and electron temperature as these quantities vary with time for case c are presented in Table 6-2. It is clear from the table that the use of condition (3-37) will give reasonable results but with some uncertainty because of the large relaxation time of the excited states (compared to helium excited states). Also the accuracy of these results depends on the accuracy of the atomic data used. Unfortunately the approximations used give cross sections and rate coefficients with some uncertainty, thus, we expect that there is large uncertainty in the result at high electron densities, where the collision processes by electron impact are important, but the results are expected to improve as the density drops, where the population is governed by radiative decay.

TABLE 6-2. Relaxation Time in seconds.

t (sec)	T_e (eV)	τ_{n_e}	τ_1	τ_2	τ_{10}	τ_{20}	τ_{36}
1.0E-12	4.308	3.3E-8	1.2E-8	1.4E-8	2.99E-10	1.58E-10	8.9E-11
1.0E-10	4.28	3.3E-8	1.2E-8	1.4E-8	3.0E-10	1.59E-10	9.0E-11
1.0E-9	4.00	3.4E-8	1.3E-8	1.5E-8	3.1E-10	1.62E-10	9.5E-11
5.0E-9	3.20	3.5E-8	2.0E-8	1.7E-8	3.6E-10	1.8E-10	1.1E-10
1.0E-8	2.7	3.7E-8	2.9E-8	1.9E-8	4.0E-10	1.9E-10	1.3E-10
5.1E-8	1.70	5.0E-8	2.4E-7	4.0E-8	7.8E-10	4.2E-10	4.1E-10
1.0E-7	1.39	6.5E-8	1.1E-6	8.5E-8	9.4E-10	5.9E-10	5.0E-10
6.2E-7	0.81	2.3E-7	7.2E-4	2.5E-6	9.0E-9	9.9E-10	9.8E-10
1.0E-6	0.58	3.6E-7	6.0E-2	7.4E-6	1.1E-8	1.13E-9	1.1E-9
2.2E-6	0.43	5.4E-7	2.3E+1	5.9E-5	1.2E-8	1.3E-9	1.9E-9

The quantity following E is the power of 10 by which the preceding number must be multiplied.

Integration of the equations was performed by using the Runge-Kutta -Gill method. The time step Δt was set to be less than one tenth of the relaxation time of the level i^* .

D) Results and Discussion

The variation of T_e with time for the three cases is shown in Fig. 6-1. It will be noticed that the variation is quite similar to that found for helium plasma in Chapter 3. The electron temperature shows very little change for $t \ll \beta$. The onset of the rapid decrease depends on individual cases. In all the three cases $|dT_e/dt|$ increases with time at first, reaches a maximum and then it decreases. Fig. 6-2 shows the electron density as a function of the time for the three cases.

Figs. 6-3 to 6-17 show the population densities vs. time for many of the levels of C III. As was the case in Chapter 3, because of the limitations of the computer program, in this case we could not go beyond $T_e < 0.4$ eV. One important difference with the results obtained for helium may be noted here. At least to the time that we have followed the three cases, there is no upturn in the population density of any of these levels.

We note here that even in the initial steady state we found that there was population inversion for some of the transitions. These transitions are as follows: $2s3p\ ^3P^o \rightarrow 2s3s\ ^3S$ ($\lambda 4650$) (Fig. 6-3), $2s4p\ ^3P^o \rightarrow 2s3d\ ^3D$ ($\lambda 2092$) (Fig. 6-6), and $2s5f\ ^3F^o \rightarrow 2s4d\ ^3D$ ($\lambda 3885$) (Fig. 6-8), $2s5s\ ^1S \rightarrow 2p3s\ ^1P^o$ ($\lambda 3507$) (Fig. 6-11).

A great many transitions in the visible and ultraviolet region show a large population inversion in all cases considered. We describe population inversion between levels for case a as a representative case, the only difference between the cases is the degree of the population inversion and the time at which the population inversion occurs.

Fig. 6-3 shows the population densities for the levels $2p^2\ ^3P$, $2s2s\ ^3S$, $2s3p\ ^3P^o$, $2s4p\ ^3P^o$ as a function of time. It can be noticed that the population density of the level $2p^2\ ^3P$ decreases more rapidly than that of $2s3p\ ^3P^o$, population inversion in the transition $2s3p\ ^3P^o \rightarrow 2p^2\ ^3P$ ($\lambda 818$) appears at $t \approx 6 \times 10^{-6}$ s and increases subsequently, with the maximum of order $2 \times 10^7\ \text{cm}^{-3}$ obtained at $T_e \sim 1.4 \times 10^4$ K, and $n_e \sim 1.2 \times 10^{14}\ \text{cm}^{-3}$. Fig. 6-3 shows there is a strong population inversion in the transition $2s3p\ ^3P^o \rightarrow 2s3s\ ^3S$ ($\lambda 4650$). The formation of the inversion is due to the probability of the collision decay of the upper working level being smaller than that of the corresponding lower level. Also, Fig. 6-3 shows there is a small population inversion in the transition $2s4p\ ^3P^o \rightarrow 2s3s\ ^3S$ ($\lambda 1256$) with maximum of order $3 \times 10^4\ \text{cm}^{-3}$ for $t \geq 2 \times 10^{-5}$ s. The corresponding plots for the cases b and c are shown in Figs. 6-4 and 6-5, respectively. These figures show

clearly that the degree of the population inversion depends on the initial conditions, with smaller initial electron temperature, the magnitude of population inversion is greater.

The population densities for the levels $2s3d\ ^3D$, $2s4p\ ^3P^o$, and $2s4f\ ^3F^o$ as a function of time are presented in Fig. 6-6. Strong population inversion between the levels $2s4p\ ^3P^o$ and $2s3d\ ^3D$ with maximum of order $3 \times 10^6\text{ cm}^{-3}$ obtained at $n_e \sim 2.3 \times 10^{14}\text{ cm}^{-3}$, and $T_e \sim 1.6 \times 10^4\text{ K}$, and exists even at larger electron densities ($n_e > 10^{15}$). Fig. 6-6 show large population inversion in the transition $2s4f\ ^3F^o \rightarrow 2s3d\ ^3D$ ($\lambda 1923$) with maximum of order $1 \times 10^6\text{ cm}^{-3}$ is obtained. The corresponding plots for the case c are presented in Fig. 6-7.

The $2s4d\ ^3D$, $2s5p\ ^3P^o$, $2p3d\ ^3P^o$, and $2s5f\ ^3F^o$ population densities as a function of time are presented in Fig. 6-8. This figure shows large population inversion in the transition $2s5f\ ^3F^o \rightarrow 2s4d\ ^3D$ ($\lambda 3885$) with maximum of order $1.3 \times 10^6\text{ cm}^{-3}$ obtained at $n_e \approx 2.6 \times 10^{14}\text{ cm}^{-3}$ and $T_e \approx 2.1 \times 10^4\text{ K}$. Large population inversion in the transitions $2s5p\ ^3P^o \rightarrow 2s4d\ ^3D$ ($\lambda 4383$) and $2p3d\ ^3P^o \rightarrow 2s4d\ ^3D$ ($\lambda 5353$) with maximum of order $9 \times 10^5\text{ cm}^{-3}$ is obtained at $t \approx 9 \times 10^{-7}\text{ s}$ and vanishes at $t \approx 1 \times 10^{-5}\text{ s}$. The population inversions in the last two transitions depend strongly on the accuracy of the cross sections involved. The formation of the population inversion in these cases is due to the large probabilities of the collision decay of the lower level $2s4d\ ^3D$ and as the electron density decreases the inversion vanishes.

Fig 6-9 show the population densities for the levels $2s3d\ ^3D$, $2s4s\ ^3S$, $2s4p\ ^3P^o$, and $2s5f\ ^3F^o$ as a function of time. Population inversion in the transition $2s5f\ ^3F^o \rightarrow 2s3d\ ^3D$ ($\lambda 1296$) appears at $t \approx 3 \times 10^{-7}\text{ s}$ and reaches maximum of order $1 \times 10^6\text{ cm}^{-3}$ at $n_e \sim 4 \times 10^{14}\text{ cm}^{-3}$, and $T_e \sim 2.3 \times 10^4\text{ K}$. Strong population inversion occurs in the transition $2s4p\ ^3P^o \rightarrow 2s4s\ ^3S$ ($\lambda 11981$) at $t \approx 2 \times 10^{-6}$, and increases subsequently, with

the maximum at $n_e \sim 2 \times 10^{14} \text{ cm}^{-3}$, and $T_e \sim 1.9 \times 10^4 \text{ K}$.

In Fig. 6-10 we present the population densities for the levels $2p3s \ ^3P^o$ and $2p3p \ ^3S$ as a function of time. Strong population inversion in the line $2p3p \ ^3S \rightarrow 2p3s \ ^3P^o$ ($\lambda 5253$) appears at $t \approx 4 \times 10^{-7} \text{ s}$ and reaches maximum at $t \approx 6 \times 10^{-6} \text{ s}$. The electron density and temperature at the maximum of inversion are $4 \times 10^{14} \text{ cm}^{-3}$ and $2.5 \times 10^4 \text{ K}$, respectively.

Fig. 6-11 shows the population densities for the levels $2p3s \ ^1P^o$, $2s3p \ ^1P^o$, $2s4p \ ^1P^o$, and $2s5s \ ^1S$. It can be noticed that the transition $2s5s \ ^1S \rightarrow 2p3s \ ^1P^o$ ($\lambda 3507$) shows large population inversion, with maximum of order 1×10^6 . Population inversion in the lines $2s5s \ ^1S \rightarrow 2s3p \ ^1P^o$ ($\lambda 1256$) and $2s5s \ ^1S \rightarrow 2s4p \ ^1P^o$ ($\lambda 6205$) appear at $t \approx 1.8 \times 10^{-5} \text{ s}$, with maximum of order $7 \times 10^4 \text{ cm}^{-3}$ at $n_e \sim 3 \times 10^{13} \text{ cm}^{-3}$, $T_e \sim 8000 \text{ K}$. The corresponding plots for case c are shown in Fig. 6-12.

Fig 6-13 shows the population densities for the levels $2s3d \ ^1D$, $2s4p \ ^1P^o$, and $2s4f \ ^1F^o$ as a function of time. Population inversion in the lines $2s4p \ ^1P^o \rightarrow 2s3d \ ^1D$ ($\lambda 2177$) and $2s4f \ ^1F^o \rightarrow 2s3d \ ^1D$ ($\lambda 2162$) appear after $t \approx 2 \times 10^{-6} \text{ s}$, and maximum of order $1 \times 10^6 \text{ cm}^{-3}$ occurs at $n_e \sim 5 \times 10^{14} \text{ cm}^{-3}$, and $T_e \sim 2 \times 10^4 \text{ K}$. Population densities as a function of time for the levels $2s4d \ ^1D$, $2s4f \ ^1F^o$, and $2s5f \ ^1F^o$ are presented in Fig. 6-14. In the initial stages the population density for the level $2s5f \ ^1F^o$ increases as the plasma expands, while the population densities for the levels $2s4d \ ^1D$ and $2s4f \ ^1F^o$ decrease, at $t \approx 3 \times 10^{-7} \text{ s}$ population inversion between $2s5f \ ^1F^o$ and $2s4d \ ^1D$ appears, with maximum of order $2 \times 10^6 \text{ cm}^{-3}$ obtained at $n_e \sim 3 \times 10^{14} \text{ cm}^{-3}$ and $T_e \sim 2 \times 10^4 \text{ K}$. Fig 6-15 shows the population densities for the levels $2p3s \ ^1P^o$, $2s3p \ ^1P^o$, and $2s4s \ ^1S$ as a function of time. The transition $2s4s \ ^1S \rightarrow 2p3s \ ^1P^o$ ($\lambda 58303$) shows strong population inversion, with maximum of order $2 \times 10^7 \text{ cm}^{-3}$ obtained at $n_e > 3 \times 10^{15} \text{ cm}^{-3}$. population inversion in the transition $2s4s \ ^1S \rightarrow 2s3p \ ^1P^o$ ($\lambda 1894$) appears at $t \approx 10^{-6} \text{ s}$ and reaches maximum of order $7 \times 10^5 \text{ cm}^{-3}$.

The electron density and temperature at the maximum of inversion are $2.5 \times 10^{14} \text{ cm}^{-3}$, and $2 \times 10^4 \text{ K}$, respectively.

The population densities of the levels $2s2p^1P^o$ and $2p^2^1D$ as a function of time are presented in Fig. 6-17. Population inversion between these levels appears at $t \approx 1.5 \times 10^{-5} \text{ s}$, and at $t \approx 2 \times 10^{-5} \text{ s}$ reaches its maximum which is of order $5 \times 10^6 \text{ cm}^{-3}$. The electron density and temperature at the maximum are $6.7 \times 10^{13} \text{ cm}^{-3}$ and 10300 K , respectively.

The nebular stage spectra of many novae (e.g. Cygni 1978, AG Peg) show $\lambda 2297$ in emission. Observations of Cygni 1978 at nebular stage with the IUE satellite have been published by Stickland et al. (1981). The nebular stage spectra showed emission lines of: He II; C II, III and IV; N II, III, IV and V; O I, III, IV and V; and Mg II. By analogy with the interpretation of solar transition region spectra, pairs of lines in the same ion were at first used to determine the temperature of formation of the lines. Thus, the lines C III $\lambda 2297$ and C III $\lambda 1909$, both assumed to be collisionally excited, yield temperatures in the range $(4 - 5) \times 10^4 \text{ K}$ in the C III region of the nova shell (Stickland et al., 1981). Subsequent work has shown that these temperatures are too large. Important clues are provided by observations of C III $\lambda 2297$ in the spectra of planetary nebulae (Harrington et al., 1981) for which the electron temperatures are known to be of order 10^4 K . At such temperatures the rate of collisional excitation is several orders of magnitude too slow to account for the observed $\lambda 2297$ intensity (Nussbaumer and Storey, 1983). The result presented in Fig. 6-17 shows clearly that the population density of $2p^2^1D$ is more than that of $2s2p^1P^o$ even at low electron density and temperature. This suggests that the observed intensity of $\lambda 2297$ can be explained easily by the mechanism presented in this chapter. In order to show the evolution of the population inversion clearly, we plot the population inversion $P(\lambda 2297)$ (P defined in Eq. 2-55) as a function of time in Fig. 6-18. The corresponding plot for the

case c is shown in Fig. 6-19.

The variation of the inverted population with initial conditions shows a behaviour similar to that found in previous chapter. The present calculations show that it is possible in practice to produce a laser on the basis of a highly-ionized carbon plasma expanding in vacuum. The results of the calculations show that the mechanism of recombination in an expanding plasma is quite effective for producing population inversion for certain transitions in C III.

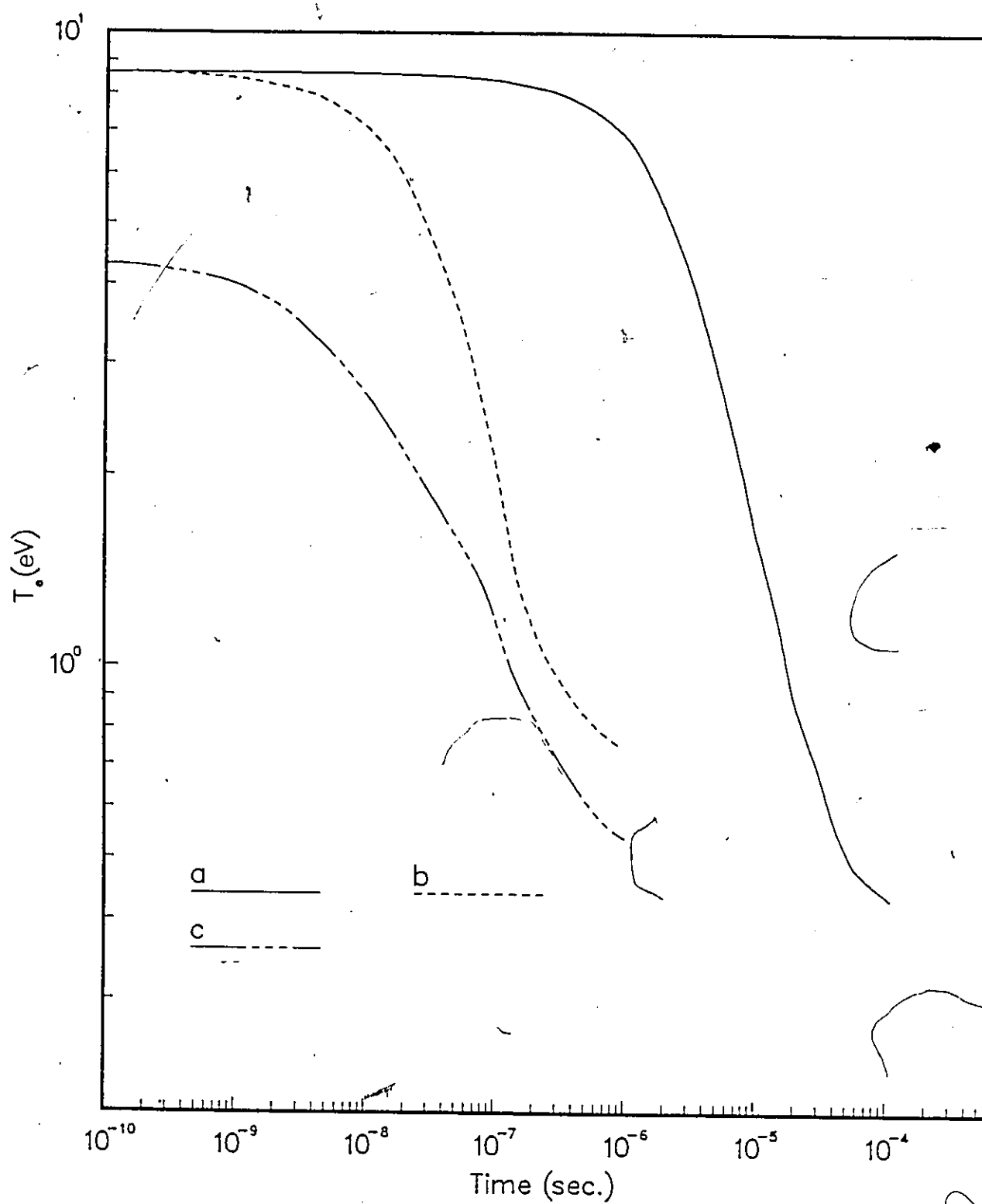


Fig. 6-1. Electron temperature vs. time for the cases a, b, c.

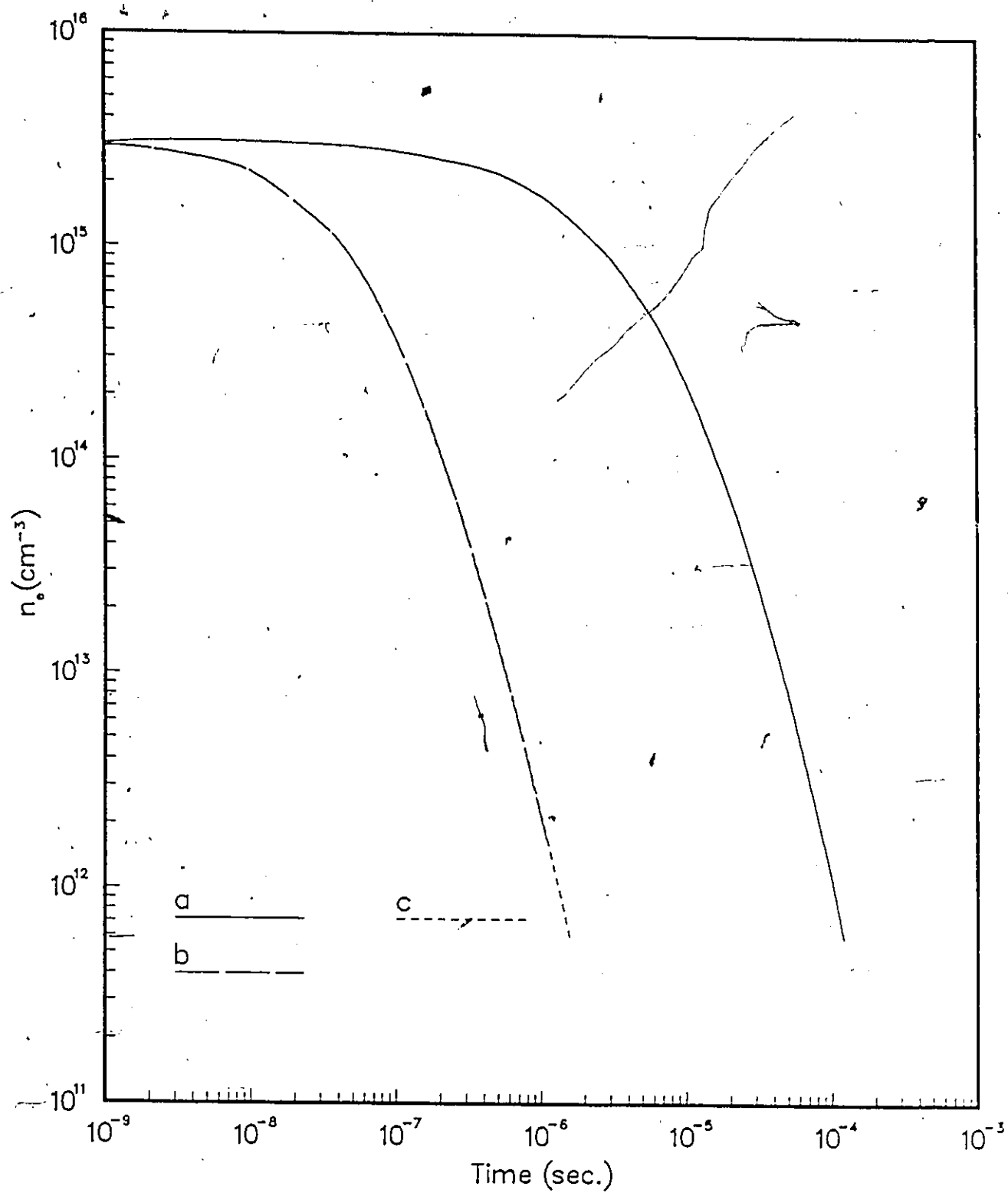


Fig. 6-2. Electron density vs. time for the cases a, b, c.

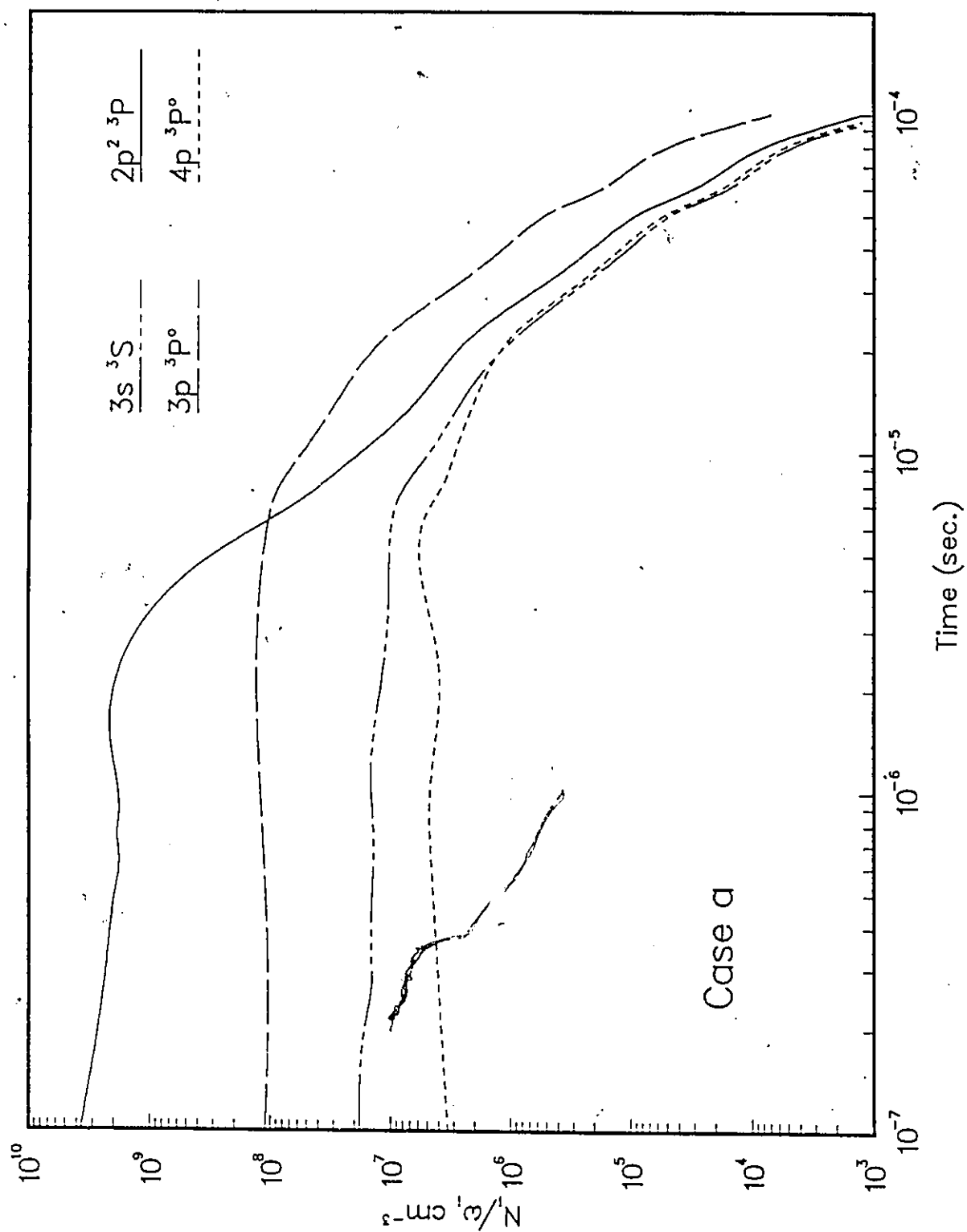


Fig. 6-3. Population densities vs. time for some levels in C III

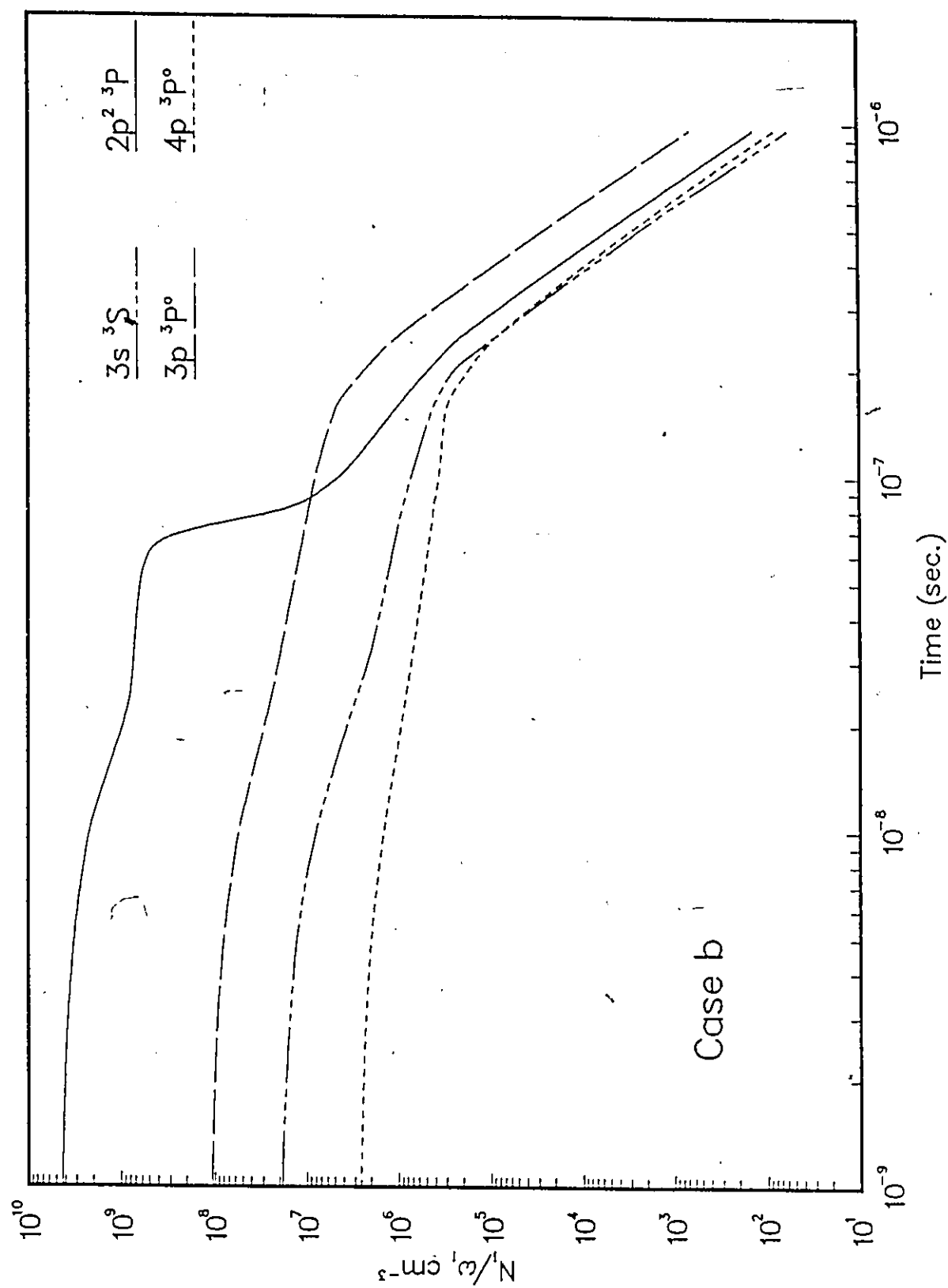


Fig. 6-4. Population densities vs. time for some levels in C III

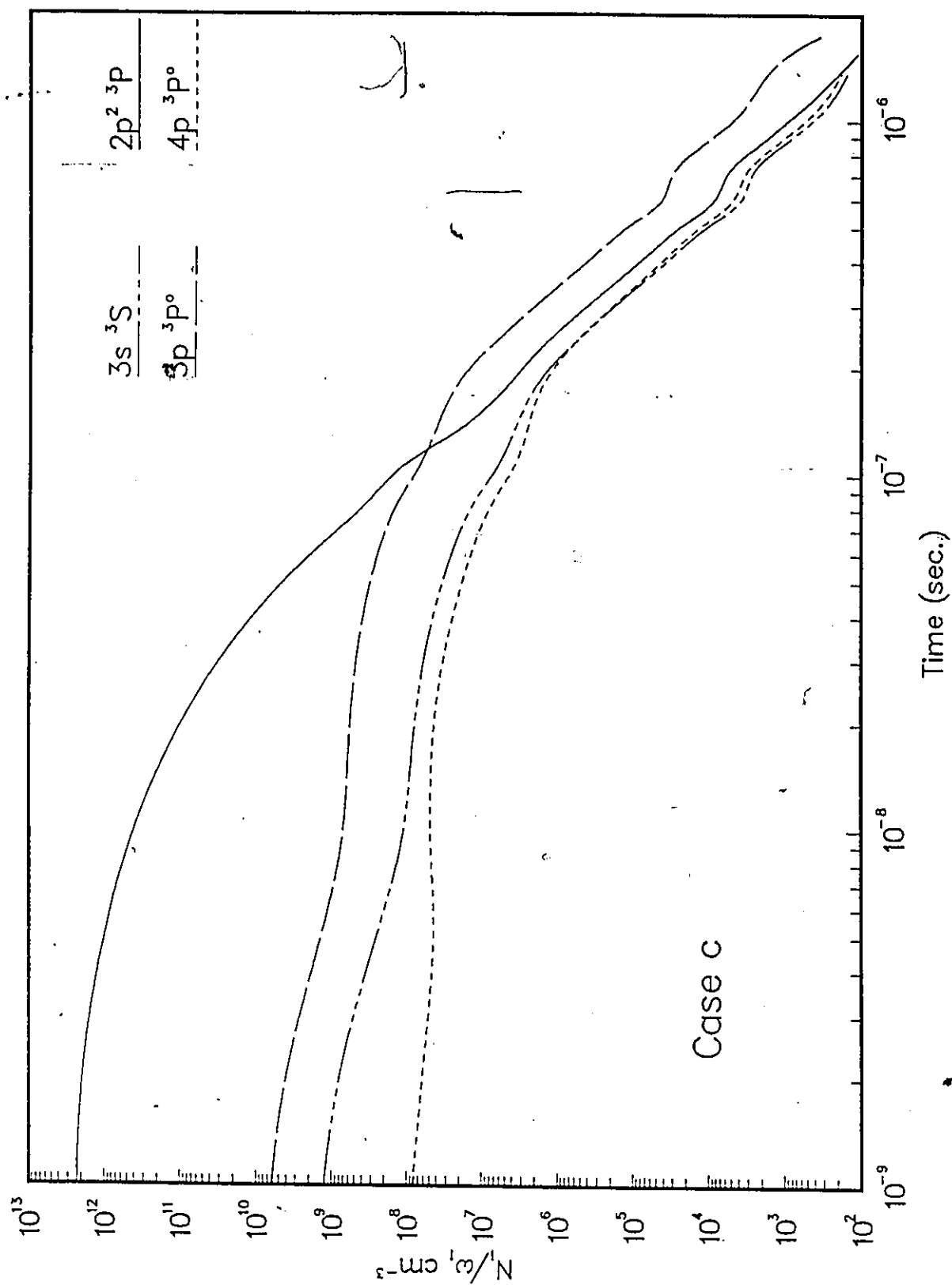


Fig. 6-5. Population densities vs. time for some levels in C III

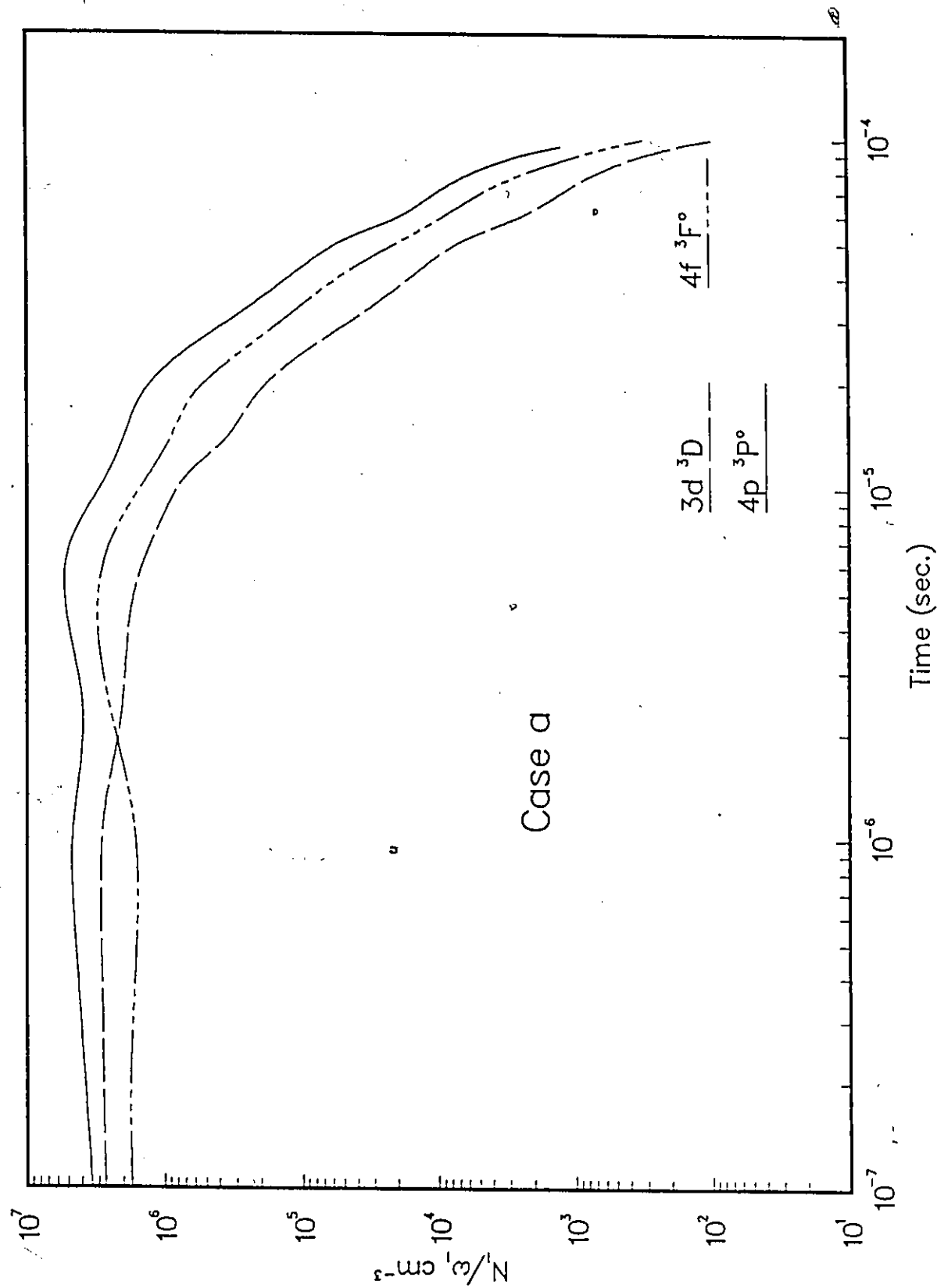


Fig. 6-6. Population densities vs. time for some levels in C III

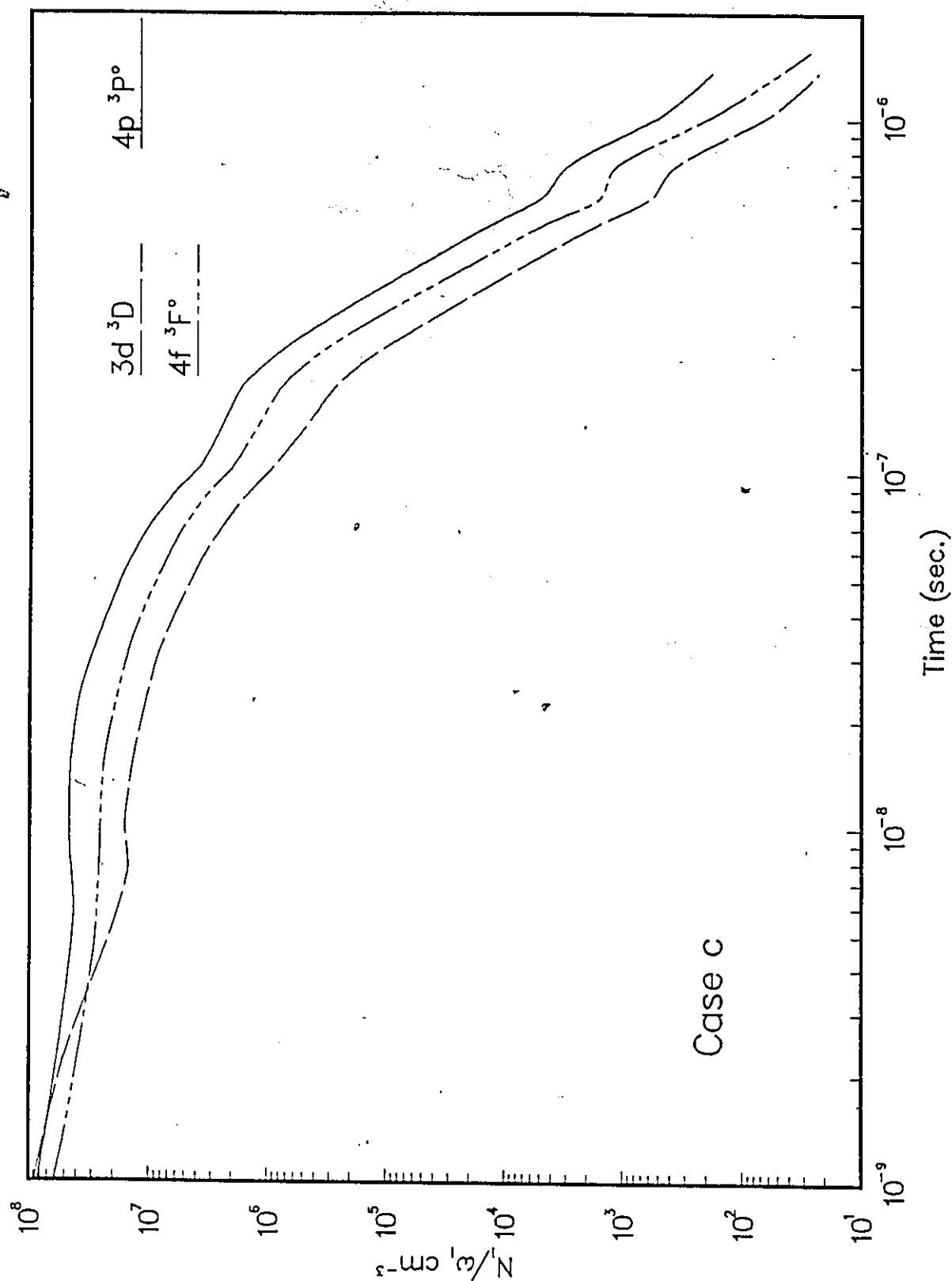


Fig. 6-7. Population densities vs. time for some levels in C III

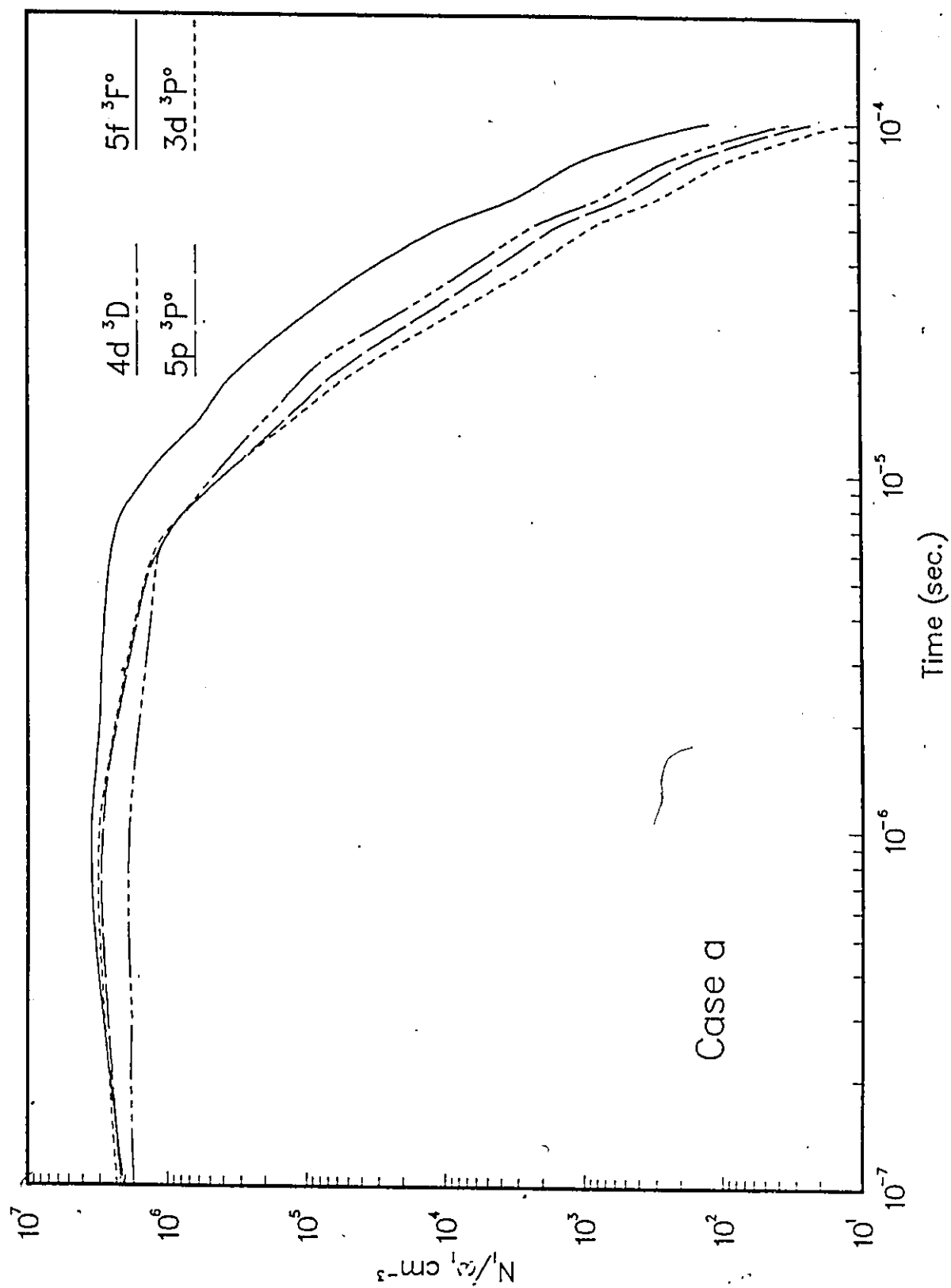


Fig. 6-8. Population densities vs. time for some levels in C III

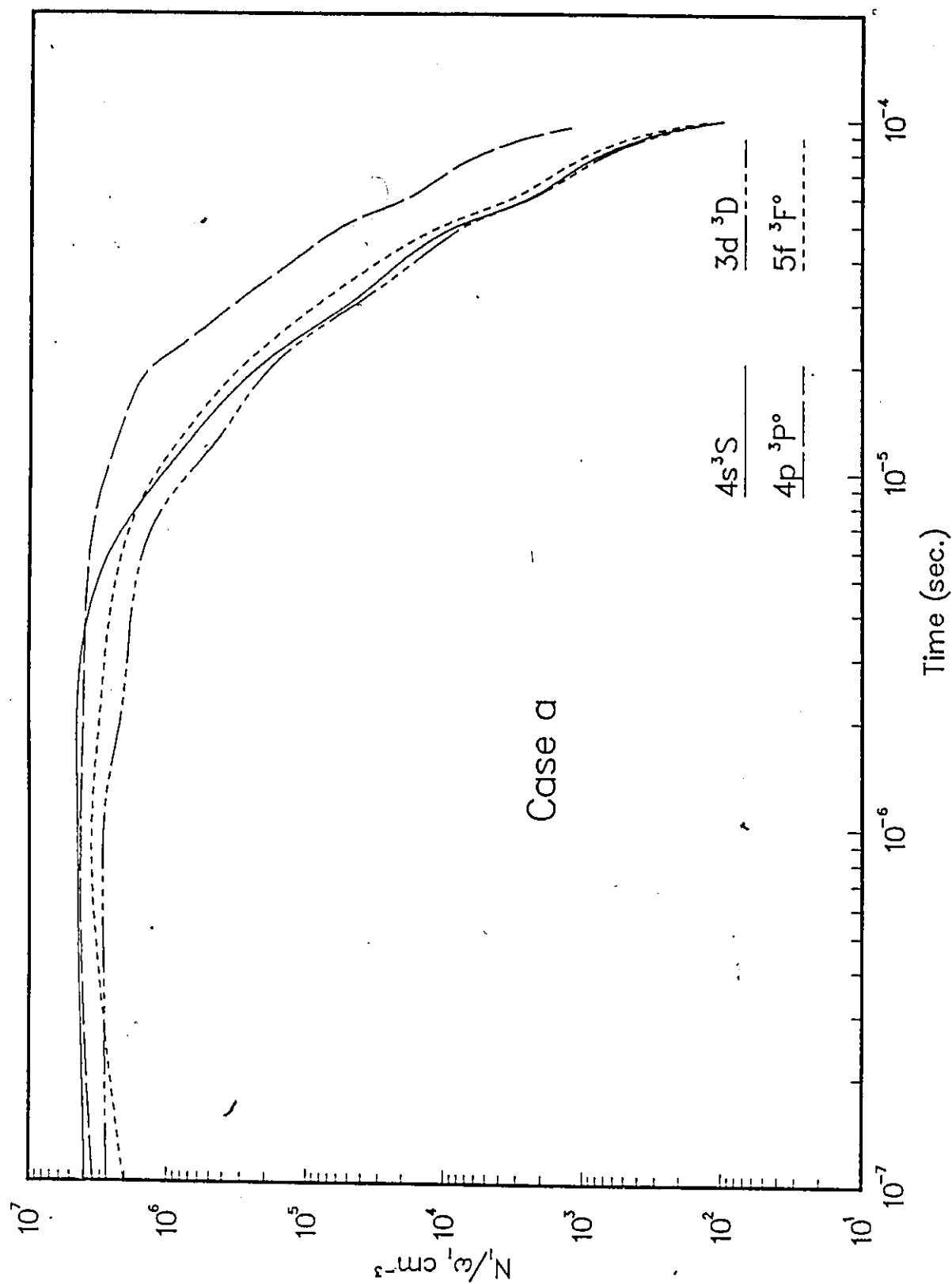


Fig. 6-9. Population densities vs. time for some levels in C III

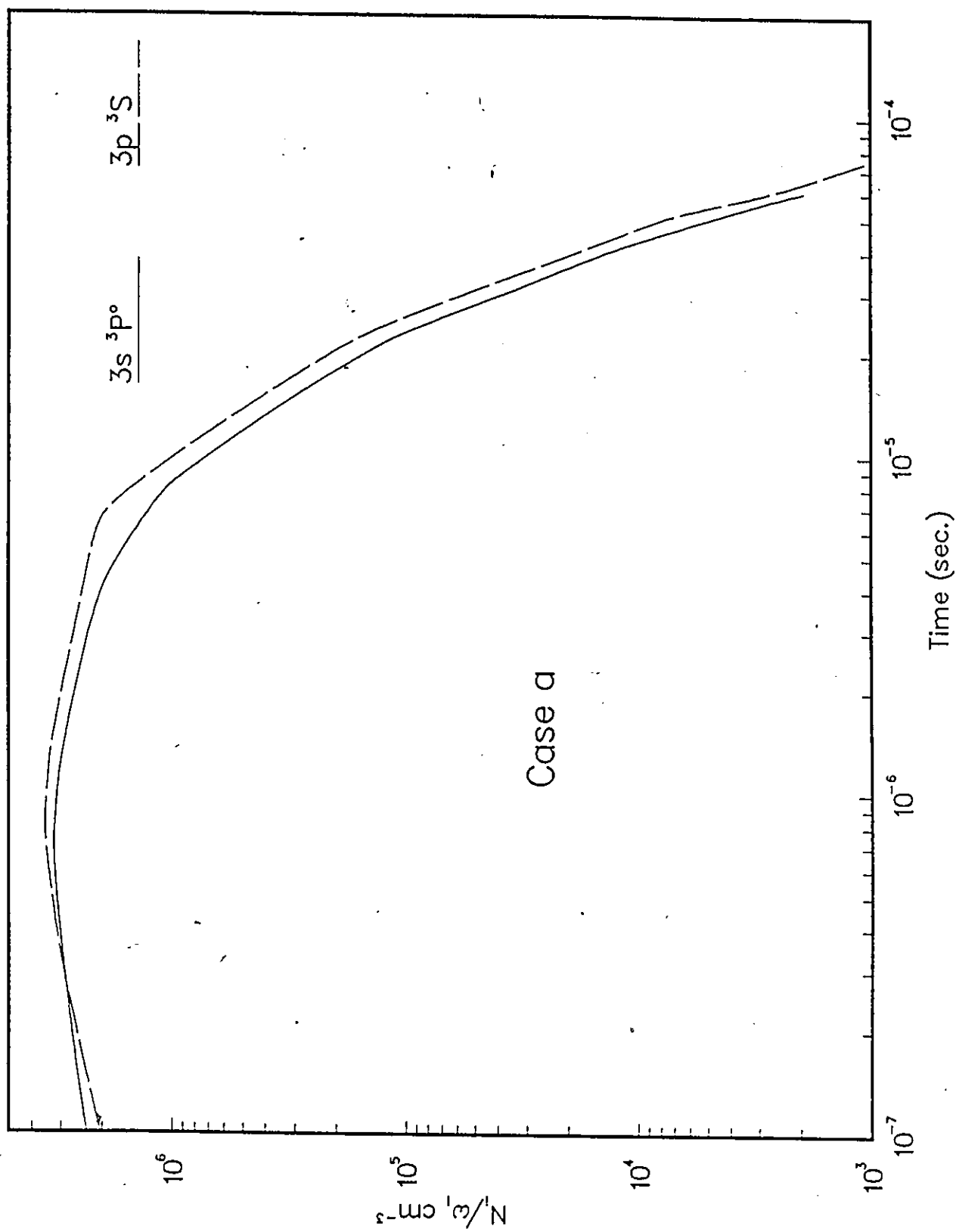


Fig. 6-10. Population densities vs. time for some levels in C III

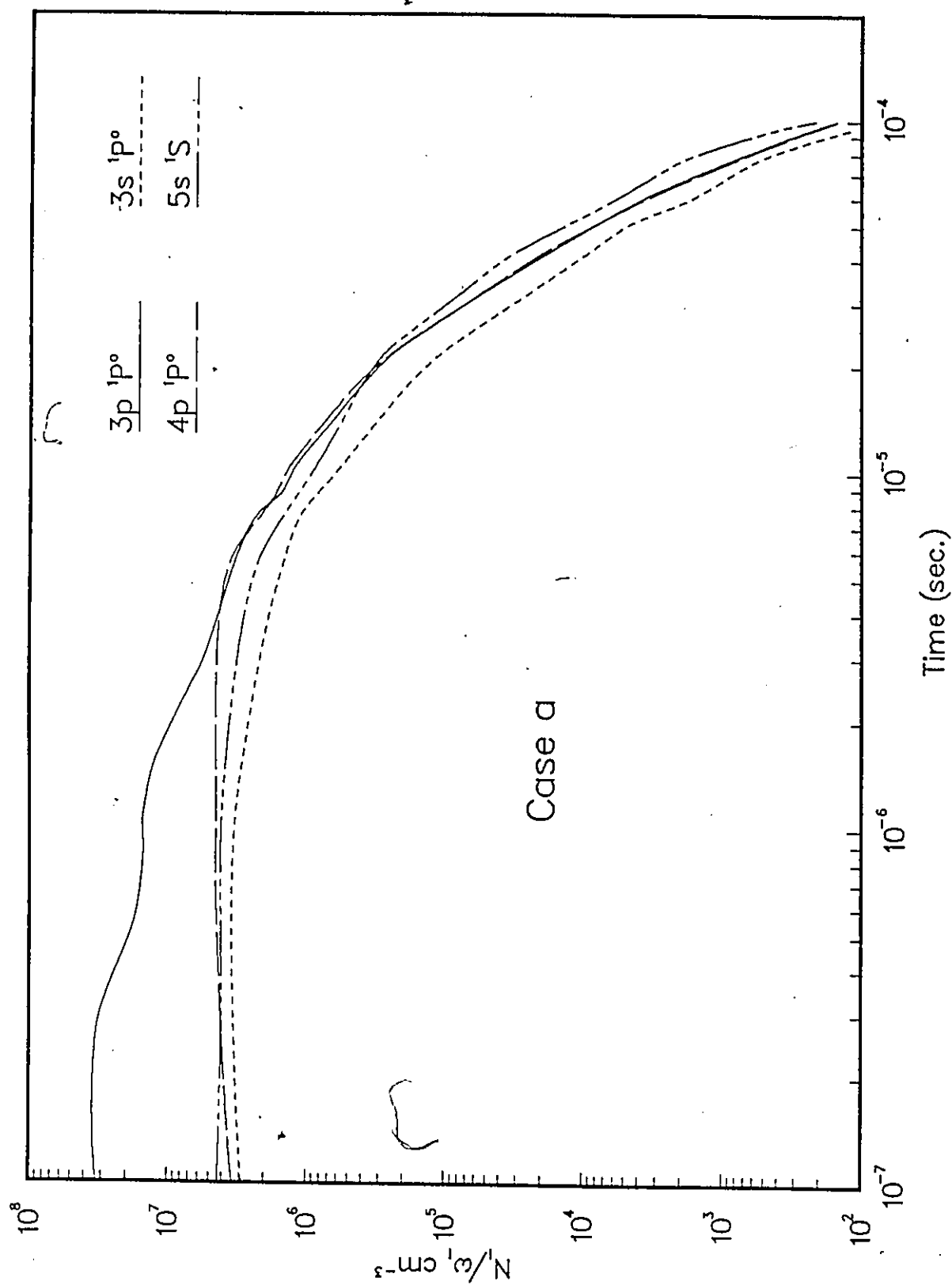


Fig. 6-11. Population densities vs. time for some levels in C III

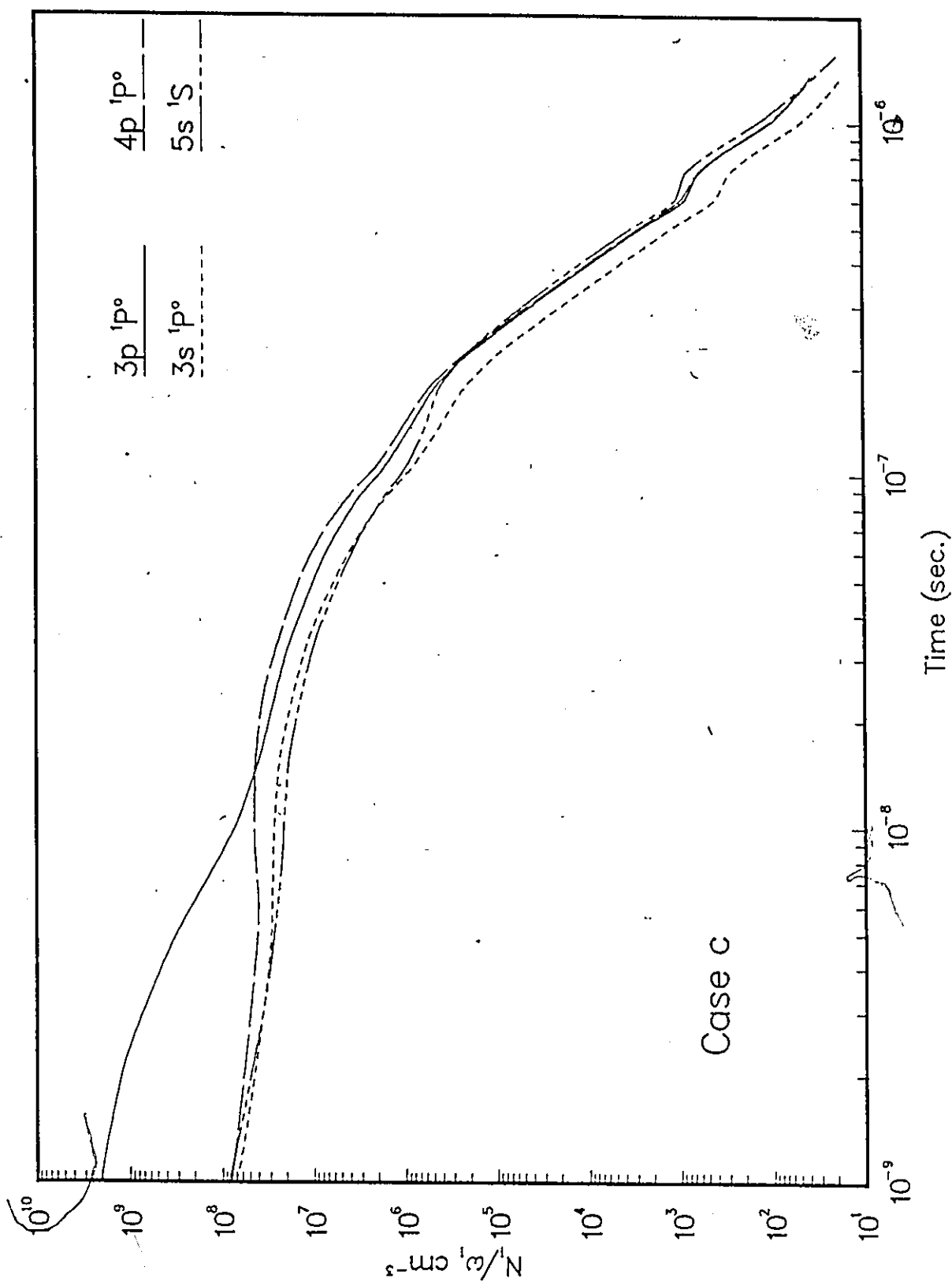


Fig. 6-12. Population densities vs. time for some levels in C III

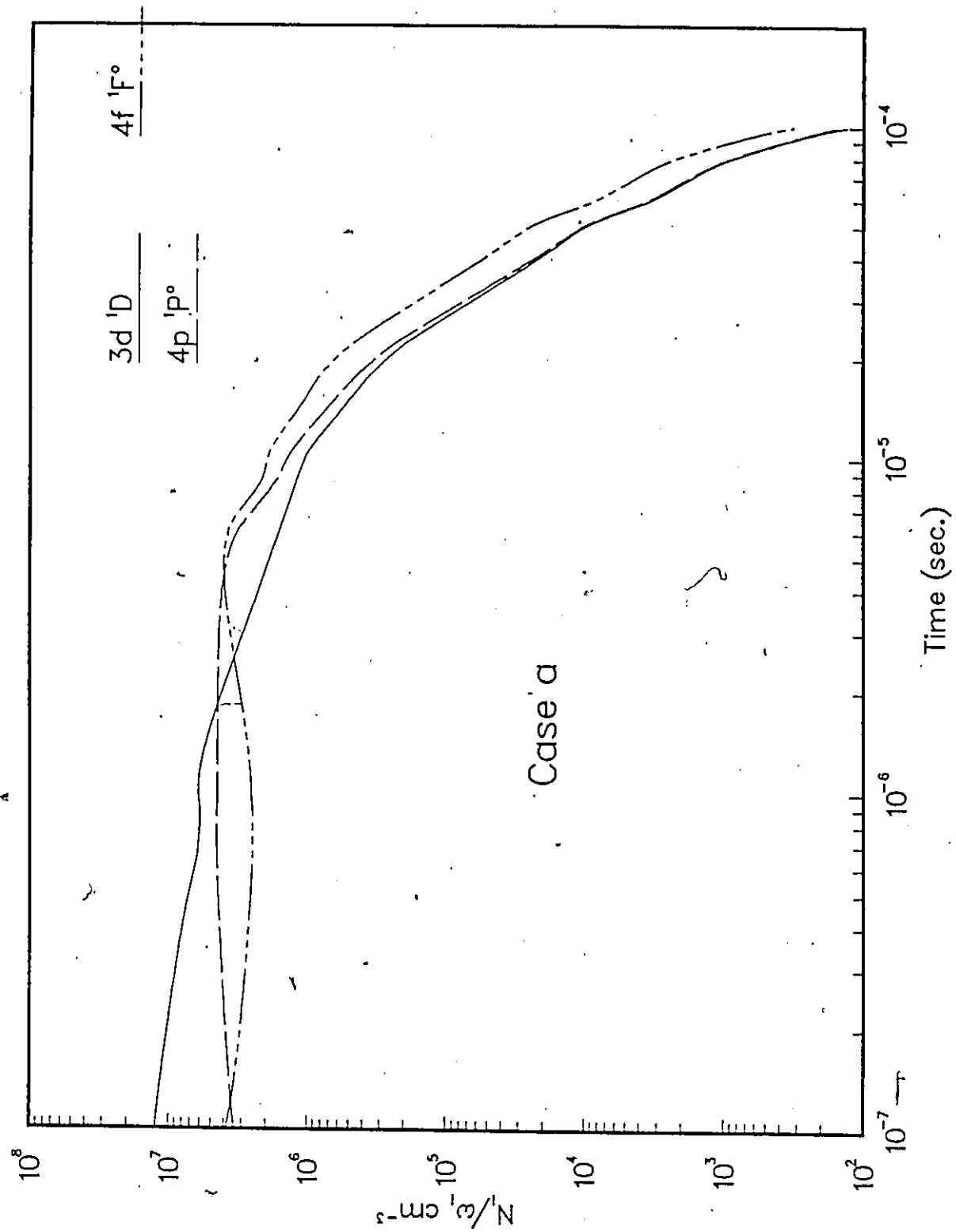


Fig. 6-13. Population densities vs. time for some levels in C III

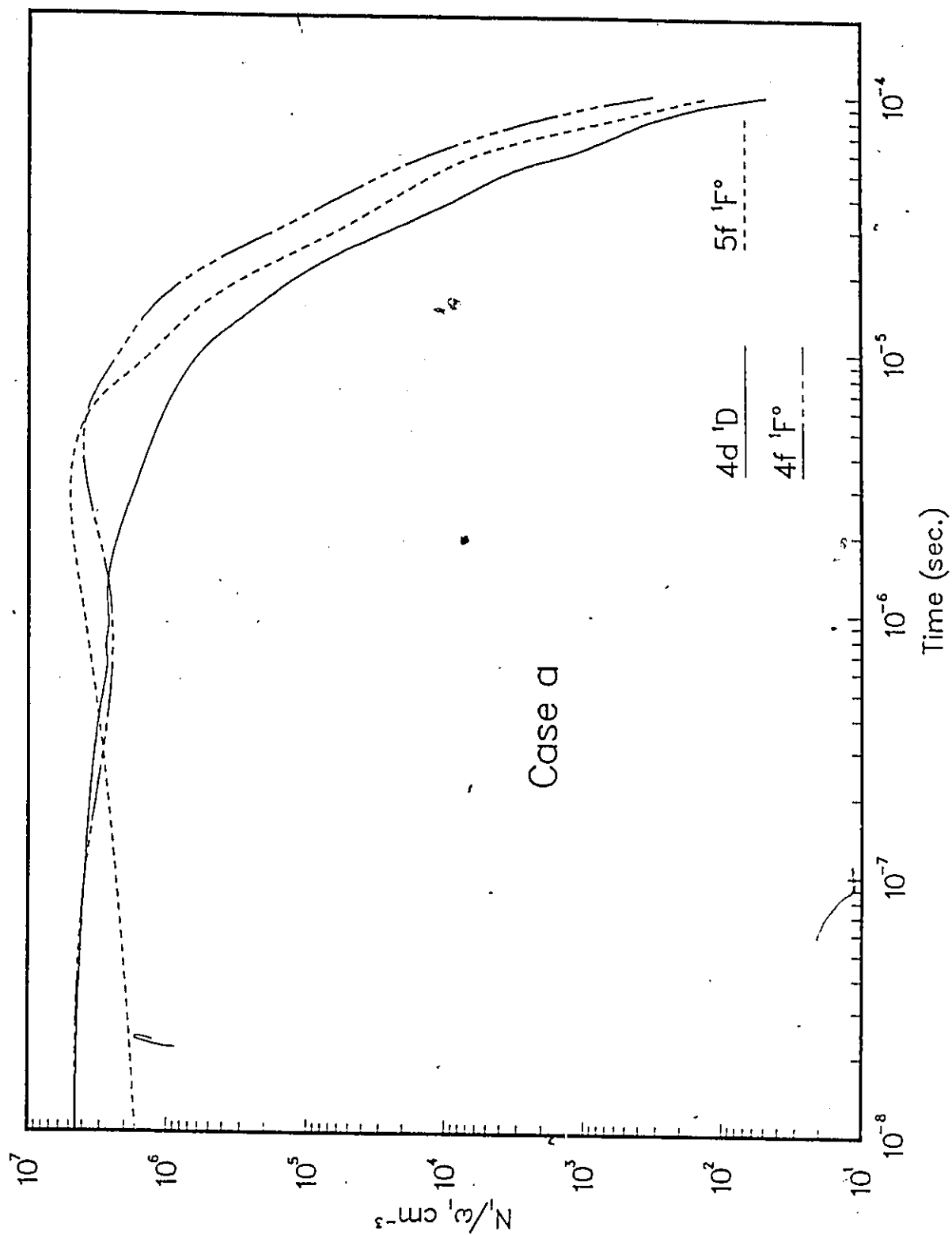


Fig. 6-14. Population densities vs. time for some levels in C III

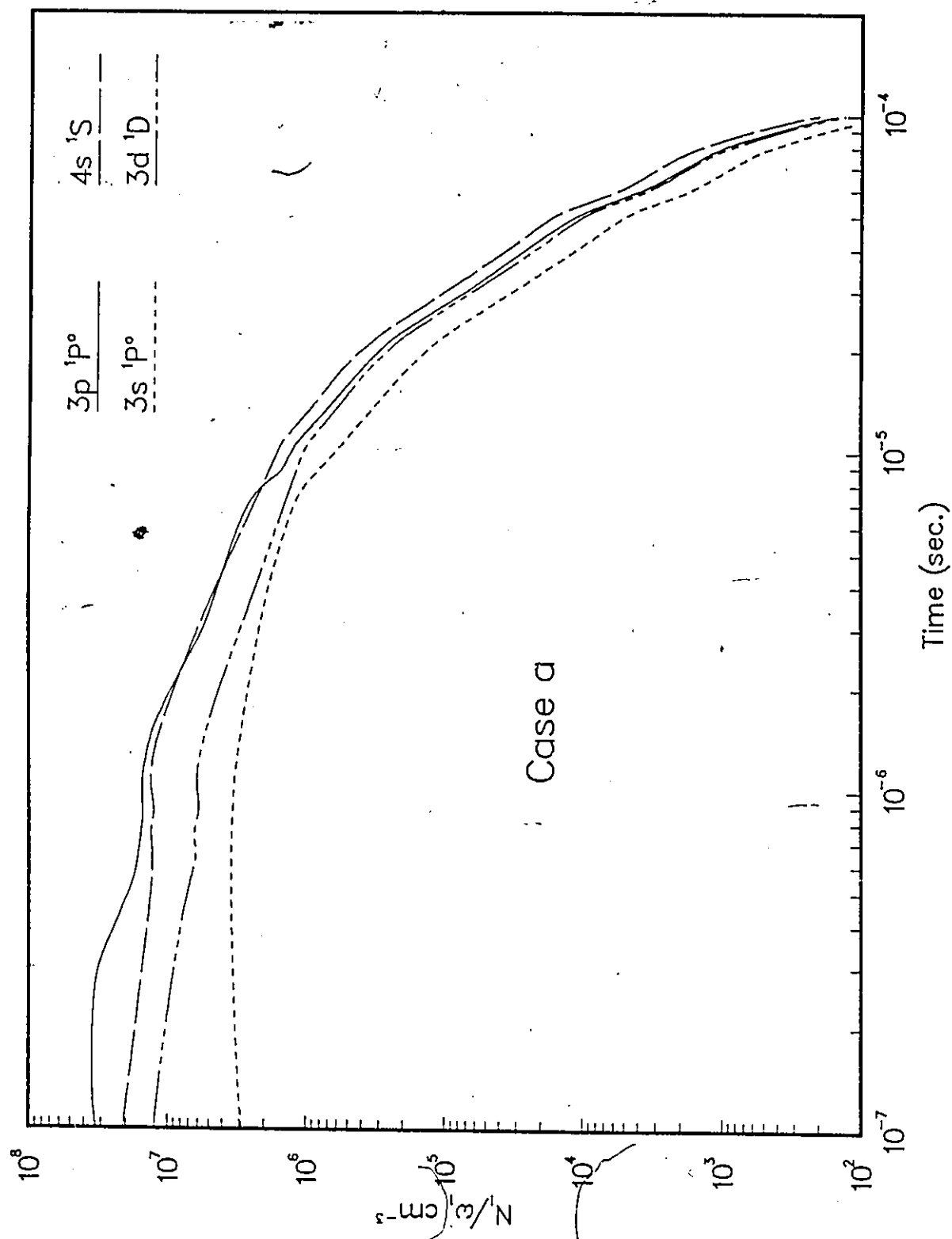


Fig. 6-15. Population densities vs. time for some levels in C III

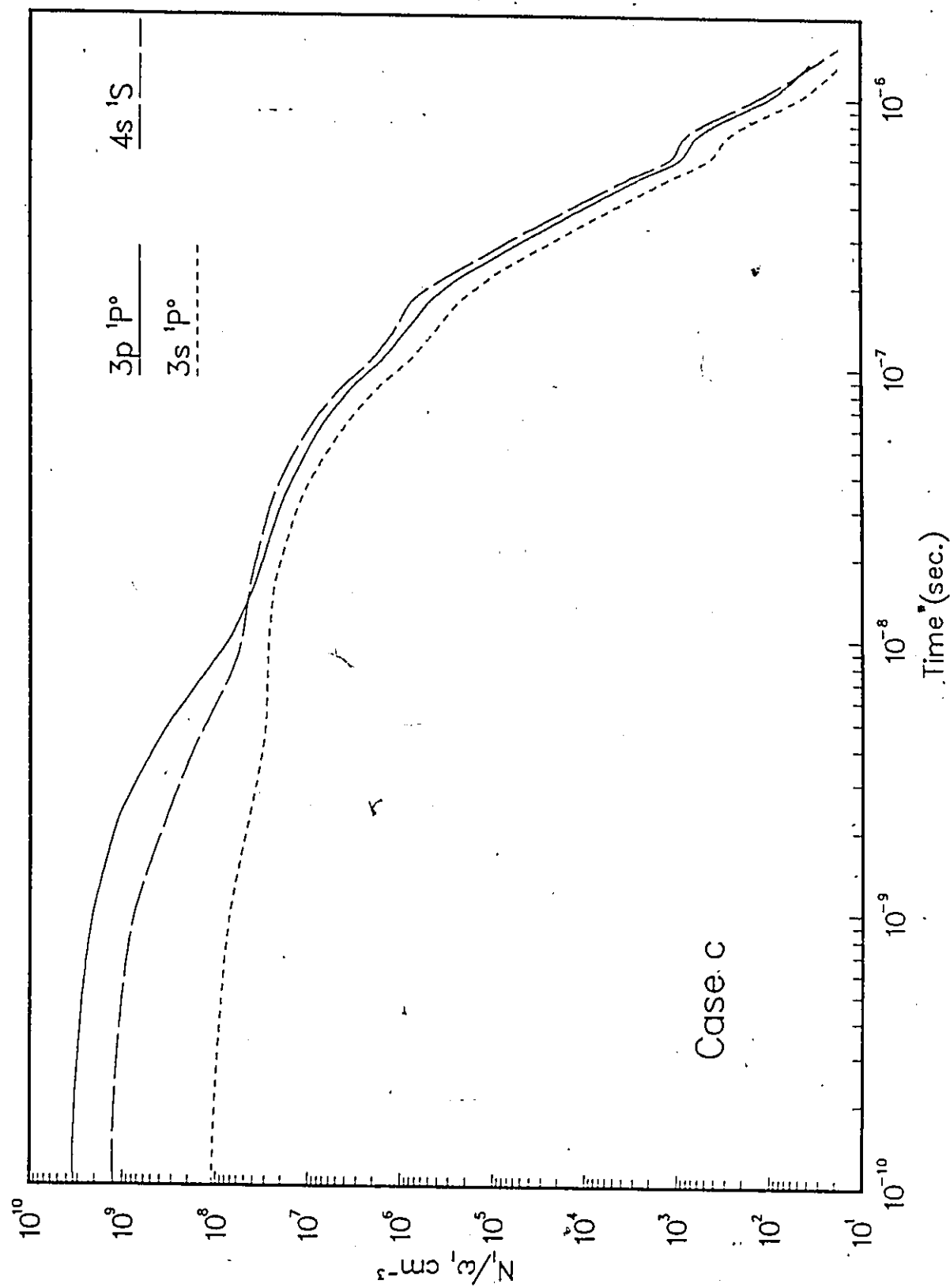


Fig. 6-16. Population densities vs. time for some levels in C III

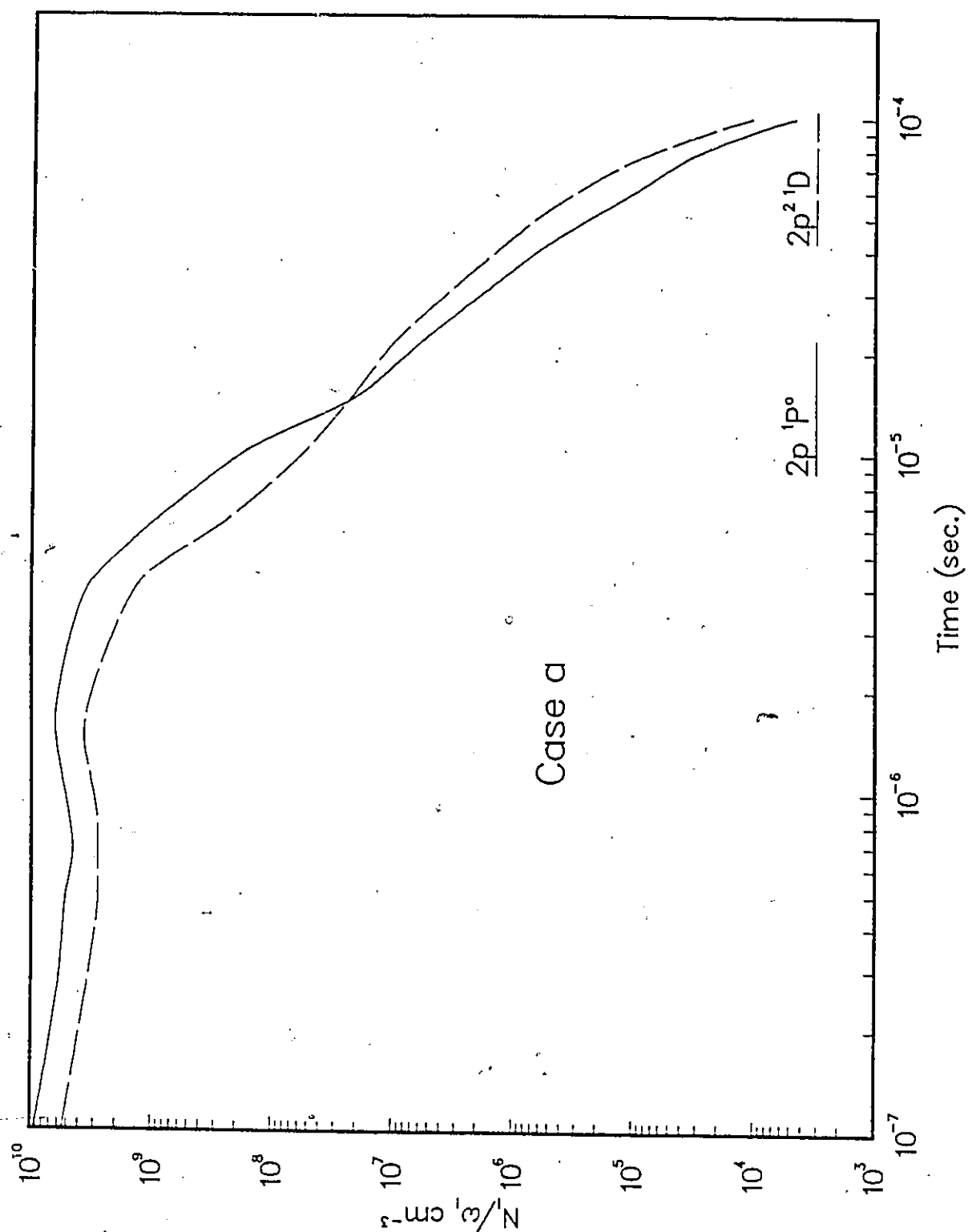


Fig. 6-17. Population densities vs. time for some levels in C III

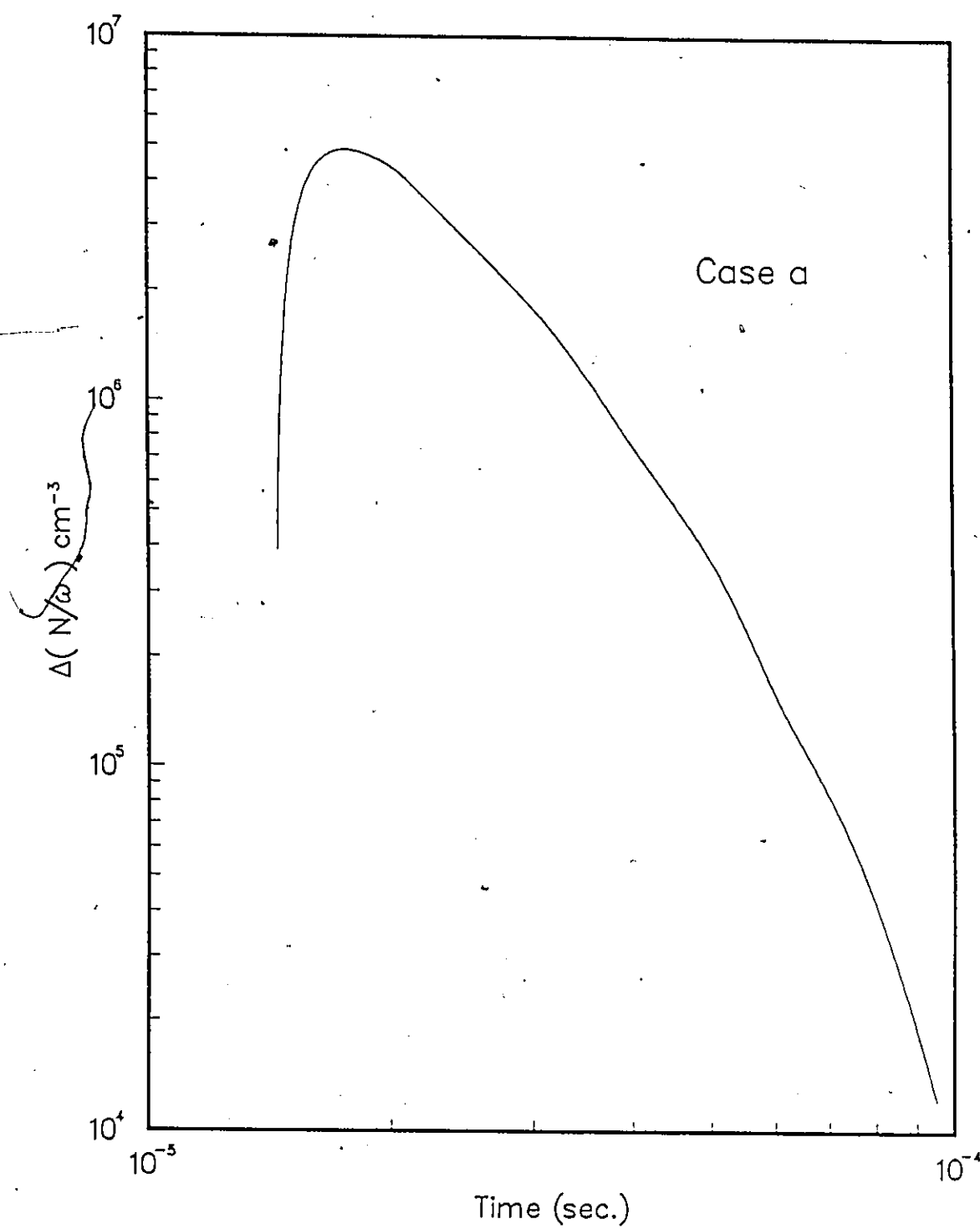


Fig. 6-18 Population inversion vs. time for $2p^2\ ^1D-2s2p\ ^1P^\circ$ line.

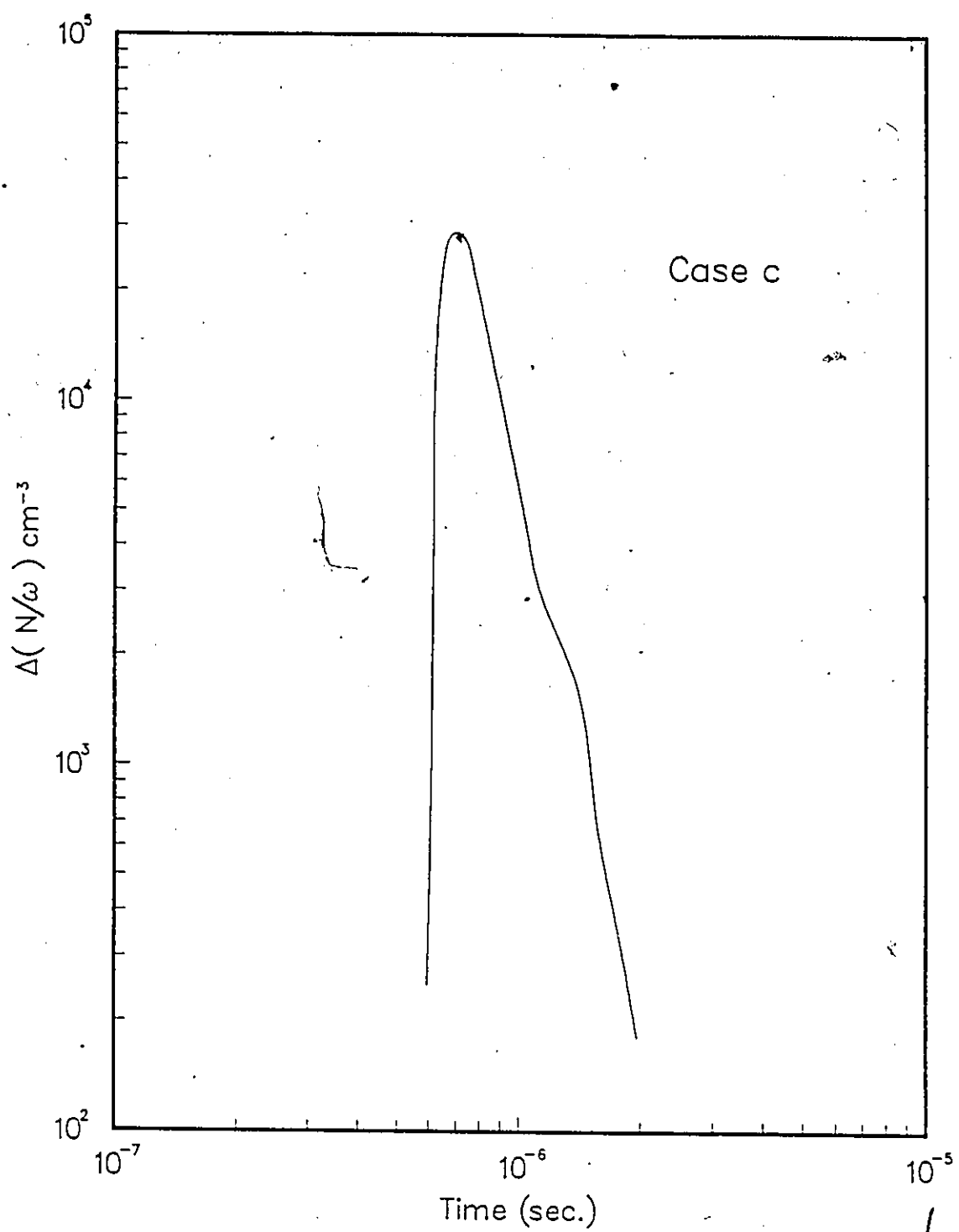


Fig. 6-19 Population inversion vs. time for $2p^2\ ^1D-2s2p\ ^1P^\circ$ line.

Chapter 7

Population inversion in a plasma interacting with an atomic gas.

A) Introduction

The population inversion in the infra-red, visible, and ultra-violet regions in an expanding plasma has already been demonstrated in the previous chapters. In this chapter, we will examine the cooling rate and the population inversion which occurs in a recombining plasma when a stationary plasma is brought into contact with a neutral gas. The geometry that we shall consider is essentially that of the TPD-I plasma machine of the Institute of Plasma Physics, Nagoya University (Otsuka *et al.*, 1975; Otsuka, 1980). Plasma flows along the axis of a cylindrical configuration and a neutral gas enters from the side (perpendicular to the axis), to interact with the plasma. Since the charged particle density in the column does not decrease along the axis as in an expanding plasma, there is the possibility of obtaining a higher gain and a VUV lasing. Experimental and theoretical investigations have been reported for generating population inversion in the TPD-I recombining plasma. Sato *et al.* (1977) observed population inversion between low lying levels of He II in the TPD-I recombining plasma column which was interacting with neutral helium gas without any expansion, and Maezawa and Sato (1980) observed population inversion between low lying levels of H atom as well as those of neutral He in the TPD-I recombining plasma when a stationary He plasma is brought into contact with neutral hydrogen gas. Furukane and Oda (1984) have investigated the processes leading to population inversion in a recombining hydrogen plasma which is interacting with a cool and dense neutral hydrogen gas by using the rate equations on the basis of CR model and the energy equations for electrons, ions and neutral particles.

We present numerical results calculated for the center axis of a helium plasma inter-

acting with cool and dense hydrogen gas.

B) Theoretical Model

We consider a simplified model of a recombining plasma by mixing a low temperature and high density gas of hydrogen with a cylindrical helium plasma of high electron temperature. Let the plasma flow along the z axis be constant with a speed of v_0 . We consider a coordinate fixed to the flow, i.e. $\frac{d}{dt} = \frac{\partial}{\partial t} + v_0 \frac{\partial}{\partial z}$.

The relaxation equations for the electronic level population of He I are given by

$$\begin{aligned} \frac{dN_i}{dt} = & -n_e N_i S_i - N_i N_1^H S_i^0 - N_1^H N_i \sum_{j \neq i}^{\infty} C_{ij}^0 - n_e N_i \sum_{j \neq i}^{\infty} C_{ij} \\ & - N_i \sum_{j=1}^{i-1} \Lambda_{ij} A_{ij} + n_e \sum_{j \neq i}^{\infty} N_j C_{ji} + N_1^H \sum_{j \neq i}^{\infty} N_j C_{ji}^0 + \sum_{j=i+1}^{\infty} N_j \Lambda_{ji} A_{ji} \\ & + \{ \Lambda_i \beta_i + \alpha_i n_e + \alpha_i^0 N_1^H \} n_e N^{+m} \equiv \Gamma_i, \quad (i = 1, 2, \dots, r) \end{aligned} \quad (7-1)$$

and for electronic level population of the hydrogen are given by

$$\begin{aligned} \frac{dN_i^H}{dt} = & -n_e N_i^H S_i^H - n_e N_i^H \sum_{j \neq i}^{15} C_{ij}^H - N_i^H \sum_{j=1}^{15} \Lambda_{ij} A_{ij}^H + n_e \sum_{j \neq i}^{15} N_j^H C_{ji}^H \\ & + \sum_{j=i+1}^{15} N_j^H \Lambda_{ji} A_{ji}^H + \{ \Lambda_i \beta_i^H + \alpha_i^H n_e \} n_e N^{H+} \equiv \Gamma_i^H, \quad (i = 1, 2, \dots, s) \end{aligned} \quad (7-2)$$

The explanation of superscripts is as follows

No superscript: He atom alone or transitions in He atom due to electronic collisions.

Superscript 0: transitions in He atom due to collisions with H atoms.

Superscript H: H atom alone or transitions in H atom due to electronic collisions.

N_i^H is the density of the hydrogen atom in level i , N^{H+} is the density of the singly ionized hydrogen, Λ_{ij} and Λ_i are the escape factors, C_{ij}^0 is the rate coefficient for excitation ($i < j$)

or de-excitation ($i > j$) from level i to j by atomic collisions, S_i^0 is the rate coefficient for ionization from level i by atomic collisions, α_i^0 is the rate coefficient for recombination by atomic collisions, C_{ij}^H and C_{ji}^H are the rate coefficients for excitation and de-excitation by electronic collisions of hydrogen, respectively. S_i^H is the hydrogenic rate coefficient for ionization from level i by electronic collisions, A_{ji}^H is the Einstein coefficient for radiative transition from level j to level i of hydrogen, β_i^H and α_i^H are the hydrogenic rate coefficient for radiative recombination three-body recombination from level i , respectively.

The rate of change of electron density n_e with time is given by

$$\frac{dn_e}{dt} = - \sum_{i=1}^r \Gamma_i - \sum_{i=1}^s \Gamma_i^H - n_e(N^{+2}\alpha^{+2} - N^{+1}S^{+1}) \quad (7-3)$$

where S^{+m} is the rate coefficient for ionization from m to $m+1$ and α^{+m} is the rate coefficient for recombination of ion m to $m-1$.

The time derivatives of the densities of He II, He III and H II are

$$\frac{dN^{+1}}{dt} = \Gamma_{+1} \quad (7-4),$$

$$\frac{dN^{+2}}{dt} = \Gamma_{+2} \quad (7-5),$$

$$\frac{dN^{H+}}{dt} = \Gamma_{H+} \quad (7-6),$$

where

$$\Gamma_{+m} = n_e[N^{+(m-1)}S^{+(m-1)} - N^{+m}(S^{+m} + \alpha^{+m}) + N^{+(m+1)}\alpha^{+(m+1)}] \quad (7-7)$$

and

$$\Gamma_{H+} = n_e[N^H S^H - N^{H+} \alpha^{H+}] \quad (7-8)$$

The following energy equation was used (Furukane and Oda, 1984)

$$\frac{d}{dt}\left(\frac{3}{2}n_k T_k\right) = Q_{inel}^k + Q_{\Delta T_k} \quad (7-9)$$

where k represents the species (electron, helium atom, hydrogen atom) under consideration.

Using Eq. (7-3), the heat-balance equation for electron can be written as follows:

$$\frac{3}{2}n_e \frac{dT_e}{dt} = Q_{inel} + Q_{inel}^H - Q_{\Delta T_e} - Q_{\Delta T_H} - \frac{3}{2}T_e \frac{dn_e}{dt} \quad (7-10)$$

The heat-balance equations for helium and hydrogen atoms are

$$\frac{3}{2}N_a \frac{dT_a}{dt} = Q_{\Delta T_a} + Q_{inel}^a \quad (7-11)$$

$$\frac{3}{2}N_a^H \frac{dT_H}{dt} = Q_{\Delta T_H} \quad (7-12)$$

where T_a and T_H are the temperature of the heavy particles in the helium plasma and of the neutral hydrogen atoms, respectively. Q_{inel} , Q_{inel}^H , and Q_{inel}^a represent the heat produced by the inelastic collision between electron-helium, electron-hydrogen and helium-hydrogen, respectively. These quantities were calculated using the following expressions:

$$Q_{inel} = - \sum_{i=2}^r \sum_{j=1}^{i-1} (E_j - E_i)(C_{ji}N_j - C_{ij}N_i) - \sum_{i=1}^r E_i S_i N_i + n_e N^{+1} \sum_{i=1}^r E_i \alpha_i \quad (7-13)$$

$$Q_{inel}^H = - \sum_{i=2}^s \sum_{j=1}^{i-1} \frac{e^2}{2a_0} (n_j^{-2} - n_i^{-2})(C_{ji}^H N_j^H - C_{ij}^H N_i^H) - \sum_{i=1}^s \frac{e^2}{2a_0} n_i^{-2} S_i^H N_i^H + n_e N^{H+} \sum_{i=1}^s \frac{e^2}{2a_0} n_i^{-2} \alpha_i^H \quad (7-14)$$

$$Q_{inel}^a = - \sum_{i=2}^r \sum_{j=1}^{i-1} (E_j - E_i) (C_{ji}^o N_j - C_{ij}^o N_i) - \sum_{i=1}^r E_i S_i^o N_i + n_e N^{+1} \sum_{i=1}^r E_i \alpha_i^o. \quad (7-15)$$

where n_i is the principal quantum number of level i . $Q_{\Delta T_e}$ and $Q_{\Delta T_H}$ are the rate of increase in the thermal energy due to the elastic collisions between electron-helium and electron-hydrogen, respectively. These rates were calculated using Eq. (3-27).

As initial conditions of the numerical calculations, we assume that the helium plasma is in a stationary state whose electron and heavy particles temperature and electron density are T_{e0} , T_{a0} , and n_{e0} and it is brought into contact with neutral hydrogen atoms which are in the ground state at an initial atom-temperature of T_{H0} . At $t = 0$, the population densities of the helium atoms were calculated using the steady-state assumption. The calculation was made for the following initial condition: $T_{e0} = 10^5$ K, $T_{a0} = 6 \times 10^4$ K, $T_{H0} = 10^3$ K, $n_{e0} = 10^{13}$ cm $^{-3}$, $N_{a0} = 10^{13}$ cm $^{-3}$, $N_{a0}^H = 10^{17}$ cm $^{-3}$.

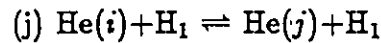
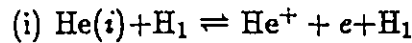
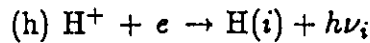
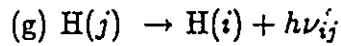
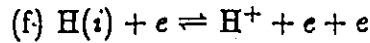
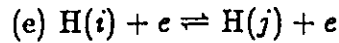
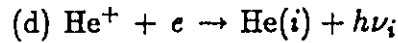
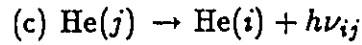
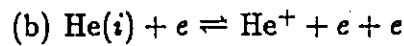
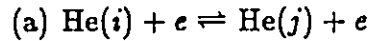
Numerical results obtained from the set of equations (7-1) to (7-6) and (7-10) to (7-12) are given as a function of time. The quasi-steady state assumption is made for all the levels $i > 5$ in hydrogen atom and for all levels $i > i^*$ in helium atom. The level i^* is determined so as to satisfy the following conditions: (1) $i \geq 11$, and (2) the relaxation time for N_i with $i \geq i^* + 1$ is less than one hundredth of an apparent relaxation time for the electron energy estimated from Eq. (7-9) (Furukane and Oda, 1984); that is

$$\frac{3}{2} n_e T_e / \left(-Q_{inel} - Q_{inel}^H - \sum_k Q_{\Delta T_k} + \frac{3}{2} T_e d\bar{n}_e/dt \right) \quad (7-16)$$

Runge-Kutta-Gill method was used in solving the set of differential equations. The time step Δt was set to be one tenth of the relaxation time for the population density of level i^* .

C) Collisional-Radiative model rate coefficients

The level system used for helium in this calculation is the same as that used in chapter 3. For hydrogen, the maximum principal quantum number for the CR is chosen to be 15 following Varshni and Lam (1976). The inelastic collisional and radiative processes considered here are as follows:



where H_1 denotes a hydrogen atom in ground state. For reaction processes (a) to (d) we used the same rate coefficients as in chapter 2 section (C). Escape factors used in this calculations were taken from Hegde and Ghosh (1977), and they are:

$$\Lambda(2^1\text{P} \rightarrow 1^1\text{S}) = 0.0013, \Lambda(3^1\text{P} \rightarrow 1^1\text{S}) = 0.01, \Lambda(4^1\text{P} \rightarrow 1^1\text{S}) = 0.07$$

$$\Lambda(5^1\text{P} \rightarrow 1^1\text{S}) = 0.2, \Lambda(6^1\text{P} \rightarrow 1^1\text{S}) = 0.5$$

all other Λ_{ij} and Λ_i assumed equal to one.

For reaction processes (e) to (j) we have used the following cross sections and rate coefficients:

1) *Spontaneous transition probability*

We consider the spontaneous transition of an electron in a hydrogen from an upper state j to a lower state i . Within the electric dipole approximation, it can be evaluated exactly using eq. (2-9). The absorption oscillator strength needed in calculating the transition probability were obtained from eq. (2-11). For the escape factors, the following values were used (Drawin and Emard, 1974):

$$\Lambda_{21} = 0.0064, \Lambda_{31} = 0.022, \Lambda_{41} = 0.076, \Lambda_{51} = 0.18,$$

$$\Lambda_{61} = 0.36, \Lambda_{71} = 0.60, \Lambda_{81} = 0.80$$

all other Λ_{ij} and Λ_i assumed equal to one.

2) *Collisional ionization and three-body recombination*

The cross section for ionization of hydrogen atom from state i by electron impact was calculated using the semi-empirical expression proposed by Drawin (1967), which gives a good fit to the available experimental data, and which is proportional to $\ln E/E$ for large values of the free electron kinetic energy E as required by quantum mechanics (Massey and Burhop, 1952, p.140).

The cross section of hydrogen is written as

$$\sigma_i(U) = 2.66\pi a_0^2 \left(\frac{I_H}{I_i} \right)^2 \zeta_i \frac{U-1}{U^2} \ln(1.25\beta_i U) \quad (7-17)$$

where I_H is the ionization energy of the hydrogen atom in its ground state, I_i is the ionization energy of the hydrogen atom in state i , $U = E/I_i$ is the kinetic energy of the incident electron in units of the threshold energy for ionization from state i , ζ_i is the effective number of electrons in i , and β_i is a correction factor of order unity. Using $I_i = Z^2/n_i^2$ (Rydbergs), and $\beta = 1$, eq. (7-17) becomes

$$\sigma_i(U) = 2.66\pi a_0^2 \left(\frac{n_i}{Z}\right)^4 S_i \frac{U-1}{U^2} \ln(1.25 U) \quad (7-18)$$

The rate coefficients were obtained by integrating the cross section over Maxwellian velocity distribution of the free electrons. The rate coefficient for the recombination of a free electron in an atomic state i with subsequent absorption of the excess energy by a neighbouring electron is obtained by the principle of detailed balancing from the rate coefficient for the inverse process of ionization by electron impact. The rate coefficients are related by the expression (Drawin, 1963)

$$\alpha_i = \frac{\omega_i}{2u_+} \frac{h^3}{(2\pi mkT)^{3/2}} e^{\frac{I_i}{kT}} S_i \quad (7-19)$$

where u_+ is the partition function of the ion before recombination, and S_i is the ionization rate coefficient from level i .

3) Collisional excitation and de-excitation

The cross section for excitation of an atomic electron from a lower state i to an upper state j by electron impact can be evaluated with a semi-empirical expression proposed by Drawin (1967):

$$\sigma_{ij}(U) = 4\pi a_0^2 \left(\frac{I_H}{E_{ij}}\right) f_{ij} G_{ij}(U) \quad (7-20)$$

where E_{ij} is the excitation energy of the $i \rightarrow j$ transition, $U = E/E_{ij}$ is the free electron kinetic energy in units of the threshold energy for excitation of the $i \rightarrow j$ transition, f_{ij} is the absorption oscillator strength of the $i \rightarrow j$ transition, and $G_{ij}(U)$ is an appropriate function giving the correct asymptotic behavior of the cross section.

Drawin proposed the following expression for $G_{ij}(U)$ in Eq. (7-20):

$$G_{ij}(U) = \alpha \frac{U-1}{U^2} \ln(1.25\beta U) \quad (7-21)$$

where α and β are adjustable parameters. Drawin suggests the values 1 and 2 for the parameters α and β , respectively.

The rate coefficient is obtained by integrating the cross section over Maxwellian velocity distribution of the free electrons. The rate coefficient for de-excitation of an atomic electron from an upper state j to a lower state i by electron impact is obtained by the principle of detailed balancing from the rate coefficient for the inverse process of excitation by electron impact. The rate coefficients are related by the expression (Drawin, 1963)

$$C_{ji}^H = \frac{\omega_i}{\omega_j} e^{E_{ij}/kT} C_{ij}^H \quad (7-22)$$

(4) Radiative recombination

The rate coefficient for the radiative recombination is calculated from an approximation proposed by Seaton (1959) for hydrogenic ions. Using the principle of detailed balancing, the rate coefficient can be obtained from the photoionization cross-section:

$$\beta_i = \frac{1}{c^2} \sqrt{\frac{2}{\pi}} \frac{2n_i^2}{(mkT_e)^{-3/2}} e^{I_i/kT_e} \int_{I_i}^{\infty} (h\nu)^2 \sigma_i(\nu) e^{-\frac{h\nu}{kT_e}} d(h\nu) \quad (7-23)$$

where σ_i is the photoionization cross section, $I_i = hRcZ^2/n_i^2$, and the other symbols have their usual meaning. The photoionization cross section is given by

$$\sigma_i(\nu) = \frac{2^6 \alpha \pi a_0^2}{3\sqrt{3}} \frac{n_i}{Z^2} \frac{g_{II}(n_i, \epsilon)}{(1 + n_i^2 \epsilon)^3} \quad (7-24)$$

where α is the fine-structure constant, $g_{II}(n_i, \epsilon)$ is the Kramers-Gaunt factor; it is of order unity, and

$$h\nu = Z^2 \left(\frac{1}{n_i^2} + \epsilon \right) \quad \text{Rydbergs} \quad (7-25)$$

with $Z^2\epsilon$ being the kinetic energy of the ejected electron.

From equations (7-23) to (7-25) we obtain

$$\beta_i = \frac{2^6}{3} \sqrt{\frac{\pi}{3}} \alpha^4 c a_0^2 Z \theta_i^{3/2} \mathfrak{R}_i(\theta_i) \quad (7-26)$$

where

$$\theta_i = \frac{I_i}{kT_e} = \frac{157890}{T_e} \frac{Z^2}{n_i^2} \quad (7-27)$$

$$\mathfrak{R}_i(\theta_i) = \int_0^\infty \frac{g_{II}(n_i, \epsilon) e^{-\theta_i u}}{(1+u)} du \quad (7-28)$$

and

$$u = n_i^2 \epsilon = Z^2 \epsilon / I_i \quad (7-29)$$

is the kinetic energy of the ejected electron in the units of the threshold energy for photoionization from state i . Numerically,

$$\beta_i = 5.197 \times 10^{-14} Z \theta_i^{3/2} \mathfrak{R}_i(\theta_i) \quad (7-30)$$

Putting the Kramers-Gaunt factor equal to unity in Eq. (7-28) gives rise to errors as large as 20%. The accuracy of radiative recombination rate coefficient is improved by using the asymptotic expansion of $g_{II}(i, \epsilon)$ (Eq. 2-54). Substituting Eq. (2-54) in Eq. (7-28), we get

$$\mathfrak{R}_i(\theta_i) = \mathfrak{R}_i^{(0)}(\theta_i) + \frac{0.1728}{i^{2/3}} \mathfrak{R}_i^{(1)}(\theta_i) - \frac{0.0496}{i^{4/3}} \mathfrak{R}_i^{(2)}(\theta_i) + \dots \quad (7-31)$$

where

$$\mathfrak{R}_i^{(0)}(\theta_i) = \int_0^\infty \frac{e^{-\theta_i u}}{1+u} du \quad (7-32)$$

$$\mathcal{R}_i^{(1)}(\theta_i) = \int_0^\infty \frac{(u-1)}{(1+u)^{5/3}} e^{-\theta_i u} du \quad (7-33)$$

and

$$\mathcal{R}_i^{(2)}(\theta_i) = \int_0^\infty \frac{u^2 + \frac{4}{3}u + 1}{(1+u)^{7/3}} e^{-\theta_i u} du \quad (7-34)$$

These integrals can be expressed in terms of well-known functions:

$$\mathcal{R}_i^{(0)}(\theta_i) = e^{\theta_i} E_1(\theta_i) \quad (7-35)$$

$$\mathcal{R}_i^{(1)}(\theta_i) = -3 + (1 + 3\theta_i) \Psi(1, 4/3; \theta_i) \quad (7-36)$$

$$\mathcal{R}_i^{(2)}(\theta_i) = -\frac{3}{2}(1 + \theta_i) + (1 + 2\theta_i + \frac{3}{2}\theta_i^2) \Psi(1, 5/3; \theta_i) \quad (7-37)$$

where $E_1(x)$ is the exponential integral, and $\Psi(a, c; x)$ is the confluent hypergeometric function (Abramowitz and Stegun, 1965).

(4) *Excitation of level i by collision with heavy particles, and the inverse process*

Drawin (1969) and Drawin et al. (1971) proposed an expression to calculate the cross sections for excitation of atom from lower level i to upper level j by collisions with heavy particles in the ground state. We used Drawin's expression in calculating the cross sections and rate coefficients for the reaction process (j). The cross sections were calculated using the following expression:

$$\sigma_{ij}^0 = 4\pi a_0^2 \left(\frac{I_H}{E_{ij}} \right)^2 \frac{m_a}{m_H} f_{ij} \frac{2m_e}{m_a + m_e} \frac{W_{ij} - 1}{\left\{ 1 + \frac{2m_a}{m_a + m_e} (W_{ij} - 1) \right\}^2} \quad (7-38)$$

where m_e , m_H , and m_a are the masses of the electron, the hydrogen atom, and the colliding particles in question, respectively. (In the case treated here $m_a \equiv m_{He}$.) W_{ij} has

the meaning of a reduced translational energy of the colliding atoms in the center-of-mass system

$$W_{ij} = \frac{E^a - |E_{ij}|}{|E_{ij}|}, \quad E^a = \frac{m_a v_a^2}{2}.$$

The quantity f_{ij} is the absorption oscillator strength for the transition $i \rightarrow j$. Integration over a Maxwellian velocity distribution yields for the excitation coefficient

$$C_{ij}^0 = 32\pi a_0^2 \left(\frac{I_H}{E_{ij}} \right)^2 f_{ij} \left(\frac{kT_a}{\pi m_a} \right)^{\frac{1}{2}} \frac{m_e m_a}{m_H (m_a + m_e)} \Psi_{m_a}(w_{ij}) \quad (7-39)$$

with $w_{ij} = E_{ij}/kT_a$. $\Psi_{m_a}(w_{ij})$ is a function depending on the mass ratio $2m_e/(m_a + m_e)$ and can be approximated by

$$\Psi_{m_a}(x) \cong \left(1 + \frac{2}{x} \right) \left(\frac{1}{1 + (2m_e/(m_a + m_e)x)^2} \right) \exp(-x). \quad (7-40)$$

The rate coefficient for the de-excitation process is then simply given by

$$C_{ji}^0 = \frac{\omega_i}{\omega_j} \exp(w_{ij}) C_{ij}^0. \quad (7-41)$$

(5) Ionization by collisions with heavy particles and three-body recombination

For process (i), we calculate the cross section and rate coefficient using the following expressions proposed by Drawin (1969), Drawin et al. (1971)

$$\sigma_i^0 = 4\pi a_0^2 \left(\frac{I_H}{E_i} \right)^2 \frac{m_a}{m_H} \xi_i \frac{2m_e}{m_a + m_e} \frac{W_i - 1}{\left\{ 1 + \frac{2m_e}{m_a + m_e} (W_i - 1) \right\}^2} \quad (7-42)$$

where $W_i = (E^a - E_i)/E_i$, and ξ_i is the number of energetically equivalent electrons in shell

i. Integration over a Maxwellian velocity distribution yields for the ionization coefficient

$$S_i^0 = 32\pi a_0^2 \left(\frac{I_H}{E_i} \right)^2 \xi_i \left(\frac{kT_a}{\pi m_a} \right)^{\frac{1}{2}} \frac{m_e m_a}{m_H(m_a + m_e)} \Psi_{m_a}(w_i) \quad (7-43)$$

where $w_i = E/kT_a$, and the function $\Psi_{m_a}(x)$ is given by eq. (7-23). The three-body recombination can be expressed in terms of the ionization coefficient

$$\alpha_i^0 = \frac{w_i}{2\omega^+} \left(\frac{m_a + m_e}{m_e m_a} \right)^{3/2} \frac{h^3}{(2\pi k)^{3/2}} \frac{S_i^0}{T_e T_a^{1/2}} \exp\{-u_i + 2(u_i w_i)^{1/2}\} \quad (7-44)$$

where $u_i = E_i/kT_e$.

D) Results and Discussion

Results for the electron, helium atom and hydrogen atom temperatures in a helium plasma which is interacting with a neutral hydrogen gas are plotted in Fig. 7-1 as a function of time. The electron temperature shows a rapid decrease with time, it drops to about 0.12 eV in 10^{-6} s. After the electron temperature reaches this value it stays almost constant. The temperature of the helium atom changes only slightly until $t \approx 10^{-8}$ s, then it rapidly decreases to about 0.13 eV. After that it starts to drop very slowly to a relaxed value of about 0.11 eV. The temperature of the hydrogen atoms stays almost constant showing only a slow increase. The rapid drop in the electron temperature demonstrates that a sufficient cooling in electron temperature can be achieved in such a plasma and conditions favorable for population inversion result, as will be seen below. In Figs. 7-2 and 7-3 we show the time evolution of the electron energy transfer rate due to inelastic collision in hydrogen and helium (Q_{inel}^H and Q_{inel}), respectively.

The population densities for the levels i ($i = 2, 3, 4$ and 5) in hydrogen atom and the electron density as a function of time are presented in Fig. 7-4. The electron density shows an increase at early time due to large ionization rate (Fig. 7-2) till $t \approx 10^{-6}$ s, and then falls due to drop in the ionization rate and increase in the recombination rate.

Initially the population densities of the levels 2, 3, 4 and 5 show a rapid increase due to excitation of the hydrogen atoms in the ground state by electron impact, and then fall due to drop in excitation rate (see Fig. 7-2). At $t \approx 1.5 \times 10^{-6}$ s the population densities of these levels show a sharp increase due to increase in the recombination flux which is however followed by a rapid decrease due to reduction in the recombination flux (see Fig. 7-2). Finally, the population inversion between the levels 4 and 3 appears after $t \approx 10^{-5}$ s and that between 5 and 3 appears after $t \approx 5 \times 10^{-5}$ s, the overpopulation density in these transitions are of the order 10^8 and 10^7 cm^{-3} , respectively. Population inversion between levels 5 and 4 appears after $t \approx 10^{-4}$ s. The rate of change in the population densities of the levels i , $\dot{N}_i \equiv dN_i^H/dt$, ($i = 2, 3$ and 4) versus t are plotted in Fig. 7-5. The solid curves represent the positive values of $\dot{N}_i$, while the dotted curves represent the negative values of $\dot{N}_i$. In Fig. 7-6 the rate of change in the density of the electron and hydrogen ion, and in the population density of the ground state of hydrogen are plotted as a function of time. The time during which $\dot{n}_e > 0$ and $\dot{n}_e < 0$ correspond to the ionizing phase and recombining phase of the plasma, respectively.

The population densities for the $1s^2 \ ^1S$, 2^3S , 2^1S , 2^3P , and 2^1P levels in helium as a function of time are presented in Fig. 7-7. At early stage "ionizing phase" the population densities of these levels change only slightly till $t \approx 10^{-7}$ s, and after that the population densities of these levels start to increase rapidly with time due to increase in the recombination rate (see Fig. 7-3). In the transient recombining phase the population densities of these levels make a very sharp increase. It is seen from Fig. 7-7 that population inversion between ground state and excited state or between two low-lying excited state can occur at the time where the population densities show the sharp increase. Unfortunately in the case examined here no such population inversion occurs for an allowed transition but it can be noticed that the population density of the metastable state 2^3S becomes greater

than that of the ground state, and the population density of 2^1S becomes greater than that of the ground state for a very short time. Figs. 7-8 and 7-9 show the time evolution of the rate of change in the population densities of the above levels. The rate of change in the density of the helium ions and the population density of the ground state versus t are presented in Fig. 7-10.

Population inversion was found to occur for a great many transitions between $n=5, 4$ and 3 (n is the principal quantum number) in helium. But we do not find any population inversion in the lines $3^1S \rightarrow 2^1P$, $3^1D \rightarrow 2^1P$, $4^1S \rightarrow 2^1P$, and $4^1D \rightarrow 2^1P$. A comparison of Figs. 7-7 and 7-12 shows that the population density of the 2^1P level stays high. This is because the main mechanism of depopulating this level is the spontaneous radiation. The radiative mechanism is extremely sensitive to reabsorption of radiation (Gordiets *et al.*, 1968b; Jones and Ali, 1978). In this calculation we allowed for reabsorption of the radiation by the lines of the principal series (transitions to the ground state). Reabsorption was taken into account approximately. Thus the allowance for reabsorption reduced the rate of depopulating this level. We present and describe the result of some transitions in helium which show population inversion.

The population densities for the 3^3S , 3^3P and 3^3D levels as a function of time are presented in Fig. 7-11. The population densities of these levels show similar behaviour to that described above. Strong population inversion between 3^3P and 3^3S appear after $t \approx 10^{-6}$ s and reaches its maximum, which is of the order of $2 \times 10^7 \text{ cm}^{-3}$, shortly after it appears. Population inversion between 3^3D and 3^3P occurs but for a very short time. Fig. 7-12 shows the population densities for the levels 3^1S , 3^1P and 3^1D as a function of time. Population inversion in the transition $3^1P \rightarrow 3^1S$ of order 10^7 cm^{-3} appears at the time the plasma changes from the ionizing phase to the recombining one (transient recombining phase). At the same time population inversion in the transition $3^1P \rightarrow 3^1D$ occurs with

maximum of order 10^6 cm^{-3} and vanishes at $t \approx 10^{-4} \text{ s}$. Fig. 7-13 shows the population densities for the levels 3^3S , $3^3 3^3\text{D}$, 4^3S and 4^3P as a function of time. Population inversions occur in the lines $4^3\text{S} \rightarrow 3^3\text{P}$, $4^3\text{P} \rightarrow 3^3\text{S}$, and $4^3\text{P} \rightarrow 3^3\text{D}$. The population inversion is of the order of $5 \times 10^8 \text{ cm}^{-3}$ at the maximum in these lines.

From Figs. 7-6 and 7-10 it will be noticed that the QSS, i.e. $\dot{N}_1^{He} + \dot{N}_1^H \approx -\dot{n}_e$, is established after $3.5 \times 10^{-6} \text{ s}$. As shown in Fig 7-4, population inversion in hydrogen takes place after QSS is established. In helium, the case is different, all the population inversion is found to occur in the transient recombining phase, which occurs at $t \approx 1.5 \times 10^{-6}$ (Fig. 7-6).

The theoretical results shown here and the experimental results (Maezawa and Sato, 1980) are in good agreement. For example: Maezawa and Sato (1980) found population inversion of order $6 \times 10^7 \text{ cm}^{-3}$ between $n=4$ and 3 in hydrogen at $T_e \sim 0.07 \text{ eV}$, $n_e \sim 2.1 \times 10^{13} \text{ cm}^{-3}$, $N^{H^+} \sim 1.9 \times 10^{13} \text{ cm}^{-3}$, $N^{He^+} \sim 2 \times 10^{12} \text{ cm}^{-3}$. Our calculated population inversion $3.45 \times 10^8 \text{ cm}^{-3}$ occurs at plasma parameters $T_e = 0.1 \text{ eV}$, $n_e = 2 \times 10^{13} \text{ cm}^{-3}$, $N^{H^+} = 4 \times 10^{13} \text{ cm}^{-3}$, $N^{He^+} = 1.26 \times 10^{12} \text{ cm}^{-3}$. But in this calculation, we do not find any population inversion between levels $n=3, 4$ and level 2 in hydrogen where the experimental results show there is population inversion. We think this discrepancy is related to the accuracy of the escape factors used to allow for reabsorption of radiation by the lines of the principal series.

From these results it is clear that the population inversion, which occurs in a recombining plasma when a stationary helium plasma is brought into contact with a neutral gas, shows a higher gain than that in an expanding plasma.

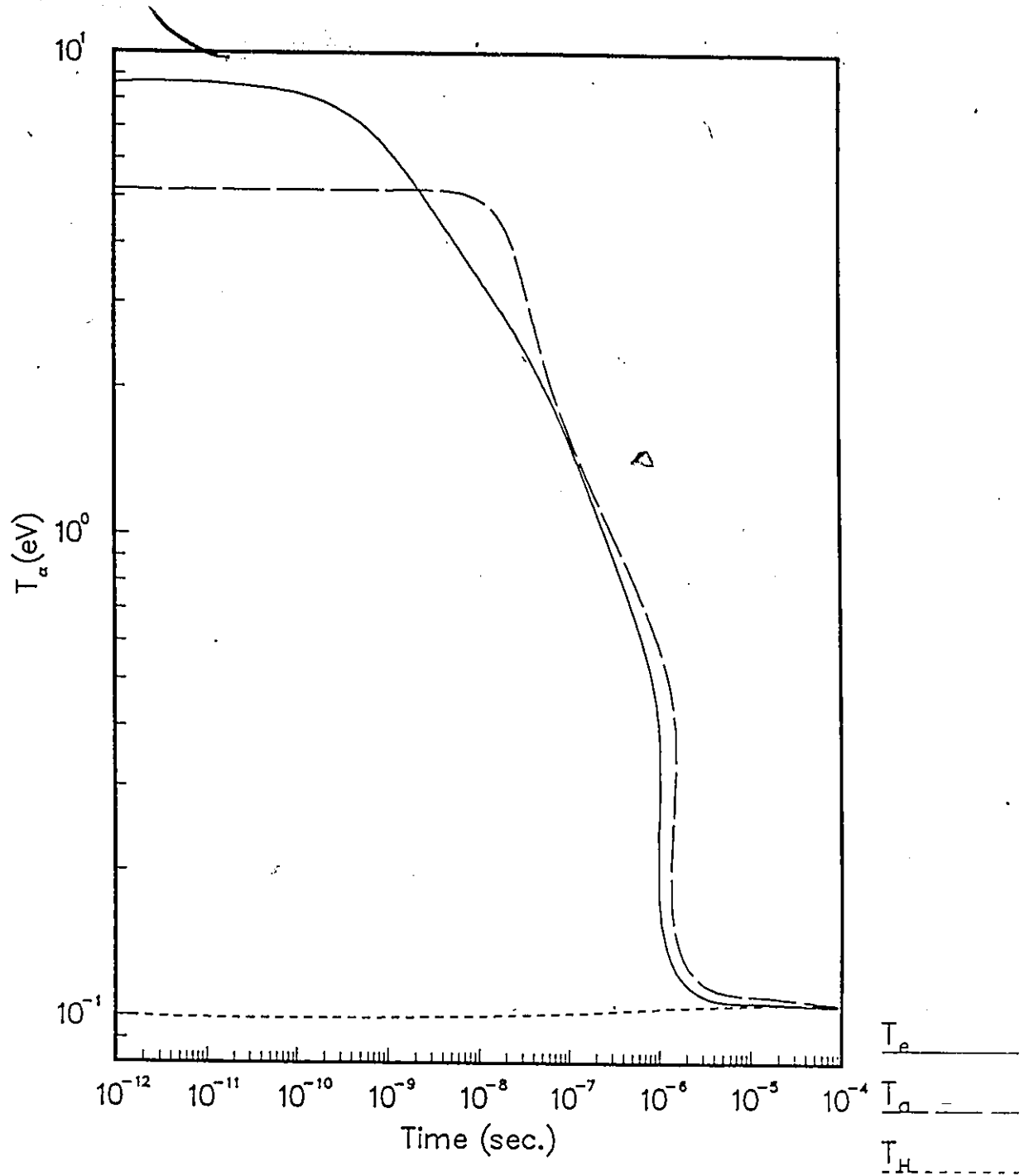


Fig. 7-1. Electron and atomic temperature vs. time

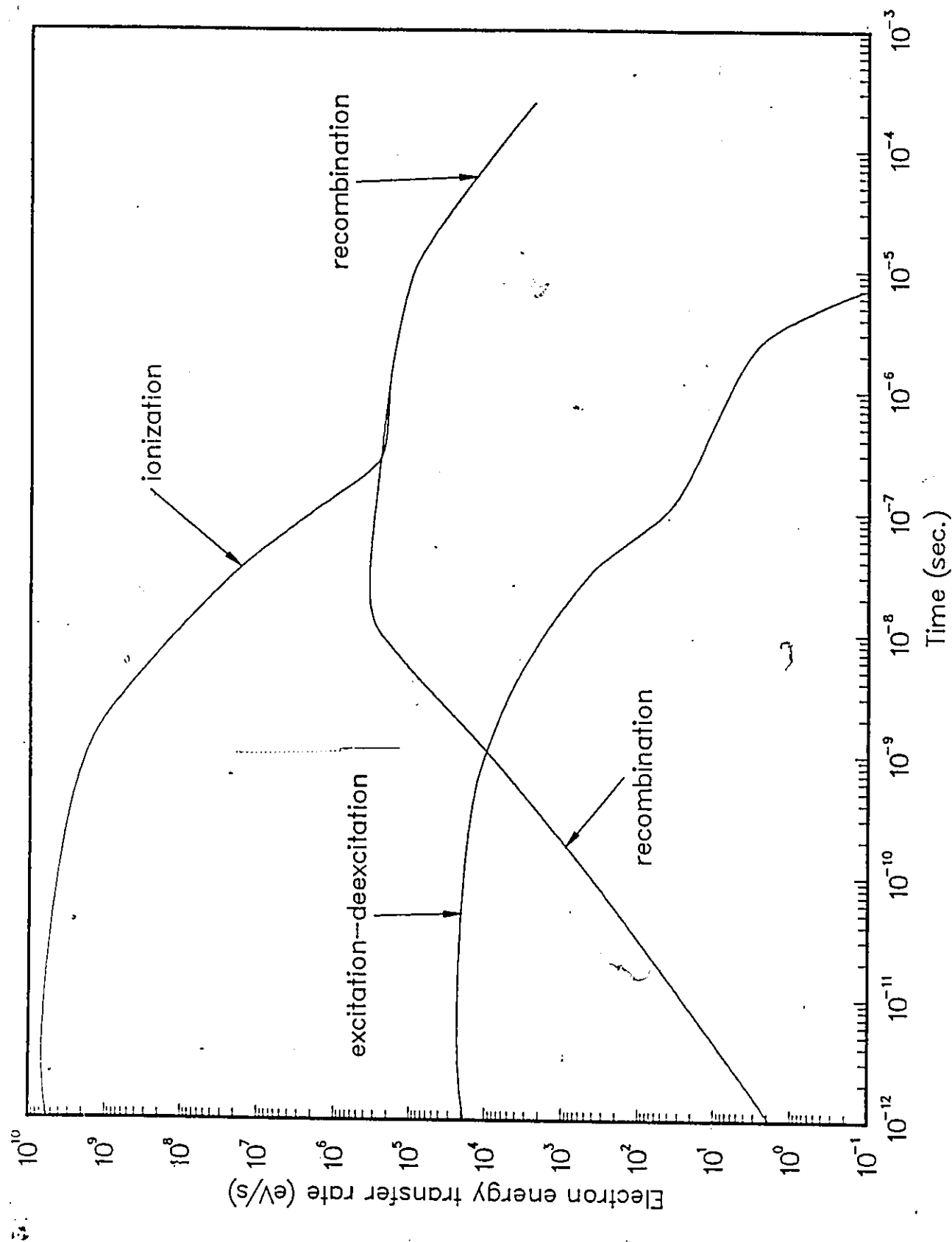


Fig. 7-2. Electron energy transfer rate due to inelastic collisions for hydrogen atom. The solid lines denote the incoming energy fluxes.

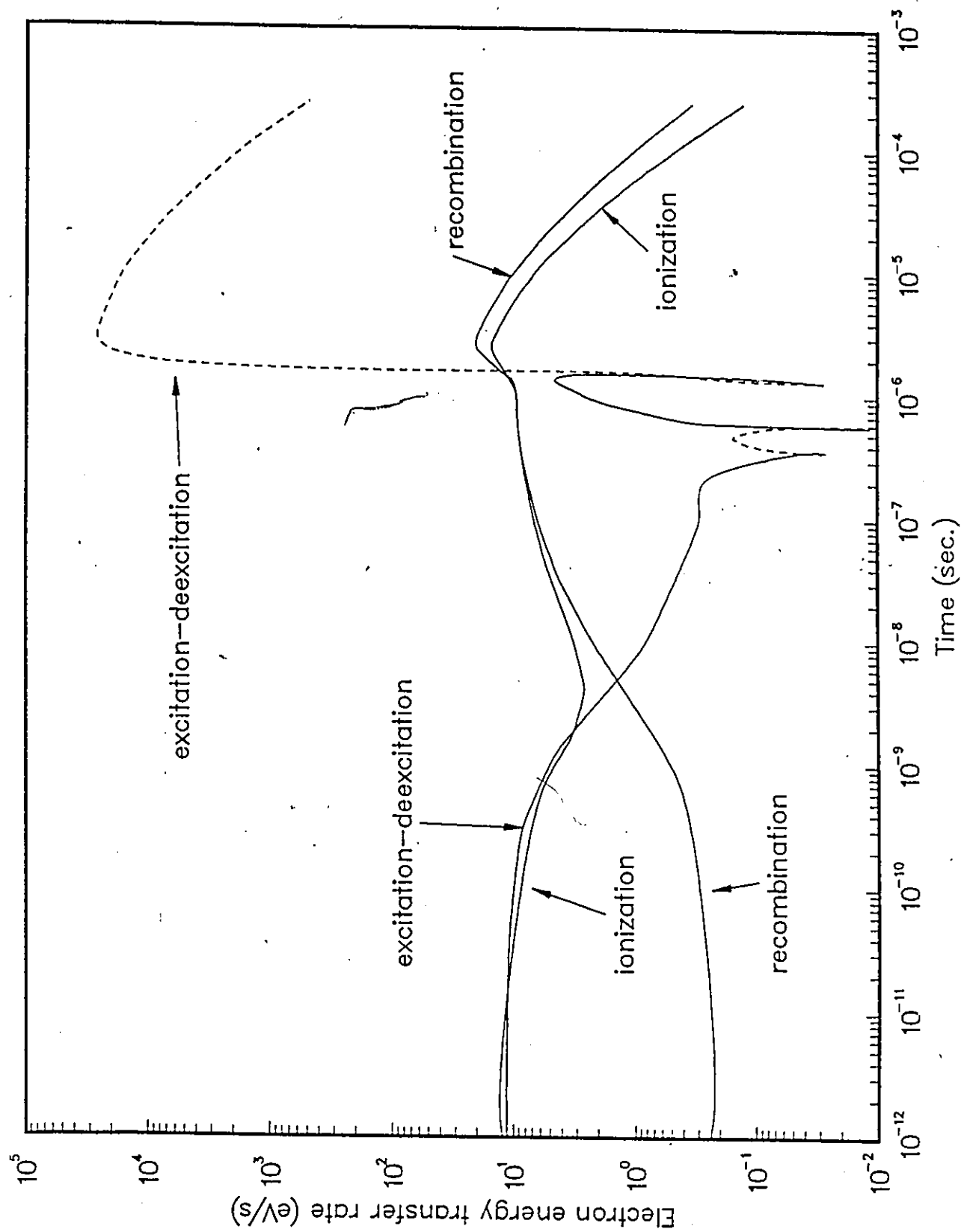


Fig. 7-3. Electron energy transfer rate due to inelastic collisions for helium atom. The solid and dashed lines denote the incoming and the outgoing energy fluxes, respectively.

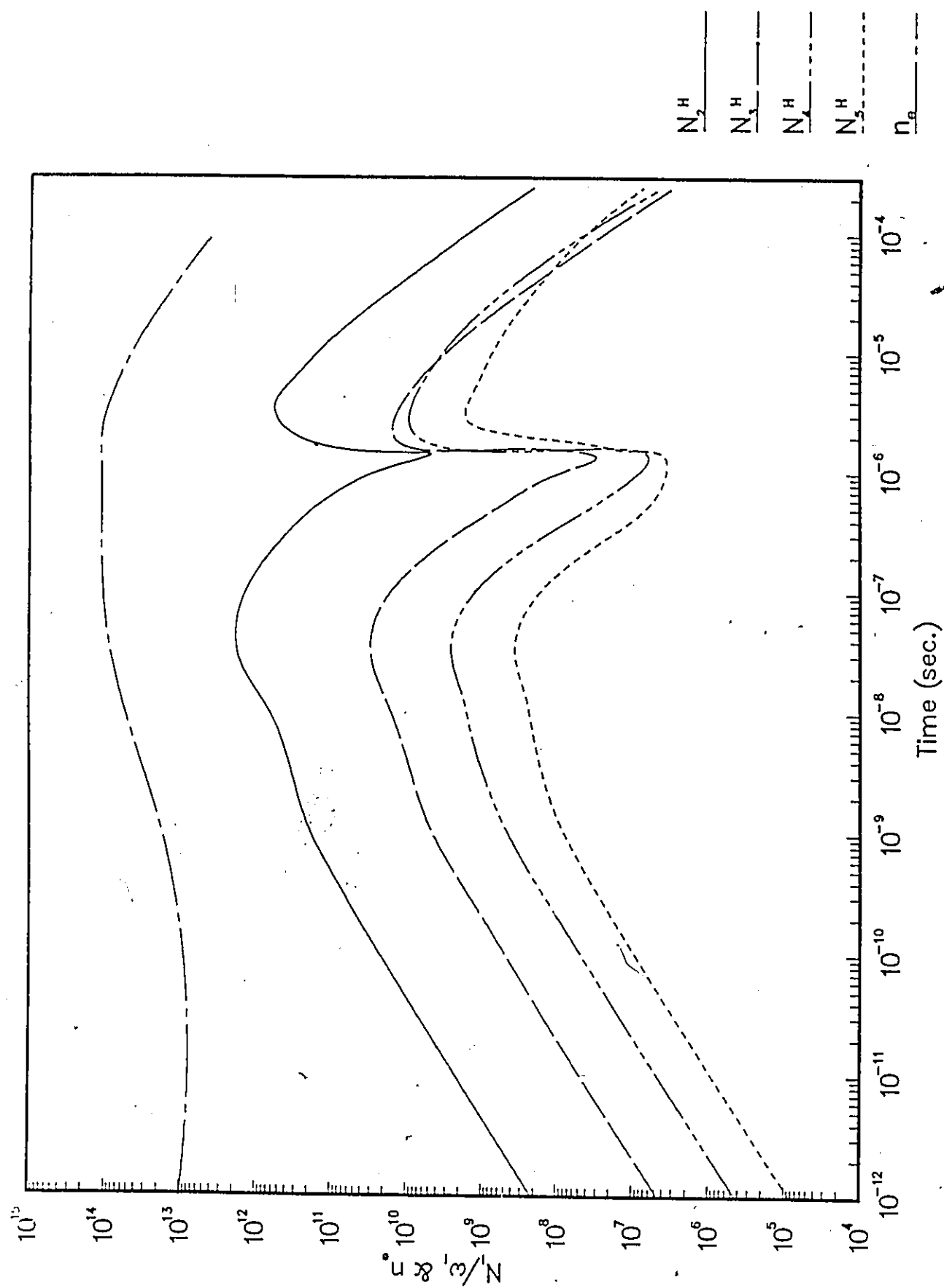


Fig. 7-4. Population densities vs. time for some levels in H and the electron density as a function of time.

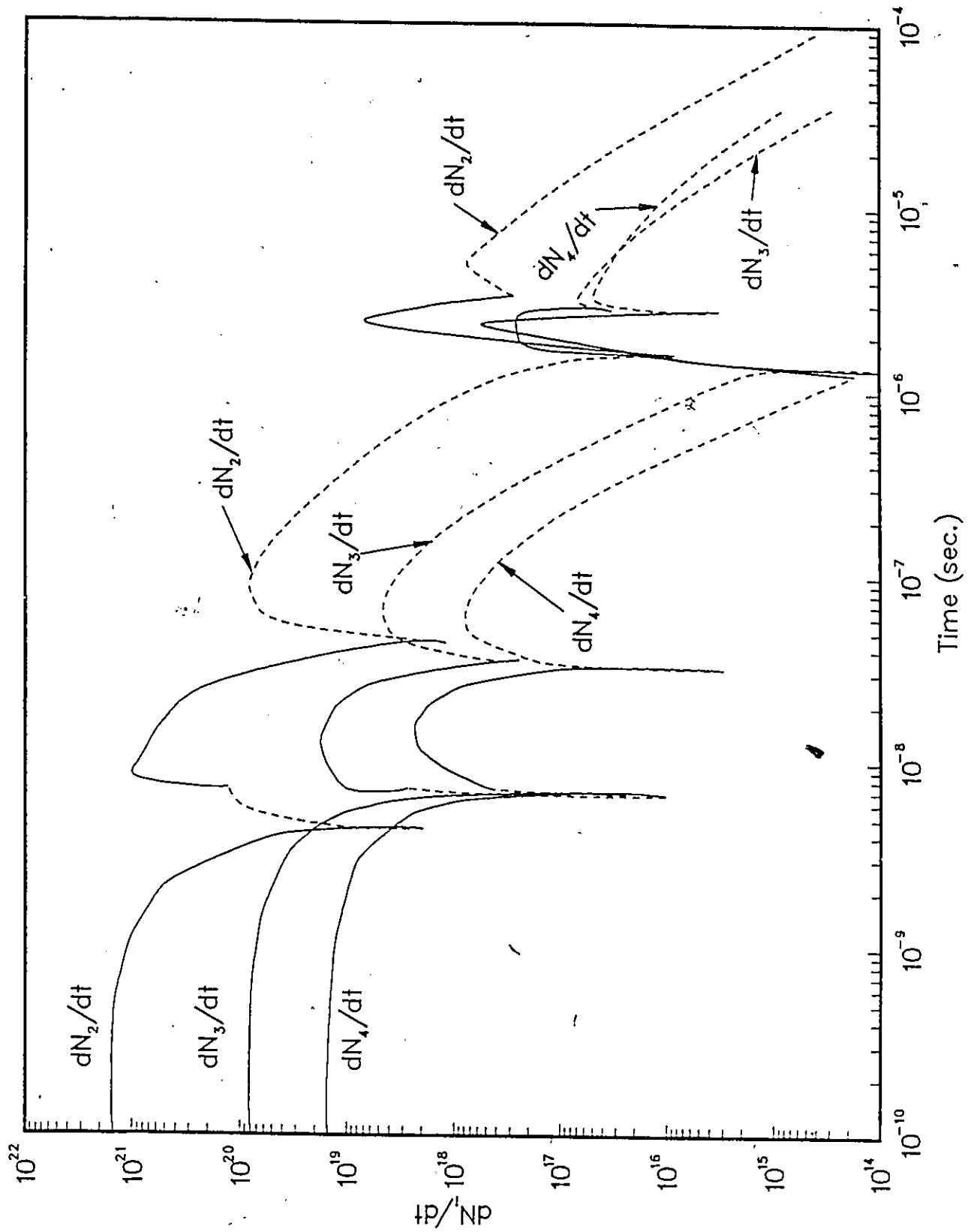


Fig. 7-5. The rate of change in the population density of levels i ($i=2, 3, 4$) of hydrogen atom. The solid and dashed lines denote growing and decreasing rates, respectively.

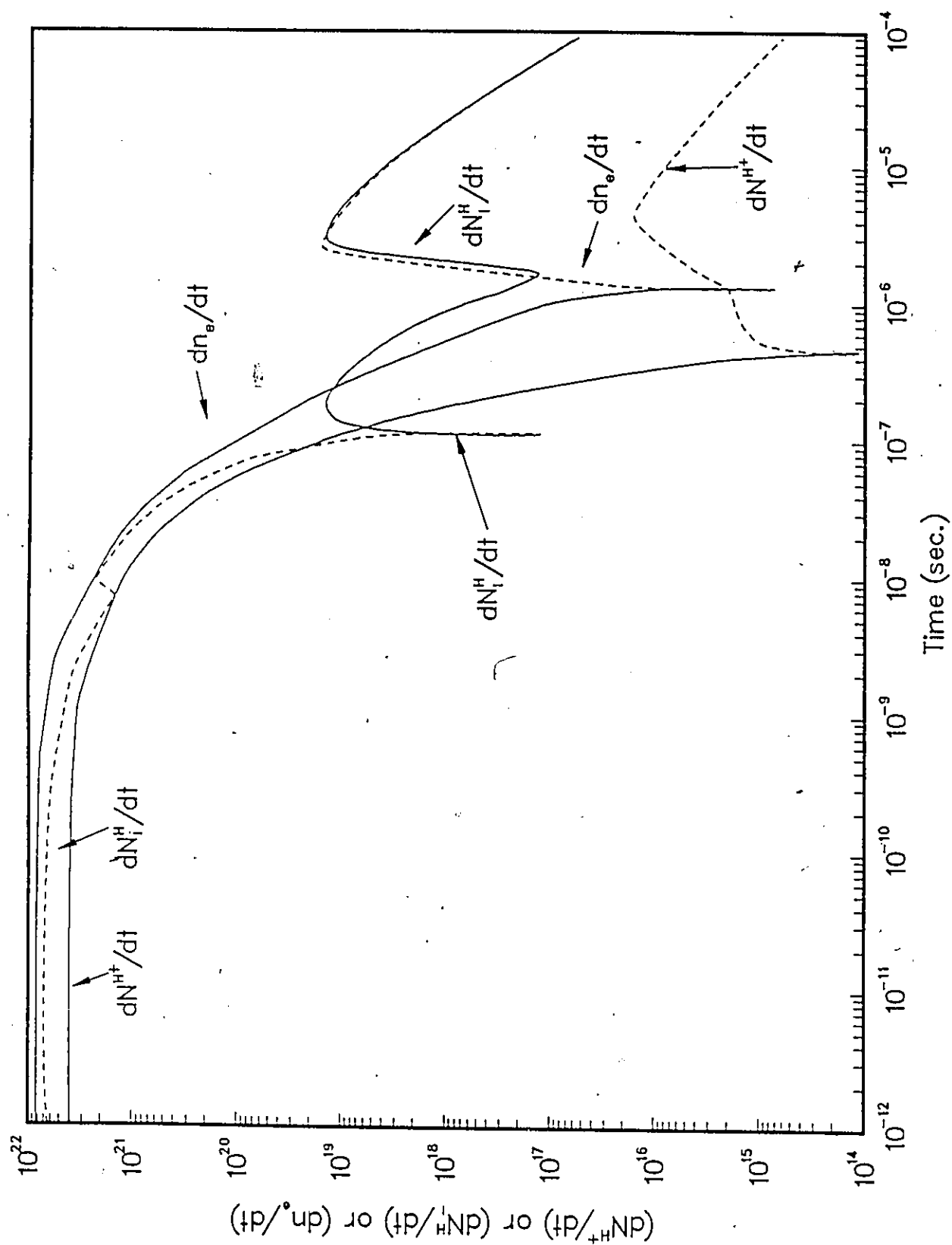


Fig. 7-6. The rate of change in the density of hydrogen ion and electron, and in the population density of the ground state of hydrogen. The solid and dashed lines denote growing and decreasing rates, respectively.

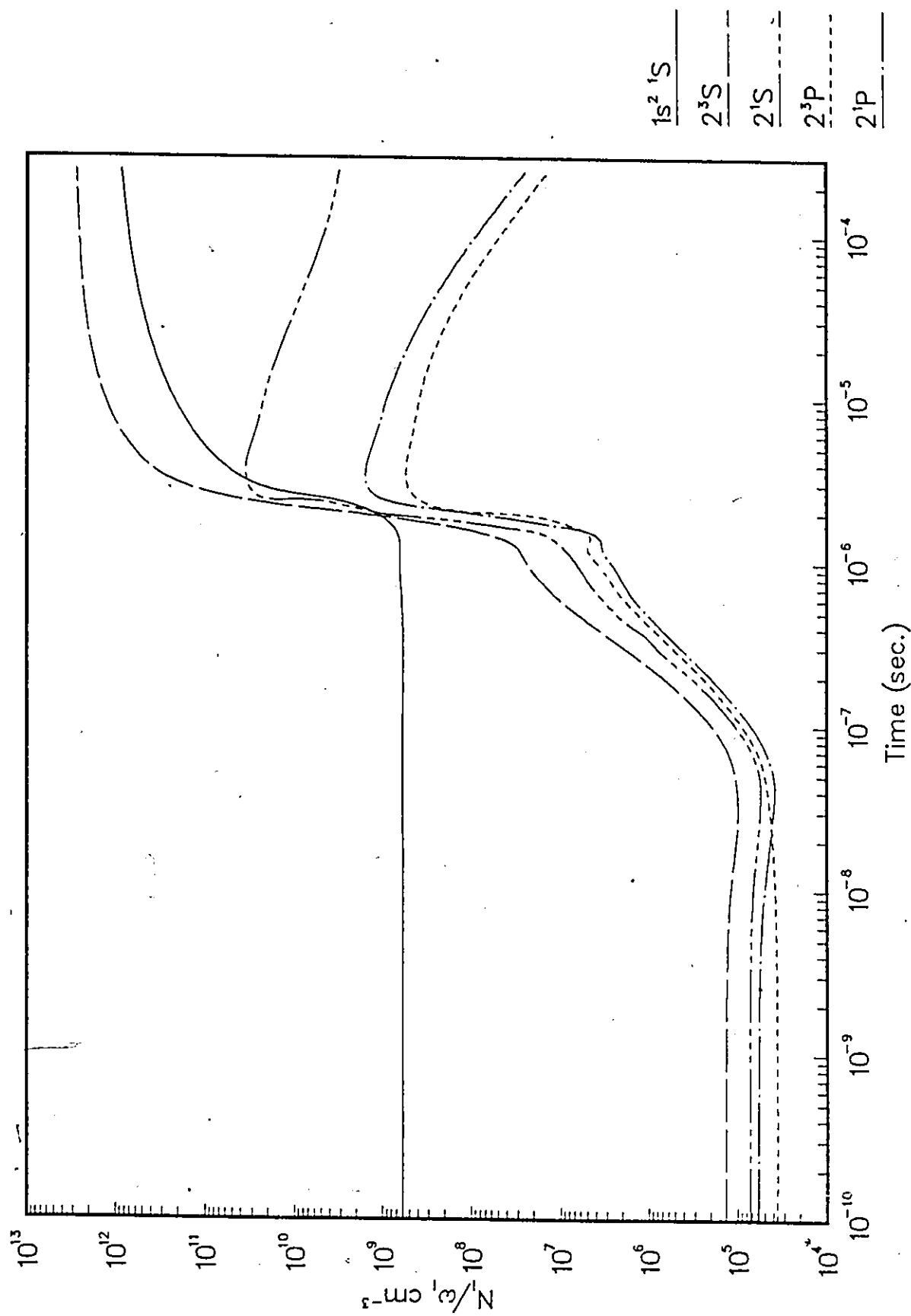


Fig. 7-7. Population densities vs. time for some levels in He I

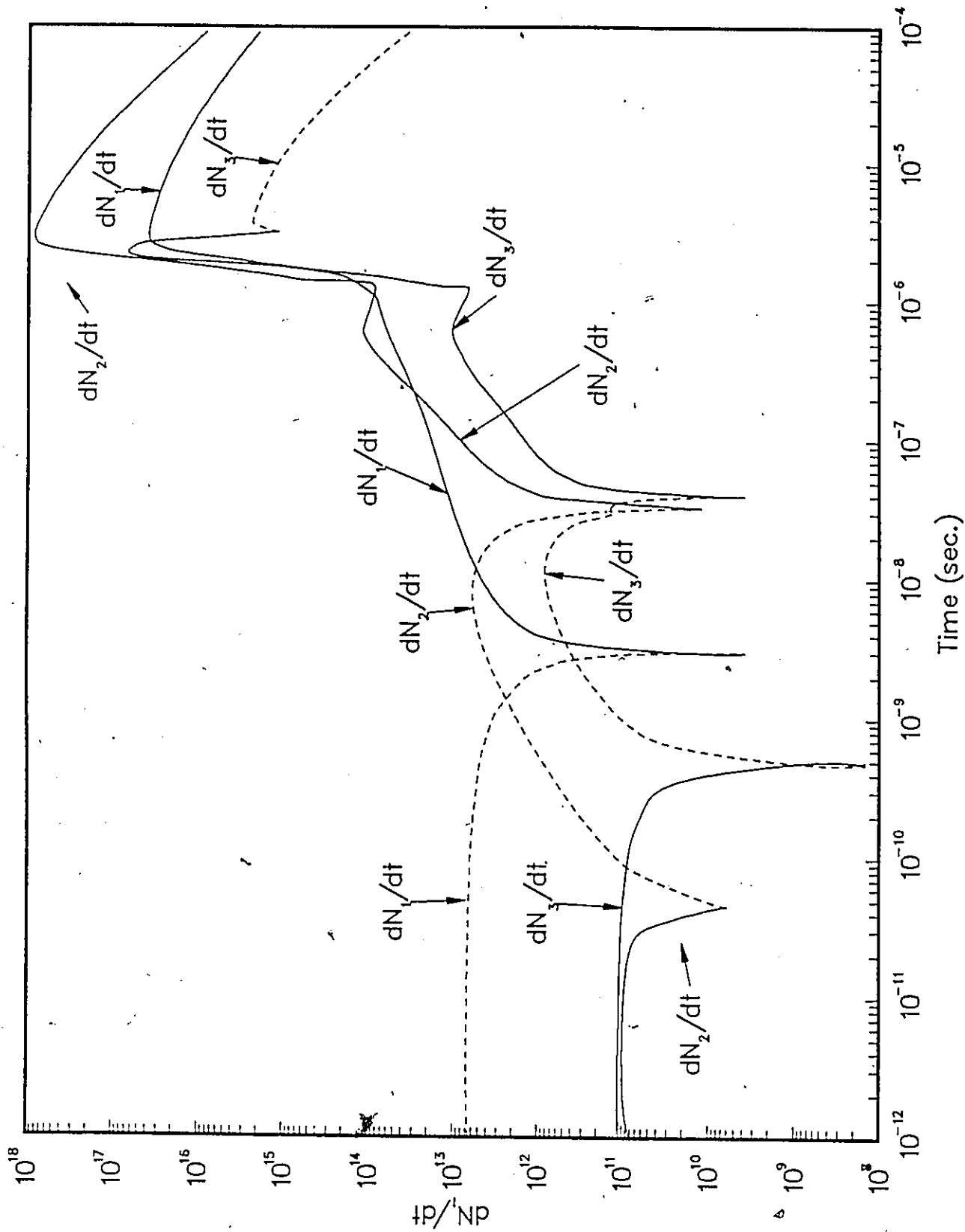


Fig. 7-8. The rate of change in the population density for the ground state and the metastable states of helium. The solid and dashed lines denote growing and decreasing rates, respectively.

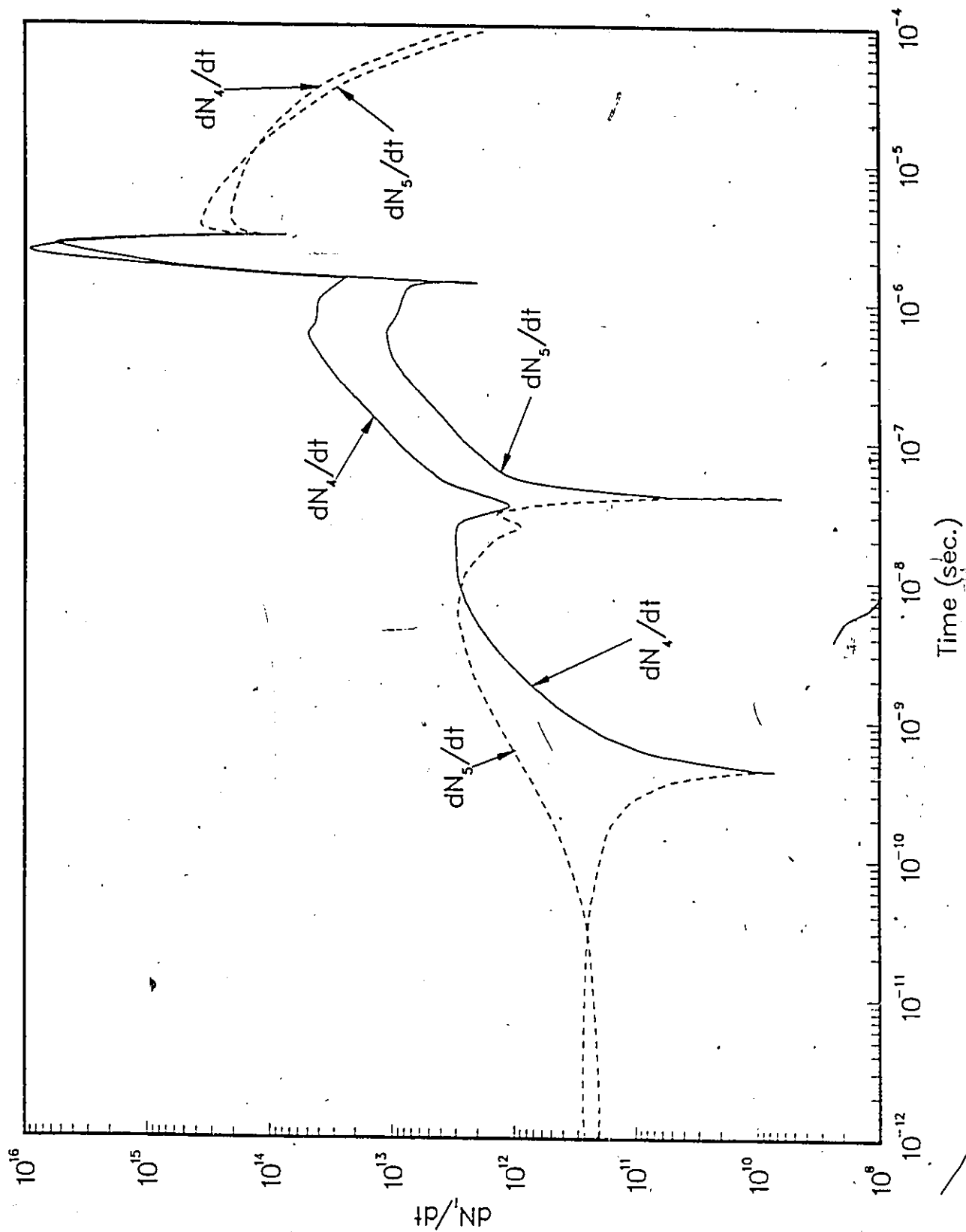


Fig 7-9. The rate of change in the population density for 2^3P (N_4) and 2^1P (N_5) levels of helium. The solid and dashed lines denote growing and decreasing rates, respectively.

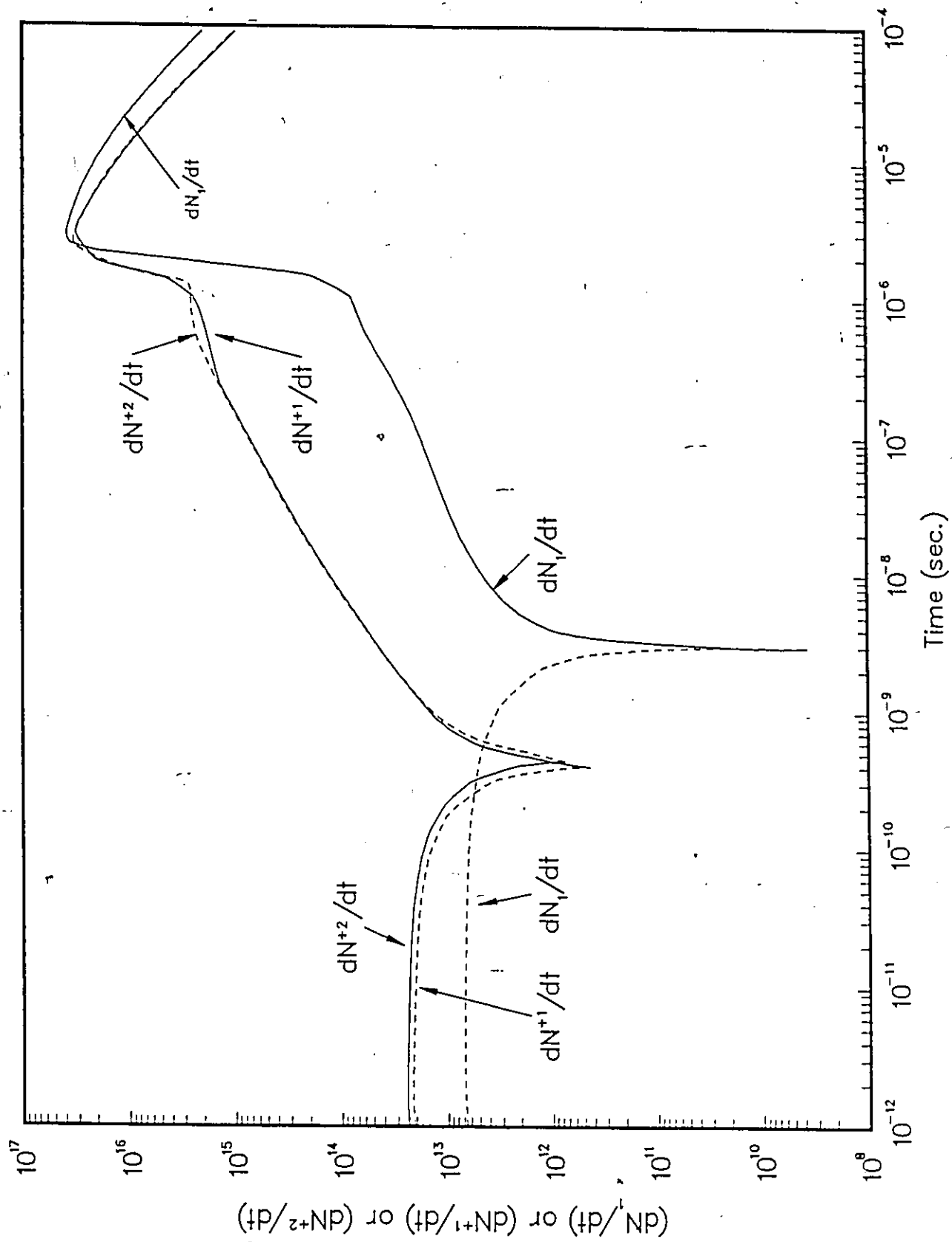


Fig. 7-10. The rate of change in the density of the helium ions and in the population density of the ground state of helium. The solid and dashed lines denote growing and decreasing rates, respectively.

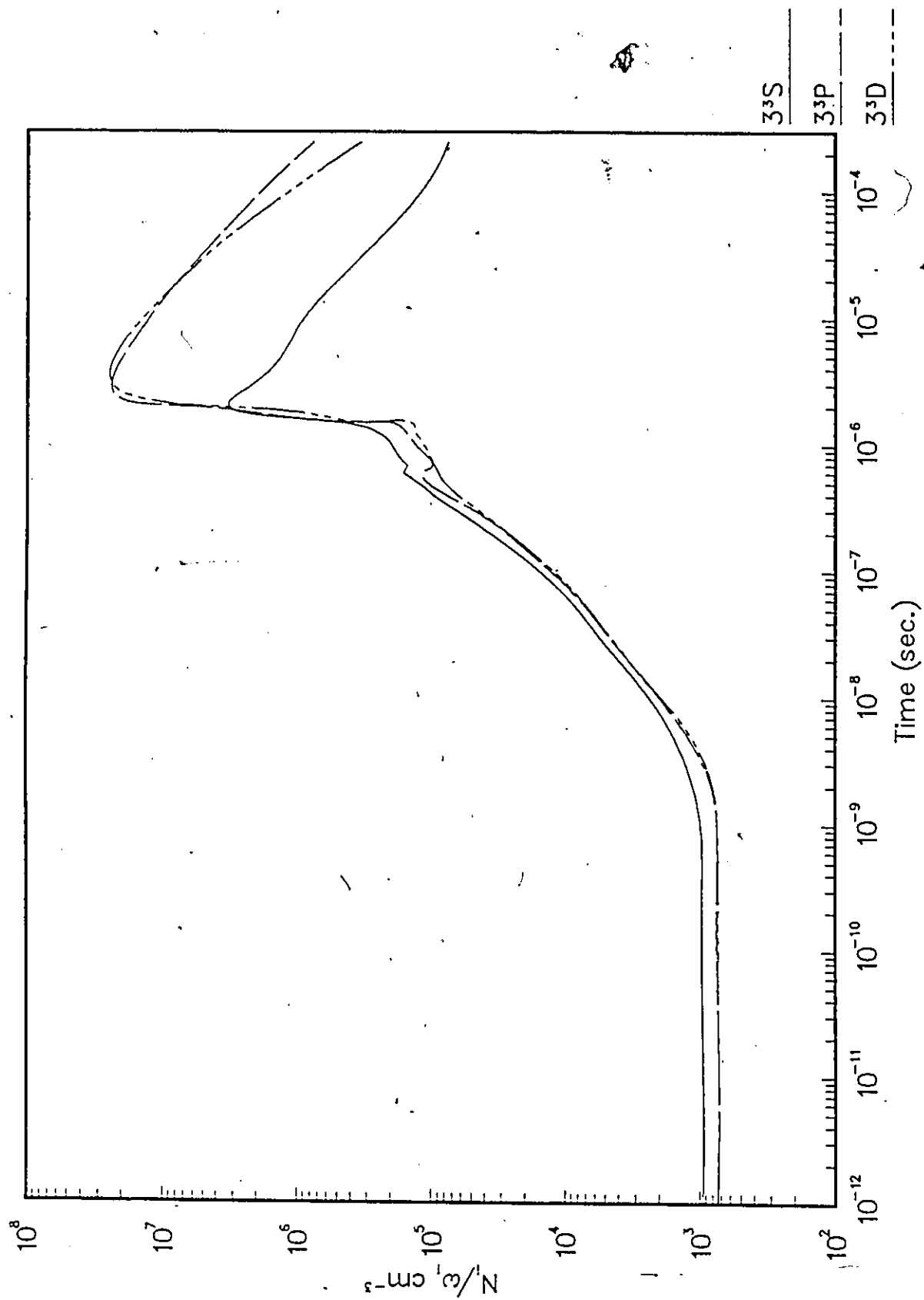


Fig. 7-11. Population densities vs. time for some levels in He I

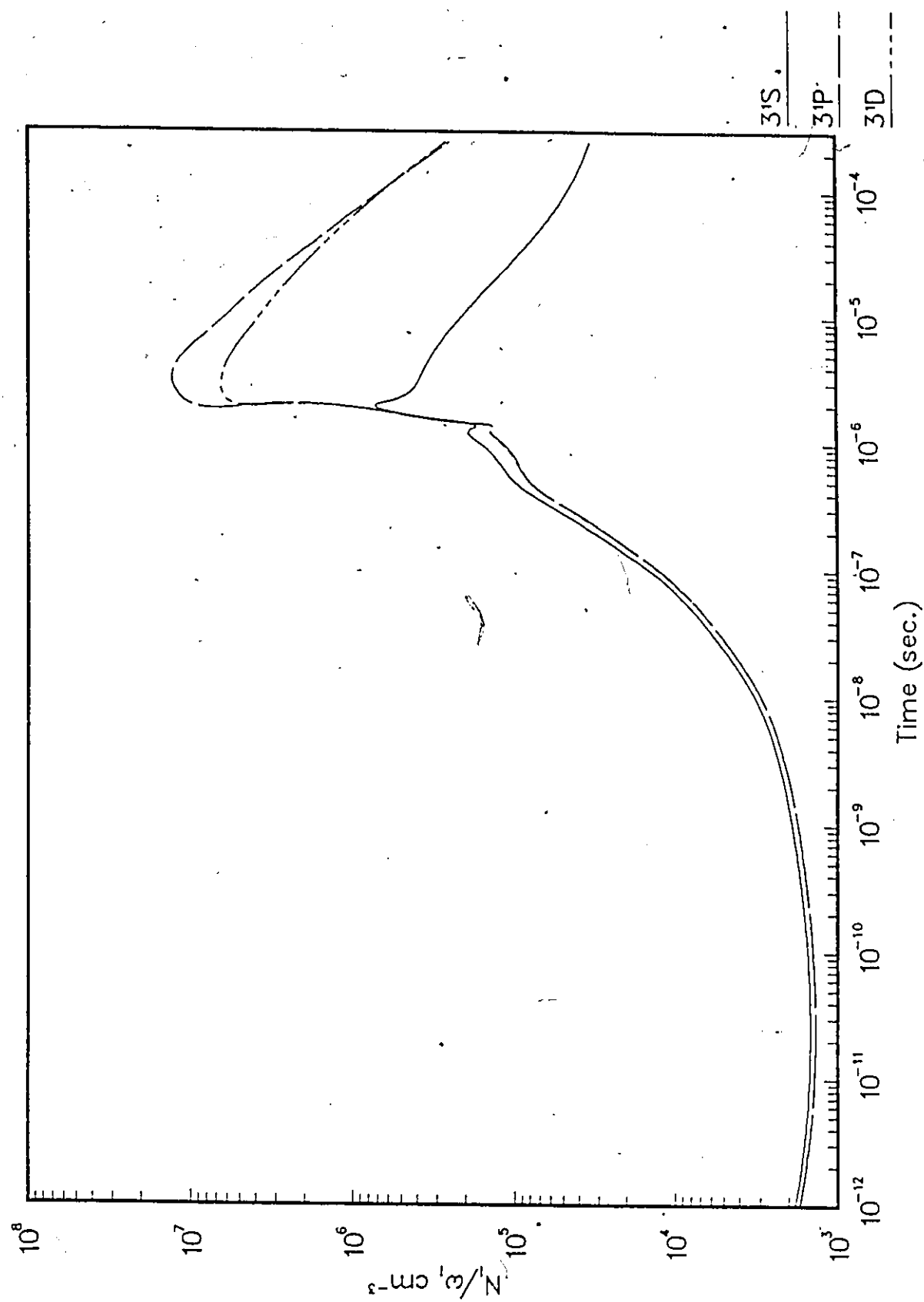


Fig. 7-12. Population densities vs: time for some levels in He I

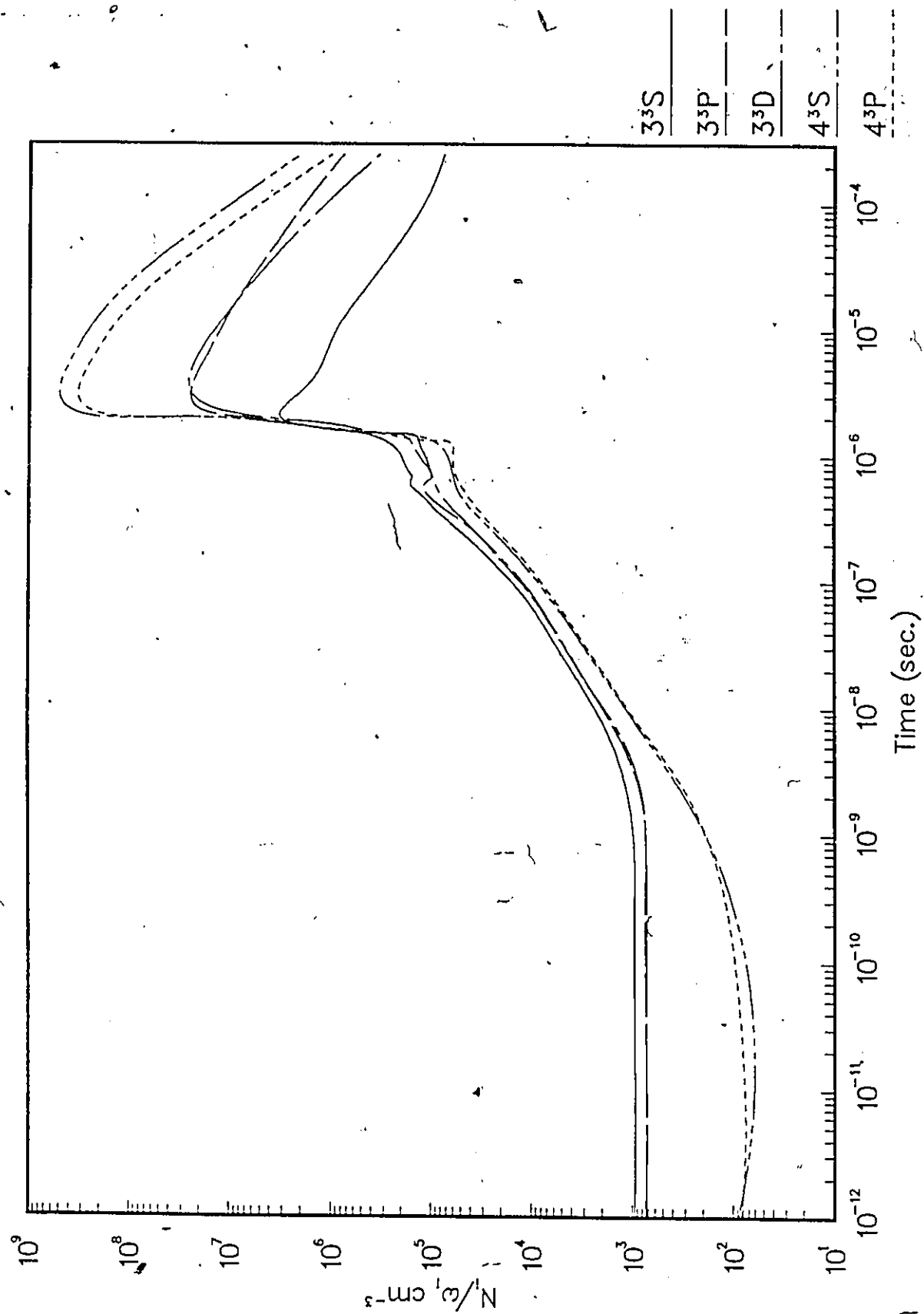


Fig. 7-13. Population densities vs. time for some levels in He I

Conclusion

Population inversions in recombining plasmas were investigated in this work and the following results were obtained:

A. Sudden expansion plasmas:

I) He I

- 1) We find that the He I $\lambda\lambda 7281, 6678$ lines arising from $3^1S \rightarrow 2^1P$ and $3^1D \rightarrow 2^1P$ transitions respectively, display strong population inversion.
- 2) In astrophysical context, the present investigation provides an understanding of the unusual strength of the He I $\lambda\lambda 7281, 6678$ emission in the Wolf-Rayet stars, and provides a strong basis for believing that laser action is responsible for it.

II) C III

- 1) Appreciable population inversion was found for only two lines C III $\lambda 4650$, and $\lambda\lambda 5273, 5254, 5244$ arising from $2s3p \ ^3P^o \rightarrow 2s3s \ ^3S$ and $2p3p \ ^3S \rightarrow 2p3s \ ^3P^o$ transitions respectively.
- 2) In Wolf-Rayet spectra, strong emission lines are observed at C III $\lambda\lambda 4650, 5263$. The available evidence on these two lines from Wolf-Rayet spectra is consistent with both possibilities, that is, presence or absence of laser action.
- 3) We do not find any population inversion for C III $\lambda 5696$ in the simple model that we have investigated.

If the expanding plasma interacts with a gas, it is possible that heavy particle interaction processes may lead to laser action in many other important lines, such as He I $\lambda 4714$ and C III $\lambda 5695$. Also improving the model by taken T_e and N to be given functions of time may lead to better understanding.

B. Free expansion plasmas (as a function of time):

I) He I

- 1) Population inversion was found to occur for a great many transitions in He I in the infra-red and visible regions. Therefore, from these results it is clear that the radiative and/or collisional depopulation of the lower working levels can work efficiently, and used for lasing in large helium plasma volumes.
- 2) The results of this calculation demonstrate that the rate of relaxation of the ns levels is lower than the corresponding rate of the $(n-1)p$ levels, and inverted population of the level pairs $ns \rightarrow (n-1)p$ can occur (inverted population of the level pairs $ns \rightarrow (n-2)p$ occurs but with lower magnitude). Also, inverted population of the level pairs $np \rightarrow (n-1)d$ can occur.
- 3) The variation of the population inversion with n_{e0} and T_{e0} showed that it depends very strongly on these parameters of the plasma. Thus, there is an optimum initial electron temperature and density at which the population inversion attains its maximum value.

II) C III

- 1) A great many transitions in C III in the visible and ultraviolet regions show a large population inversion. The present calculations show that it is possible in practice to produce a laser in ultraviolet region on the basis of a highly-ionized carbon plasma expanding in vacuum.
- 2) Population inversion was found in some transitions in C III even in the initial steady state. These transitions are as follows: $2s3p \ ^3P^o \rightarrow 2s3s \ ^3S$ ($\lambda 4650$), $2s4p \ ^3P^o \rightarrow 2s3d \ ^3D$ ($\lambda 2092$), and $2s5f \ ^3F^o \rightarrow 2s4d \ ^3D$ ($\lambda 3885$), $2s5s \ ^1S \rightarrow 2p3s \ ^1P^o$ ($\lambda 3507$).
- 3) C III $\lambda 2297$ line arising from $2p^2 \ ^1P \rightarrow 2s2p \ ^1P^o$ has been observed in emission in many novae at the nebular stage with intensity greater than the expected intensity.

The present investigation shows that the observed intensity can be explained by using this theoretical model.

- 4) The degree of the population inversion depends on the initial conditions, with higher initial electron temperature, the magnitude of population inversion in C III is lower.

C. Helium plasma interacting with hydrogen gas:

- 1) Under the initial conditions considered here, the QSS was established after $t \sim 2 \times 10^{-6}$ s. In other words, the population densities change rapidly in time during the transient recombining phase.
- 2) Population inversion in hydrogen cannot be expected in the transient recombining phase, but is realized only in QSS. In helium, the case is different, all the population inversion is found to occur in the transient recombining phase, which occurs at $t \sim 1.5 \times 10^{-6}$ s.
- 3) Fig 7-3 shows the importance of the de-excitation processes in producing population inversion in helium. The results of the calculation show clearly that the population inversion of the level pairs $ns \rightarrow (n-1)p$ can result from a difference between the scale times for the collisional decay of these levels.
- 4) The theoretical results shown here and the experimental results (Maezawa and Sato, 1980) are in very good agreement.

A study of plasma which undergoes both cooling mechanisms simultaneously, that is, expansion and interaction with a cool and dense gas, is expected to provide a better and direct understanding to the problem of intensity anomalies in the spectra of Wolf-Rayet and Of stars and novae.

Appendix A

Ionization equilibrium of helium

The relative concentrations of He, He⁺, and He⁺⁺ of monatomic non-LTE plasma under statistical equilibrium are calculated approximately with the model of House (1964). Since the plasma is not in LTE, the individual physical processes contributing to the ionization equilibrium must be considered. House (1964) calculated the ionization equilibrium of elements between hydrogen and iron, over a wide range of temperatures, including the processes of collisional ionization, radiative and collisional recombination. The model is based on the following assumptions: (1) Each stage of ionization of element X consists of only a ground state and a continuum. (2) The monatomic plasma is optically thin. Furthermore, the collisional excitation followed by auto-ionization and di-electronic recombination processes are neglected, which under certain conditions, can restrict the applicability of the model.

Let S^{+m} represent the total rate coefficient for ionization from m -times ionized atom of element X to $m+1$ and α_{tot}^{+m} represent that for recombination of ion $m+1$ to m . Then under statistical equilibrium, we have

$$N^{+m} S^{+m} = N^{+(m+1)} \alpha_{tot}^{+m} \quad (\text{A-1})$$

where N^{+m} and $N^{+(m+1)}$ are the density of ions m and $m+1$, respectively. The collisional ionization rate coefficient is calculated with the following simple approximated formula (Allen, 1961):

$$S^{+m} = 1.15 \times 10^{-8} f \frac{\zeta_m}{I_m^2} n_e \sqrt{T} e^{-I_m/kT} \quad (\text{A-2})$$

where ζ_m is the number of electron in the outer shell of ion m , I_m is the ionization potential of ion m in eV,

$$f = 3.1 - \frac{1.2}{z_m} - \frac{0.9}{z_m^2}, \quad (\text{A-3})$$

z_m is the core charge of ion m , and all other symbols have their usual meaning. The three-body recombination rate coefficient is obtained from the condition of detailed balancing

$$\alpha_{three}^{+m} = \left(\frac{N^{+m}}{N^{+(m+1)}} \right) S^{+m} \quad (\text{A-4})$$

where S^{+m} is the collisional ionization rate coefficient (Eq. A-2), and $(N^{+m}/N^{+(m+1)})$ is given by the Saha-Boltzmann equation:

$$\frac{N^{+m}}{N^{+(m+1)}} = \left(\frac{h^2}{2\pi m_e k} \right)^{3/2} \frac{n_e}{T_e^{3/2}} \frac{U_m}{2U_{m+1}} \exp(I_m/kT_e), \quad (\text{A-5})$$

U is the partition function. The radiative recombination rate coefficient has been calculated using the well known formula of Elwert (1952) given by

$$\alpha_{rad.c.}^{+m} = 5.16 \times 10^{-14} f_1 \left(\frac{I_H}{kT_e} \right)^{1/2} \frac{I_m}{I_H} n n_e G_1(I_m/kT) g \quad (\text{A-6})$$

where

$$G_1(X) = X_m \exp(X_j) E_1(X_m), \quad (\text{A-7})$$

n is the principal quantum number of ground state of lower stage of ionization, I_m is the ionization potential of ion of charge $+m$ in eV, I_H is the ionization potential of hydrogen, $E_1(x)$ is the first exponential integral, $f_1 = 0.8$, $g = 3$. The values of f_1 and g come from Allen (1961). The total recombination rate is given by

$$\alpha_{tot}^{+m} = \alpha_{rad.}^{+m} + \alpha_{threc.}^{+m} \quad (A-8)$$

The fraction of the atoms of element X that have been ionized m times is given by $N^{+m} / \sum_m N^{+m}$.

Appendix B

Oscillator strength calculation

The absorption oscillator strength for the $n'\ell' \rightarrow n\ell$ transition is expressed in term of the line strength S :

$$f_{n'\ell',n\ell} = \frac{2}{3} \frac{m}{\hbar^2 e^2} \frac{E^{n\ell, n'\ell'}}{2(2\ell' + 1)} S_{n'\ell',n\ell} \quad (\text{B-1})$$

$S_{n'\ell',n\ell}$ is in atomic units ($a_0^2 e^2$).

If LS-coupling is applicable, then the line strength can be separated as follows (Bates and Damgaard, 1949):

$$S_{n'\ell',n\ell} = \mathcal{L}(M) \mathcal{L}(\mathcal{L}) \sigma_{n'\ell',n\ell}^2 \quad (\text{B-2})$$

where $\mathcal{L}(M)$ represents the strength of the multiplet, and $\mathcal{L}(\mathcal{L})$ the relative strength of the spectral line within the multiplet. The numerical values of these factor may be obtained from tables given by Goldberg (1935, 1936), and White and Eliason (1933) or Russell (1963). The line strengths are summed over J and j' , and the following expressions are obtained (Condon and Shortley, 1935):

$$S_{n'\ell',n\ell-1} = 2(2\ell + 1)\ell(2\ell - 1)\sigma_{n'\ell',n\ell-1}^2 \quad (\text{B-3})$$

$$S_{n'\ell',n\ell+1} = 2(2\ell + 1)(\ell + 1)(2\ell + 1)\sigma_{n'\ell',n\ell+1}^2 \quad (\text{B-4})$$

The transition intergral $\sigma_{n'\ell',n\ell}^2$ is related to the radial matrix element $\mathfrak{R}_{n'\ell'}^{n\ell}$ by

$$\sigma_{n'\ell',n\ell}^2 = \frac{1}{4\ell^2 - 1} [\mathfrak{R}_{n'\ell'}^{n\ell}]^2 \quad (a_0^2 e^2) \quad (\text{B-5})$$

ℓ being the greater of the two azimuthal quantum numbers involved in the transition and

$$\mathfrak{R}_{n'\ell'}^{n\ell} = \int_0^\infty R_i(r) R_f(r) r dr. \quad (\text{B-6})$$

$R_i(r)/r$ and $R_f(r)/r$ are the normalized radial wave functions of the valence electron in the initial and final states expressed in atomic units, respectively. The calculation of $S_{n'\ell',n\ell}$, and hence of $f_{n'\ell',n\ell}$, therefore requires only the evaluation of $\sigma_{n'\ell',n\ell}^2$. Using the Coulomb approximation (CA) proposed by Bates and Damgaard (1949), $\sigma_{n'\ell',n\ell}^2$ is evaluated as follows: In the standard central field model the functions R_i and R_f satisfy a differential equation of the form

$$\frac{d^2 R}{dr^2} + \left(2V - \frac{\ell(\ell+1)}{r^2} - \epsilon \right) R = 0 \quad (\text{B-7})$$

where V is the potential of the atom or ion and ϵ is the energy of the state. Replacing the potential V by its asymptotic Coulomb form z/r , z being the core charge of the ion. The differential equation for R thus becomes

$$\frac{d^2 R}{dr^2} + \left(\frac{2z}{r} - \frac{\ell(\ell+1)}{r^2} - \epsilon \right) R = 0 \quad (\text{B-8})$$

A solution of this satisfying the boundary condition

$$R \longrightarrow 0 \quad \text{as} \quad r \longrightarrow \infty \quad (\text{B-9})$$

can be written as

$$R = \frac{W_{n^*, \ell + \frac{1}{2}}(2zr/N^*)}{[n^{*2} \Gamma(n^* + \ell + 1) \Gamma(n^* - \ell)/z]^{1/2}} \quad (\text{B-10})$$

where n^* is the effective principal quantum number defined by

$$n^* = \frac{z}{\sqrt{\epsilon}} \quad (\text{B-11})$$

and $W_{n^*, \ell + \frac{1}{2}}$ is Whittaker function, a particular confluent hypergeometric function.

The asymptotic behavior of the Whittaker function is

$$W_{n^*, \ell + \frac{1}{2}}(2zr/n^*) \approx \left(\frac{2zr}{n^*}\right) e^{-zr/n^*} \left\{1 + \sum_{t=1}^{\infty} \frac{a_t}{r^t}\right\} \quad (\text{B-12})$$

where

$$a_1 = \frac{n^*}{2z} [\ell(\ell+1) - n^*(n^*-1)] \quad (\text{B-13})$$

$$a_t = a_{t-1} \left\{ \frac{n^*}{2tz} [\ell(\ell+1) - (n^*-t)(n^*-t+1)] \right\} \quad (\text{B-14})$$

Combining Eqs. (B-11) and (B-12), we can then write

$$R(r) \simeq \sum_{t=0}^{\infty} C_t(n^*, \ell) x^{1/2} (zr)^{n^*-t} e^{-zr/n^*} \quad (\text{B-15})$$

where

$$C_t(n^*, \ell) = \frac{b_t}{\sqrt{n^{*2}} \Gamma(n^* + \ell + 1) \Gamma(n^* - \ell)} \left(\frac{2}{n^*}\right)^{n^*-t} \quad (\text{B-17})$$

$$b_t = \frac{1}{t!} \prod_{j=1}^t (\ell(\ell+1) - (n^*-j+1)(n^*-j)) \quad (\text{B-18})$$

The radial matrix element given by Eq. (B-6) thus becomes

$$\mathfrak{R}_{n^* \ell'}^{n^* \ell} = \frac{1}{z} \sum_{t'=0}^{\infty} \sum_{t=0}^{\infty} C_{t'}(n^*, \ell') C_t(n^*, \ell) \int_0^{\infty} (zr)^y e^{-zr \left(\frac{n^* + n^*}{n^* n^*}\right)} d(zr) \quad (\text{B-19})$$

where

$$y = n'^* + n^* + 1 - t' - t. \quad (\text{B-20})$$

The integral in Eq. (B-19) is evaluated using the formula (Spiegel, 1968)

$$\int_0^\infty X^n e^{-aX} dX = \frac{\Gamma(n+1)}{a^{n+1}} \quad (\text{B-21})$$

Thus Eq. (B-19) becomes

$$\mathfrak{R}_{n'\ell}^{n\ell} = \frac{1}{z} \sum_{t'=0}^\infty \sum_{t=0}^\infty C_{t'}(n'^*, \ell') C_t(n^*, \ell) \Gamma(y+1) \left(\frac{n'^*}{n'^* + n^*} \right)^{y+1} \quad (\text{B-22})$$

Bates and Damgaard (1949) terminate the sum in Eq. (B-22) by using a physical argument. In the sum over the integral of Eq. (B-19), all the terms for which the powers of $zr < 2$ are neglected because the main contribution from these terms comes from regions close to the origin where Coulomb approximation does not necessarily hold and the use of asymptotic expansions is not valid. We thus neglect those terms of Eq. (B-22) for which

$$t' + t > n'^* + n^* - 1 \quad (\text{B-23})$$

The range of allowed values of $t' + t$ is

$$0 \leq t' + t \leq p \quad (\text{B-24})$$

where p is the integer part of $(n'^* + n^* - 1)$. Using the following transformation (Rainville, 1960):

$$\sum_{t=0}^\infty \sum_{t'=0}^\infty A(t', t) = \sum_{t=0}^\infty \sum_{t'=0}^t A(t', t - t'). \quad (\text{B-25})$$

Equation (B-22) can be written

$$\mathfrak{R}_{n'\ell}^{n\ell} = \frac{1}{z} \mathcal{F}(n'^* \ell', n^* \ell) \sum_{t=0}^p (-1)^t \mathcal{N}(n'^* \ell', n^* \ell) \Gamma(n'^* + n^* + 2 - t) \left(\frac{n'^* + n^*}{2n'^*} \right)^t \quad (\text{B-26})$$

where

$$\mathcal{F}(n'^* \ell', n^* \ell) = \frac{1}{4} \frac{[2n'^*/(n'^* + n^*)]^{n^*+1}}{\sqrt{\Gamma(n'^* + \ell' + 1) \Gamma(n'^* - \ell')}} \frac{[2n^*/(n'^* + n^*)]^{n'^*+1}}{\sqrt{\Gamma(n^* + \ell + 1) \Gamma(n^* - \ell)}} \quad (\text{B-27})$$

$$\mathcal{N}(n'^* \ell', n^* \ell) = \sum_{t'=0}^t \frac{1}{t'!(t-t')!} \left(\frac{n'^*}{n^*} \right)^{t'} \prod_{i=1}^{t'} q_i(n'^* \ell') \prod_{j=1}^{t-t'} q_j(n^* \ell) \quad (\text{B-28})$$

$$q_i(n'^* \ell') = (n'^* - i + 1)(n'^* - i) - \ell'(\ell' + 1) \quad (\text{B-29})$$

$$q_j(n^* \ell) = (n^* - j + 1)(n^* - j) - \ell(\ell + 1) \quad (\text{B-30})$$

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