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KINETIC STUDIES OF THE KRF LASER. (U)

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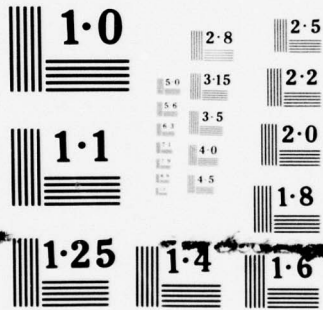
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KINETIC STUDIES OF THE K_rF LASER
FINAL TECHNICAL REPORT

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March 1977

Prepared By

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and M. L. Bhaumik
Advanced Laser Research Laboratory

For

Office of Naval Research
Department of the Navy

Contract N00014-76-C-0777

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REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM	
1. REPORT NUMBER 14 NRTC-77-29R ✓	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER	
4. TITLE (and Subtitle) 6 Kinetic Studies of the KrF Laser,	9	5. TYPE OF REPORT & PERIOD COVERED Final Technical Report, 29 March 1976-28 Feb 1977	
7. AUTHOR(s) 10 W. B. Lacina, R. S. Bradford, Jr. and M. L. Bhaumik	15	6. PERFORMING ORG. REPORT NUMBER NRTC 77-29R	
9. PERFORMING ORGANIZATION NAME AND ADDRESS Northrop Research and Technology Center 3401 West Broadway Hawthorne, California 90250		8. CONTRACT OR GRANT NUMBER(s) N00014-76-C-0777 new	
11. CONTROLLING OFFICE NAME AND ADDRESS Office of Naval Research Department of the Navy Arlington, Virginia 22217	11	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 121107	
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office) -- 12/69p.		12. REPORT DATE March 1977	
		13. NUMBER OF PAGES 64	
		15. SECURITY CLASS (of this report) Unclassified	
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE --	
16. DISTRIBUTION STATEMENT (of this Report) Distribution of this document is unlimited			
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report) --			
18. SUPPLEMENTARY NOTES --			
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) Laser Kinetics High Power Excimer Small Signal Gain Rare Gas Halide E-Beam KrF Modeling			
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) The small signal gain coefficient for KrF in a high pressure, e-beam excited mixture of Ar/Kr/F ₂ has been measured at different pressures using an oscillator-amplifier configuration. Kinetic modeling of the electrically excited KrF laser system has been carried out using a sophisticated and comprehensive computer analysis which couples molecular and electron kinetics, radiative extraction, and external driving circuit. Comparisons of the results of kinetic modeling with small signal gain measurements have been made, and reasonable agreement is obtained.			

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KINETIC STUDIES OF THE KrF LASER

Contract Number: N00014-76-C-0777

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Office of Naval Research
Department of the Navy
801 N. Quincy Street
Arlington, Virginia 22217

Effective Date of Contract: 29 March 1976 - 28 February 1977

Amount of Contract: \$39,406.00

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INDEXED	<input type="checkbox"/>
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1.0 SUMMARY

The overall objective of this program has been the investigation of the fundamental physical mechanisms of electrically excited, high pressure rare gas halide excimer laser systems, such as KrF, which are based upon bound-free transitions. The specific purpose of this study was to attain a theoretical understanding of the KrF system in order to optimize efficiency and output extraction in present devices and to predict scalability to higher powers and larger devices. This requires an understanding of the kinetic reaction scheme and determination of the appropriate rate constants, and to obtain this information a wide range of experimental and theoretical work is needed, some of which is currently in progress. For the present program, efforts have been concentrated on theoretical kinetic modeling and experimental measurements of small signal gain coefficients. During the period of investigation, the following specific tasks were performed:

- 1) The small signal gain coefficient for KrF in a high pressure, e-beam excited mixture of Ar/Kr/F₂ has been measured at different pressures using an oscillator-amplifier configuration. The value for the small signal gain coefficient was found to vary from 0.13 to 0.35 cm⁻¹ over the range of parameters investigated.
- 2) Kinetic modeling of the electrically excited KrF laser system has been carried out using a sophisticated and comprehensive computer analysis which couples molecular and electron kinetics, radiative extraction, and external driving circuit. All relevant reactions and species which are currently believed to contribute to the kinetics have been

included in this analysis, and the best current estimates of corresponding rate constants are used.

- 3) Comparisons of the results of kinetic modeling with small signal gain measurements have been made, and reasonable agreement is obtained. The sensitivity of the reactions included in the kinetic scheme has been investigated.

2.0 INTRODUCTION

The recent success of the KrF laser represents a breakthrough in the attainment of high power uv visible lasers. By pumping a dye laser with the newly developed KrF laser, a blue-green laser appears feasible with output in the multikilowatt range with an overall efficiency exceeding 1%. The development of this dye laser will represent a two orders of magnitude improvement in laser output over present devices at these wavelengths.

In order to realize the full potential of the KrF laser, the mechanism of operation must be understood. Different mechanisms have been proposed to explain the KrF laser operation in a high pressure e-beam pumped system. To elucidate the reactions which form KrF^* , the small signal gain has been measured for various conditions and compared with a sophisticated computer model which predicts the gain for these conditions.

Experimental measurement of the gain utilized simultaneous excitation of the oscillator and amplifier cavity by the same e-beam to avoid the problem of synchronizing short pulses. Details of the experiment are discussed in Section 3.1.

In addition, a computer analysis of the KrF system has been carried out. In general, the straightforward attempt to write the subroutines which define molecular kinetics for a complicated reaction scheme is a difficult task, and the resulting computer program would have little flexibility for analysis of any system except those in a very limited class. Having anticipated the necessity for a powerful and general analytical capability, a much more sophisticated approach was taken.

Under IR&D funding, a generalized computer code was developed which itself synthesizes all the necessary subroutines for kinetics analysis. Details of the capabilities of this code and its application to the present program are discussed in Section 3.2.

3.0 TECHNICAL REPORT

The small signal gain is an essential parameter for predicting the scaling of the KrF laser. The mechanism of operation may also be best understood by comparing measured small signal gain with the results of kinetic modeling. The experiments and computer predictions are presented in the following sections.

3.1 KrF Gain Measurements

The experiments were carried out using two independent gas cells ($1 \text{ cm}^2 \times 10 \text{ cm}$ extracted optical volume) stacked side by side and simultaneously pumped with a Pulserad 110A e-beam which provides an output of 1 MeV for 20 ns at 500 A/cm^2 . Each cell was fitted with AR windows, one cell was used as oscillator with external optics while the other served as an amplifier. The output from the oscillator was directed into the amplifier with a prism after 10% was split off by a beam splitter and measured with a F4000 UVG S-1 photodiode. After passing through the second cell, the amplified signal was measured by a second photodiode.

Both photodiodes had a 10X neutral density filter and quartz diffuser over the photo cathode. The pair of diodes were calibrated at 249 nm on a relative basis with radiation from the oscillator using several shots. The amplifier photodiode was placed 1 m from the amplifier output to reduce the detection of spontaneous emission. The addition of various neutral density filters to the oscillator beam allowed the power into the amplifier to be varied over a wide range. A schematic layout of the experiment is shown in Figure 1.

Gain measurements were taken over several mixture ratios and pressure ranges. A typical data run is shown in Figure 2. For each of

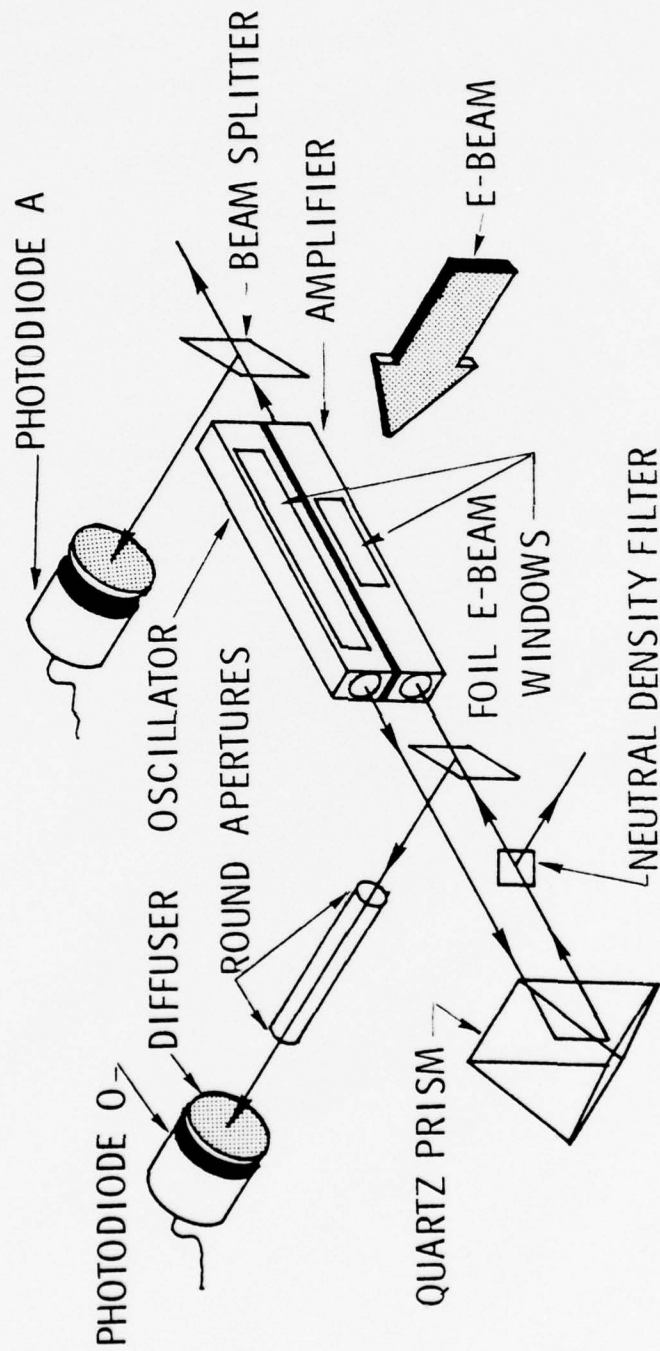


Figure 1. Schematic Diagram of the KrF Gain Measurement

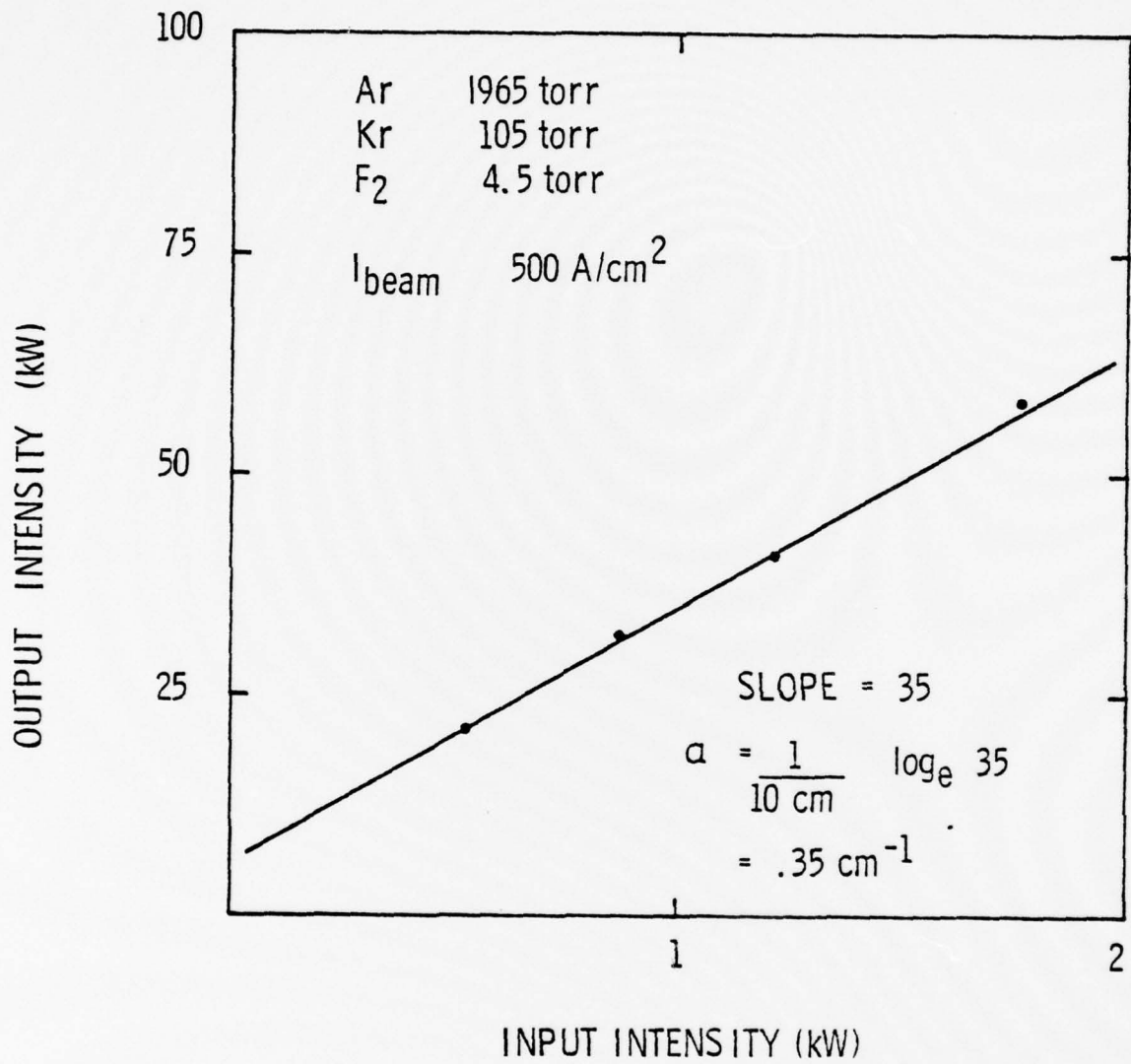


Figure 2. Typical KrF Gain Data

the following cases, with 500 A/cm^2 beam current, the Kr partial pressure held constant while the F_2 partial pressure was varied and vice versa.

The gain was also calculated from the kinetics code described in the next section for the pressures indicated in Tables I, II, and III. From the data, the optimum mixture is Ar:Kr: F_2 (1965:105:4.5 Torr) with a measured gain of 0.35 cm^{-1} . More Kr causes KrF^* loss while less inhibits KrF^* production. The best amplifier performance also coincides with the best laser performance. That is, the mixture with the highest gain as an amplifier is also the best mixture for the oscillator.

3.2 KrF Kinetic Modeling

In order to theoretically model the KrF laser, it is necessary to construct a coupled analysis containing electron and molecular kinetics, optical radiation fields, and an external driving circuit. However, KrF is only one of a broad class of several promising schemes for uv or visible lasers which are currently under investigation (or which will be pursued in the future), and it is impractical to construct new computer codes for the analysis of each new kinetic reaction scheme. The straightforward approach to write the rate subroutines which define the molecular kinetics for a complicated reaction scheme is a time consuming task, and the resulting computer program has little flexibility for analysis of any system except those in a very limited class. Furthermore, as understanding of the reaction scheme evolves, addition of new reactions (or deletion of old reactions) may be required in addition to simple modification of rate constants. Thus, such a code would itself have to be revised in a continuing manner, rather than merely executed with revised input values for rate constants.

Table I. KrF Gain Measurement Data at Constant
Kr Pressure (207 Torr) for various F₂ Pressures

F ₂ Torr	Ar Torr	Measured Gain (cm ⁻¹)	Calculated Gain (cm ⁻¹)
9.0	1860	0.30	0.27
4.5	1860	0.33	0.26
2.2	1655	0.29	0.22

Table II. KrF Gain Measurement Data at Constant
F₂ Pressure (4.5 Torr) for Various Kr Pressures

Kr Torr	Ar Torr	Measured Gain (cm ⁻¹)	Calculated Gain (cm ⁻¹)
105	1965	0.35	0.34
207	1860	0.33	0.26
415	1655	0.27	0.17

Table III. KrF Gain Measurement Data Constant for
 Various Total Pressures as a Function of Kr and F₂ Pressures

Ar Torr	Kr Torr	F ₂ Torr	Measured Gain (cm ⁻¹)
1654	415	9.0	0.24
1654	415	4.5	0.27
1965	105	9.0	0.32
1965	105	4.5	0.35
931	105	4.5	0.31
931	105	2.2	0.30
414	105	2.2	0.24
414	105	1.1	0.18
982	52	4.5	0.25
982	52	2.2	0.28
465	52	2.2	0.19
465	52	1.1	0.15
491	25	2.2	0.16
491	25	1.1	0.13

Therefore, in order to obtain a more powerful analytical capability, a generalized code which itself synthesizes a coupled analysis (as described above) has been developed. This code automatically generates its own subroutines for analysis of the molecular kinetics by translating symbolic reactions into computer-coded equations. Thus, for the most complicated reaction scheme containing an arbitrary number of kinetic collision processes and interacting species, it is possible to construct the complete computer code required with virtually no effort. All that is required is to provide an input deck, arbitrarily long, consisting of pairs of cards, the first containing a reaction, followed by the second containing the forward and reverse rate constants. The syntax for the reactions is very flexible, with a free format that specifies the reaction just as it would normally be written. The content of each reaction is analyzed, and the appearance of each new species is recognized and its name stored. The syntax of each reaction is subjected to numerous tests to detect errors. If the reaction is determined to be acceptable, it is translated into appropriate expressions in the generation of synthesized subroutines. Otherwise, diagnostic comments are produced. Program generation and execution are protected by automatic exit (by input request) if specified error conditions are encountered.

There are several obvious advantages to this approach. First of all, there is simplicity and the minimization of the possibility of error. For example, approximately 70 reactions are currently believed to contribute to the KrF reaction kinetics, and to write subroutines for such a complicated system would not be a simple task. Secondly, the program diagnoses error conditions in the

reaction syntax which may not have been noticeable or which may be overlooked. For example, duplicate reactions are detected (even when written backwards), charge particle and heavy particle conservation is insured, detail balance relations for binary collision processes are enforced, and miscellaneous other error conditions are detected. Secondary electron collision processes are recognized and properly coupled to the electron kinetics analysis, except for the case with no discharge, in which case their rate constants can be defined by input. Finally, the subroutines are constructed in such a way that null operations are completely eliminated (e.g., if no input rate constant is provided, no translation of the corresponding term occurs), and in such a way as to optimize execution efficiency.

For a given system, the required analysis includes the coupled system of equations consisting of 1) the Boltzmann transport equation for the electron energy distribution function to describe electron kinetics, 2) the master equations for the population densities of the electrons, ions, neutrals, excimers, and 3) circuit equations to describe the external driving circuit. It is usually the case that rate constants involved in molecular kinetic reaction schemes can vary over several orders of magnitude, and therefore, the resulting master equations become a "stiff" system of differential equations. Therefore, the approach which has been taken is to employ a multistep integration technique developed by Gear for solution of such equations. This method automatically adjusts the integration step size as the solution proceeds, in such a way that required accuracy conditions are maintained. The Gear method requires subroutines not only for the rates of change of the population densities, dn_i/dt , but also for the Jacobian, $\delta(\dot{n}_i) / \delta n_j$, as a function of time. Because numerical evaluation of the Jacobian is not satisfactory, it is necessary to generate

both such subroutines symbolically in the synthesis section of the program, where the reaction scheme is translated into computer-coded equations.

Figure 3 presents a schematic flow diagram of the present approach. The rate constants initially assumed in the generation of the program can be changed in the subsequent execution, if desired. The main purpose of the rate constants in the initial input deck is to define whether the forward and/or reverse process is to be included, for if a zero rate constant is entered for other than secondary electron collisions, no translation of the forward (or backward) term occurs in the generated subroutines. If correct values of the rate constants are known, they may be entered for once and for all in the original reaction input data deck.

After the kinetics code has been synthesized, initial conditions and experimental parameters are entered and the analysis is executed. The entry of control parameters, experimental parameters, revised rate constants, initial conditions, etc., is quite flexible, and permits the code to be executed for a variety of situations of interest. In pure e-beam excitation cases, rate constants for secondary electron processes default to zero, but can be specified by input if desired. This makes it possible to use the same general code for both discharge and e-beam excitation conditions. The integration of the coupled set of equations over the total pulse length is carried out with the Gear technique which automatically adjusts its step size. However, the total pulse length is divided into 50 subintervals at which time the electron kinetics are updated, and a variety of output options can be specified. Sample output from a typical run is presented below, where comparison with experimental data is made.

GENERALIZED SYNTHESIS LASER KINETICS CODE

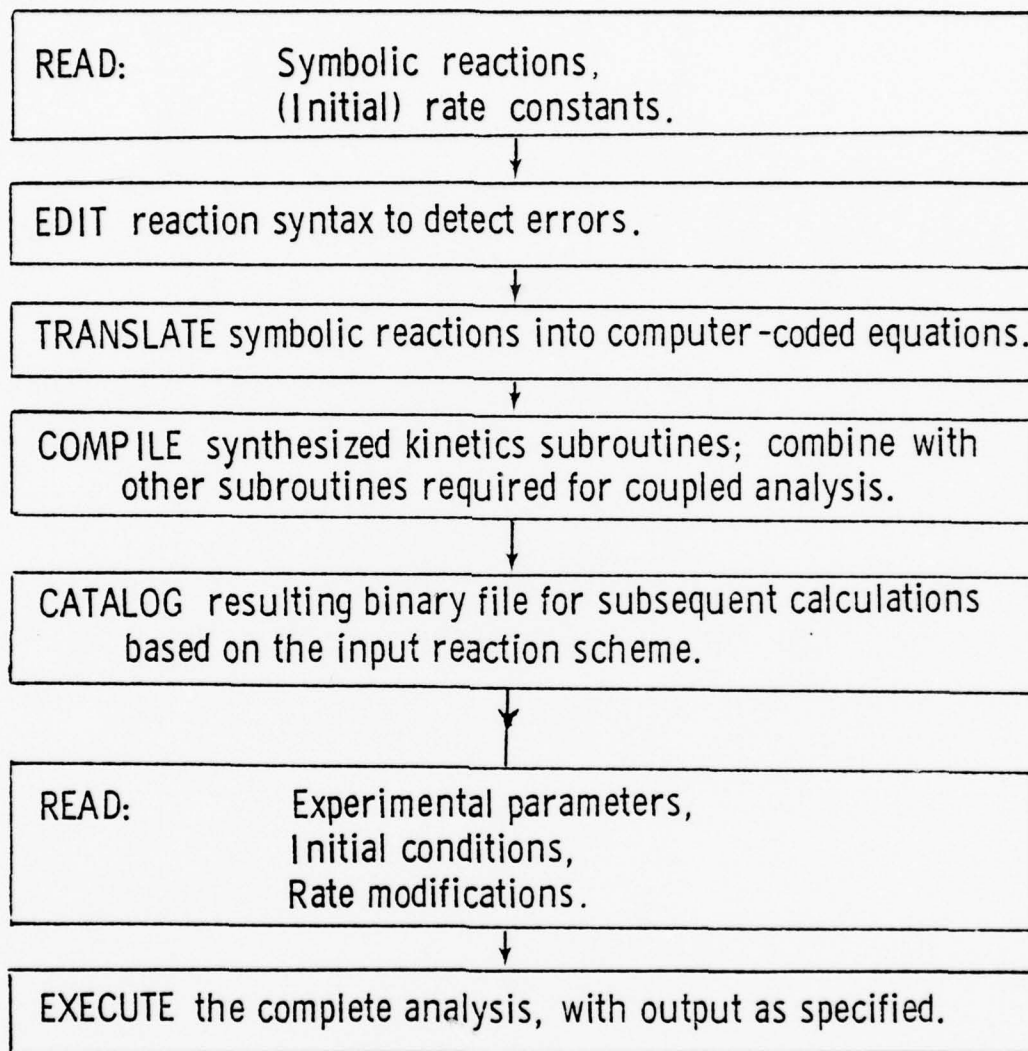


Figure 3 Laser Kinetics Code Flow Diagram

The molecular kinetic processes required for the KrF system are summarized in Figure 4, which is a reproduction of the input data deck which defines the reaction scheme. Figure 5 is a reproduction of output summarizing details and comments about the reaction scheme generated during synthesis of the subroutines for the rates, and Figure 6 presents the results of an edit of the reaction scheme. The KrF kinetic processes include excitation of excited states and ions of Ar and Kr by secondary and high energy e-beam electrons, fluorine attachment, formation and quenching of several excimers, charge transfer, electron and negative F⁻ ion recombination with positive ions, miscellaneous replacement reactions, a variety of energy transfer collisions and quenching processes, spontaneous radiative decay, and stimulated emission and absorption in the active gain medium. Figure 7 illustrates the input data deck for execution of the analysis, and Figure 8 summarizes the modified rate constant input data. Input parameters have been chosen to make comparison with experimental data for an Ar/Kr/F₂ = 1965/105/4.5 Torr mixture pumped with a 500 A/cm² e-beam (nominally 1 MeV). Effective cross sections for electron-beam excitation of excited states and ions of Ar and Kr are taken to be those of Berger and Seltzer, defined by

$$\sigma_{\text{eff}}^{\dagger} \langle u \rangle N_0 / M = 1.4 \text{ MeV cm}^2 / \text{g}$$

where $\langle u \rangle \sim 26$ eV is the average energy loss in an ionizing collision, $N_0 = 6 \times 10^{23}$ is Avogadro's number, and M is the molecular weight of the gas. (The effective cross section for excited states is taken to be a factor of 3.5 smaller.) The stimulated emission cross section for KrF* has been taken to be

$$\sigma = \frac{\lambda^2}{8 \pi c \tau \Delta \bar{\nu}} \sim 2.0 \times 10^{-16} \text{ cm}^2$$

SUMMARY OF CARD IMAGES FOR INPUT DATA DECK

CARD NO.	1	2	3	4	5	6	7	8
41	1234567890123456789012345678901234567890123456789012345678901234567890							
42	3.2E-10	• E	• KR*	• KR				
43	4.00 E-08	• E	• AR*	• AR				
44	4.00 E-08	• E	• AR*	• AR				
45	4.00 E-08	• E	• AR*	• AR				
46	1.00 E-10	• E	• AR2*	• M				
47	1.00 E-10	• E	• AR2*	• M				
48	1.0E-32	• KR	• M	• ARKR*	• M			
49	1.0E-32	• KR	• M	• ARKR*	• M			
50	1.0E-32	• KR	• M	• ARKR*	• M			
51	5.5E-32	• KR	• M	• ARKR*	• M			
52	1.0E-32	• KR	• M	• ARKR*	• M			
53	1.0E-32	• KR	• M	• ARKR*	• M			
54	1.0E-32	• KR	• M	• ARKR*	• M			
55	1.00 E-10	• F	• ARF*	• AR				
56	1.0E-06	• F	• ARF*	• AR				
57	1.0E-06	• F	• ARF*	• AR				
58	1.0E-06	• F	• ARF*	• AR				
59	1.0E-06	• F	• ARF*	• AR				
60	1.0E-06	• F	• ARF*	• AR				
61	1.0E-06	• F	• ARF*	• AR				
62	1.0E-06	• F	• ARF*	• AR				
63	1.0E-06	• F	• ARF*	• AR				
64	1.0E-06	• F	• ARF*	• AR				
65	1.0E-06	• F	• ARF*	• AR				
66	1.0E-06	• F	• ARF*	• AR				
67	1.0E-06	• F	• ARF*	• AR				
68	1.0E-06	• F	• ARF*	• AR				
69	1.0E-06	• F	• ARF*	• AR				
70	1.0E-06	• F	• ARF*	• AR				
71	1.0E-06	• F	• ARF*	• AR				
72	7.20 E-10	• F2	• ARF*	• F				
73	7.20 E-10	• F2	• ARF*	• F				
74	7.50 E-10	• F2	• ARF*	• F				
75	7.50 E-10	• F2	• ARF*	• F				
76	6.20 E-12	• M	• ARKR*	• M				
77	6.20 E-12	• M	• ARKR*	• M				
78	4.00 E-33	• KR	• AR	• AR	• KR*			
79	4.00 E-33	• KR	• AR	• AR	• KR*			
80	4.00 E-33	• KR	• AR	• AR	• KR*			

BOHME ET AL, J. CHEM. PHYS. 52, 5094 (1970)
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 HILL, GUTCHECK, HUESTIS, ET AL, SRI REPORT, 1974.
 HUGHES LASL ASPEN 9/76
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 VELAZCO, KULTS, SETSER, JCP 65, 3469 (1976)
 VELAZCO, KULTS, SETSER, JCP 65, 3469 (1976)
 PIPER, SETSER, CLYNE, JCP 63, 4018 (1975)
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Figure 4 (Continued)

SUMMARY OF CARD IMAGES FOR INPUT DATA DECK

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83	...	3.0E-10						
84	...	ARF*	KR	KRF*	AR			
85	...	1.50 E-10						
86	...	AR2*	F	ARF*	AR			
87	...	3.0E-10						
88	...	KR2*	F	KRF*	KR			
89	...	3.0E-10						
90	...	AR2*	F2	AR2F*	F			
91	...	2.50 E-10						
92	...	ARKR*	F2	KRF*	AR	F		
93	...	6.00 E-10						
94	...	ARKR*	F2	ARKRF*	F			
95	...	3.0E-10						
96	...	KR2*	F2	KR2F*	F			
97	...	3.00 E-10						
98	...	AR2F*	F2	AR	AR	F	F2	
99	...	1.00 E-09						
100	...	ARKRF*	F2	AR	KR	F	F2	
101	...	1.00 E-09						
102	...	KR2F*	F2	KR	KR	F	F2	
103	...	1.00 E-09						
104	...	KRF*	KR	AR	KR2F*	AR		
105	...	2.00 E-33						
106	...	ARF*	AR	AR	AR2F*	AR		
107	...	2.00 E-33						
108	...	ARKRF*	KR	KR2F*	AR			
109	...	1.00 E-10						
110	...	KRF*	F2	KR	F	F2		
111	...	1.00 E-09						
112	...	ARF*	F2	AR	F	F2		
113	...	1.00 E-09						
114	...	AR2F*	KR	KRF*	AR	AR		
115	...	1.0E-10						
116	...	AR*	M	AR*	M			
117	...	1.00 E-10						
118	...	KR*	M	KR*	M			
119	...	1.00 E-10						
120	...	ARF*	AR	F				

Figure 4 (Continued)

SUMMARY OF CARD IMAGES FOR INPUT DATA DECK

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125	3.0E*06						
126	KR2*	KR	*	KR			
127	3.30 E 06						
128	AR2F*	AR	*	AR	*	F	
129	2.00 E 08						
130	ARKRF*	AR	*	KR	*	F	
131	5.00 E 07						
132	KR2F*	KR	*	KR	*	F	
133	6.70 E 07						
134	KRF*	KR	*	F	*	MNU	
135	1.60 E 08						
136	KRF*	RAD	*	KR	*	F	*
137	2.50 E-16						
138	F2	RAD	*	F	*	F	
139	1.50 E-20						
140	F	RAD	*	F	*	E	
141	5.40 E-18						
142	AR2(1)*	RAD	*	AR	*	AR(1*)	
143	1.50 E-17						
144	KR2(1)*	RAD	*	KR	*	KR(1*)	
145	1.00 E-17						

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Figure 4 (Continued)

SUMMARY OF INPUT REACTIONS AND RATE CONSTANTS (SEC-1, CH3/SEC, CM6/SEC, ... OR CM2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

I	REACTION(I) (IGNORED REACTIONS ARE NOT NUMBERED)	RATE CONSTANTS		RATE REFERENCES AND/OR COMMENTS
		KF(I)	KR(I)	
1	AR • E • AR • E	(COMPUTED)	(COMPUTED)	SCHAPER, SCHEIBNER, BEITR. AUS PLASMA PHYS. 9, 45 FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE RATE IS OBTAINED FROM E- KINETICS ANALYSIS
2	KR • E • XR • E	(COMPUTED)	(COMPUTED)	SCHAPER, SCHEIBNER, BEITR. AUS PLASMA PHYS. 9, 45 FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE RATE IS OBTAINED FROM E- KINETICS ANALYSIS
3	KR • E • KR • E	(COMPUTED)	(COMPUTED)	60.E-16 CM2 AT 1.6 EV THRESHOLD ASSUMED. FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE RATE IS OBTAINED FROM E- KINETICS ANALYSIS
4	AR • E • AR • E	(COMPUTED)	(COMPUTED)	60.E-16 CM2 AT 2 EV THRESHOLD ASSUMED. FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE RATE IS OBTAINED FROM E- KINETICS ANALYSIS
5	AR • E • AR(•) • E • E	(COMPUTED)	(COMPUTED)	7.E-16 CM2 AT 4.2 EV THRESHOLD ASSUMED. FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE REACTION IS IGNORED -- KR = 0.
6	KR • E • KR(•) • E • E	(COMPUTED)	(COMPUTED)	10.E-16 CM2 AT 4.0 EV THRESHOLD ASSUMED. FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE REACTION IS IGNORED -- KR = 0.
7	F2 • E • F • F-	(COMPUTED)	(COMPUTED)	HOFLAND, AEROSPACE CORP. FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE REACTION IS IGNORED -- KR = 0.
8	AR2 • E • AR • AR • E	1.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
9	KR2 • E • KR • KR • E	1.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
10	AR • HE- • AR • HE-	3.3000E-18	3.3000E-18	
11	AR • HE- • AR(•) • HE- • E	1.2000E-17		
12	KR • HE- • KR • HE-	6.0000E-18	6.0000E-18	3 X BERGER, SELTZER; STOP = 1.7 MEVCM2/GM AT 300 K REVERSE REACTION IS IGNORED -- KR = 0.
13	KR • HE- • KR(•) • HE- • E	2.4000E-17		REVERSE REACTION IS IGNORED -- KR = 0.

Figure 5

SUMMARY OF INPUT: REACTIONS AND RATE CONSTANTS (SEC-1, CN3/SEC, CM6/SEC, ... OR CM2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

I	REACTION(I) (IGNORED REACTIONS ARE NOT NUMBERED)	RATE CONSTANTS KF(I)	RATE CONSTANTS KR(I)	RATE REFERENCES AND/OR COMMENTS
14	AR(+) * AR * M * AR2(+) * M	2.5000E-31		REVERSE REACTION IS IGNORED -- KR = 0.
15	AR(+) * KR * M * ARKR(+) * M	2.5000E-31		REVERSE REACTION IS IGNORED -- KR = 0.
16	KR(+) * KR * M * KR2(+) * M	3.0000E-31		REVERSE REACTION IS IGNORED -- KR = 0.
17	KR(+) * AR * M * ARKR(+) * M	1.0000E-31		REVERSE REACTION IS IGNORED -- KR = 0.
18	AR(+) * KR * AR * KR(+) * M	3.0000E-11	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
19	AR2(+) * KR * KR(+) * AR * AR	7.5000E-10		BOHME ET AL, J. CHEM. PHYS. 52, 5094 (1970) REVERSE REACTION IS IGNORED -- KR = 0.
20	ARKR(+) * KR * KR2(+) * AR	3.2000E-10	X E(-E/KT)	BOHME ET AL, J. CHEM. PHYS. 52, 5094 (1970) REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
21	KR2(+) * E * KR * KR	4.0000E-08		MEHR, BIONDI (TE = 30,000 K) REVERSE REACTION IS IGNORED -- KR = 0.
22	AR2(+) * E * AR * AR	4.0000E-08		MEHR, BIONDI (TE = 30,000 K) REVERSE REACTION IS IGNORED -- KR = 0.
23	AR * AR * AR * M * AR2 * M	1.0000E-32		HILL, GUTCHECK, HUESTIS, ET AL, SRI REPORT, 1974. REVERSE REACTION IS IGNORED -- KR = 0.
24	AR * KR * M * ARKR * M	1.0000E-32		REVERSE REACTION IS IGNORED -- KR = 0.
25	KR * KR * M * KR2 * M	5.5000E-32		HUGHES LASL ASPEN 9/76 REVERSE REACTION IS IGNORED -- KR = 0.
26	KR * AR * M * ARKR * M	1.0000E-32		REVERSE REACTION IS IGNORED -- KR = 0.
27	ARKR * KR * KR2 * AR	1.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
28	AR2(+) * F- * ARF * AR	1.0000E-06	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
29	AR2(+) * F- * AR2F*	1.0000E-06		REVERSE REACTION IS IGNORED -- KR = 0.
30	AR(+) * F- * ARF*	1.0000E-06		REVERSE REACTION IS IGNORED -- KR = 0.

Figure 5 (Continued)

SUMMARY OF INPUT: REACTIONS AND RATE CONSTANTS (SEC-1, CM3/SEC, CM6/SEC, . . . OR CM2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

I	REACTION(I) (IGNORED REACTIONS ARE NOT NUMBERED)	RATE CONSTANTS KF(I)	RATE CONSTANTS KR(I)	RATE REFERENCES AND/OR COMMENTS
31	KR2(*) * F -> KRF * * KR	1.0000E-06	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
32	KR2(*) * F -> KR2F*	1.0000E-06		REVERSE REACTION IS IGNORED -- KR = 0.
33	KR(*) * F -> KRF*	1.0000E-06		REVERSE REACTION IS IGNORED -- KR = 0.
34	ARKR(*) * F -> KRF * * AR	1.0000E-06	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
35	ARKR(*) * F -> ARKRF*	1.0000E-06		REVERSE REACTION IS IGNORED -- KR = 0.
36	KR * * F2 -> KRF * * F	7.2000E-10	X E(-E/KT)	VELAZCO, KOLTS, SETSER, JCP 65, 3469 (1976) REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
37	AR * * F2 -> ARF * * F	7.5000E-10	X E(-E/KT)	VELAZCO, KOLTS, SETSER, JCP 65, 3469 (1976) REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
38	AR * * KR -> AR * * KR*	6.2000E-12	X E(-E/KT)	PIPER, SETSER, CLYNE, JCP 63, 4018 (1975) REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
39	AR * KRF * * M -> ARKRF * * M	4.0000E-33		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
40	AR2 * * KR -> AR * * KR*	8.0000E-11		ZAMIR (PRIV. COMMUN. TO SRI) REVERSE REACTION IS IGNORED -- KR = 0.
41	AR2 * * AR2* -> AR2(*) * AR * AR * E	3.0000E-10		REVERSE REACTION IS IGNORED -- KR = 0.
42	ARF * * KR -> KRF * * AR	1.5000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
43	AR2 * * F -> ARF * * AR	3.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
44	KR2 * * F -> KRF * * KR	3.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
45	AR2 * * F2 -> AR2F * * F	2.5000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
46	ARKR * * F2 -> KRF * * AR * F	6.0000E-10		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
47	ARKR * * F2 -> ARKRF * * F	3.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.

Figure 5 (Continued)

SUMMARY OF INPUT: REACTIONS AND RATE CONSTANTS (SEC-1), CM3/SEC, CM6/SEC, ... OR CM2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

I	REACTION(I) (IGNORED REACTIONS ARE NOT NUMBERED)	RATE CONSTANTS KF (I)	RATE CONSTANTS KR (I)	RATE REFERENCES AND/OR COMMENTS
48	KR2* * F2 * KR2F* * F	3.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
49	AR2F* * F2 * AR * AH * F * F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
50	ARKRF* * F2 * AR * KH * F * F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
51	KR2F* * F2 * KR * KR * F * F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
52	KRF* * KR * AR * KR2F* * AR	2.0000E-13		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
53	ARF* * AR * AR * AR2F* * AR	2.0000E-33		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
54	ARKRF* * KR * KH2F* * AR	1.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
55	KRF* * F2 * KR * F * F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
56	ARF* * F2 * AR * F * F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
57	AR2F* * KR * KH2F* * AR * AR	1.0000E-10		REVERSE REACTION IS IGNORED -- KR = 0.
58	AR* * M * AR* * M	1.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
59	KR* * M * KR* * M	1.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
60	ARF* * AR * F	3.3000E-07		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
61	AR2* * AR * AR	3.8000E-06		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
62	ARKR* * AR * KR	3.0000E-06		REVERSE REACTION IS IGNORED -- KR = 0.

Figure 5 (Continued)

SUMMARY OF INPUT REACTIONS AND RATE CONSTANTS (SEC-1), CM3/SEC, CM6/SEC, . . . OR CM2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

I	REACTION(I)	RATE CONSTANTS KF(I)	KR(I)	RATE REFERENCES AND/OR COMMENTS
63	KR2 * KR * KR	3.3000E+06		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
64	AR2F * AR * AR * F	2.0000E+08		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
65	ARKRF * AR * KR * F	5.0000E+07		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
66	KR2F * KR * KR * F	6.7000E+07		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
67	KRF * KR * F * HNU	1.6000E+08		HAY, DUNNING (6 NS LIFETIME) REVERSE REACTION IS IGNORED -- KR = 0. NO REVERSE REACTION ALLOWED FOR RADIATIVE DECAY.
68	KRF * RAD * KR * F * RAD	2.5000E-16		LASER TRANSITION REVERSE REACTION IS IGNORED -- KR = 0.
69	F2 * RAD * F * F	1.5000E-20		REVERSE REACTION IS IGNORED -- KR = 0.
70	F * RAD * F * E	5.4000E-18		A. MANDL, PHYS REV A3, 251 (1971) REVERSE REACTION IS IGNORED -- KR = 0.
71	AR2(+) * RAD * AR * AR(*)	1.5000E-17		STEVENS (PARK CITY CONFERENCE) REVERSE REACTION IS IGNORED -- KR = 0.
72	KR2(+) * RAD * KR * KR(*)	1.0000E-17		ESTIMATED, BUT NOT CURRENTLY UNDERSTOOD REVERSE REACTION IS IGNORED -- KR = 0.

OF 72 INPUT REACTIONS SCANNED, 72 WERE RETAINED (MAXIMUM ALLOWED = 200) AND 0 WERE IGNORED FOR REASONS ITEMIZED IN THE TABLE. OF THOSE RETAINED, 7 REQUIRE RATES FROM AN E- KINETICS ANALYSIS. 24 SEPARATE SPECIES WERE ENCOUNTERED (MAXIMUM ALLOWED = 30).

Figure 5 (Continued)

SUMMARY OF REACTIONS FOR WHICH EACH SPECIES OCCURS: NIYPE = 24
 (THIS EDIT PERMITS RAPID DELETION OF ANY SPECIES FROM THE KINETIC SYSTEM)

I	GAS(I)	REACTIONS CONTAINING GAS(I)
1	RAD	68, 69, 70, 71, 72,
2	E(-)	1, 2, 3, 4, 5, 6, 7, 8, 9, 11, 13, 21, 22, 41, 70,
3	AR	1, 8, 10, 11, 14, 17, 18, 19, 20, 22, 23, 26, 27, 28, 34, 38, 39, 40, 41, 42, 43, 46, 49, 50, 52, 53, 54, 56, 57, 60, 61, 62, 64, 65, 71,
4	AR*	1, 4, 5, 10, 22, 23, 24, 37, 38, 58,
5	KR	2, 9, 12, 13, 15, 16, 18, 19, 20, 21, 24, 25, 27, 31, 38, 40, 42, 44, 50, 51, 52, 54, 55, 57, 62, 63, 65, 66, 67, 68, 72,
6	KR*	2, 3, 6, 12, 21, 25, 26, 36, 38, 40, 59,
7	KR**	3, 59,
8	AR**	4, 58,
9	AR(+)	5, 11, 14, 15, 18, 30, 71,
10	KR(+)	6, 13, 16, 17, 18, 19, 33, 72,
11	F2	7, 36, 37, 45, 46, 47, 48, 49, 50, 51, 55, 56, 69,
12	F	7, 36, 37, 43, 44, 45, 46, 47, 48, 49, 50, 51, 55, 56, 60, 64, 65, 66, 67, 68, 69, 70,
13	F-	7, 28, 29, 30, 31, 32, 33, 34, 35, 70,
14	AR2*	8, 23, 40, 41, 43, 45, 61,
15	KR2*	9, 25, 27, 44, 48, 63,
16	AR2(+)	14, 19, 22, 28, 29, 41, 71,
17	ARKR(+)	15, 17, 20, 34, 35,
18	KR2(+)	16, 20, 21, 31, 32, 72,
19	ARKR*	24, 26, 27, 46, 47, 62,

Figure 6

SUMMARY OF REACTIONS FOR WHICH EACH SPECIES OCCURS: NTYPE = 24
 (THIS EDIT PERHAPS RAPID DELETION OF ANY SPECIES FROM THE KINETIC SYSTEM)

I	GAS(I)	REACTIONS CONTAINING GAS(I)
20	ARF*	28, 30, 37, 42, 43, 53, 56, 60,
21	AR2F*	29, 45, 49, 53, 57, 64,
22	KRF*	31, 33, 34, 36, 39, 42, 44, 46, 52, 55, 57, 67, 68,
23	KR2F*	32, 48, 51, 52, 54, 66,
24	ARKRF*	35, 39, 47, 50, 54, 65,

Figure 6 (Continued)

SUMMARY OF CARD IMAGES FOR INPUT DATA DECK

CARD NO. 1 2 3 4 5 6 7 8
 123456789012345678901234567890123456789012345678901234567890

1 \$CONTROL
 2 \$PARAM
 3 \$OPTICAL \$
 4 \$CIRCUIT
 5
 6
 7
 8 \$SHATES
 9
 10
 11
 12
 13
 14
 15
 16 \$AR
 17 \$KR
 18 \$F2
 19 \$AR*
 20 \$AR*
 21 \$AR(*)
 22 \$KR*
 23 \$KR*
 24 \$KR(*)
 25 \$F-
 26 \$AR*
 27 \$KR*
 28 \$AR2*
 29 \$KR2*
 30 \$AR2(*)
 31 \$KR2(*)
 32 \$AR2F*
 33 \$AR2F*
 34 \$AR2F(*)
 35 \$KR2F*
 36 \$AR2F*

IO(16) = 5.0E-05, LIMIT=40\$
 IPULSE = 50.E-09\$
 TR = 15.0.
 TF = 10.
 ENERGY = 1000.*
 BEAM = 500.\$
 KF(7) = 1.0E-07.
 KF(23) = 2.0E-07.
 KF(22) = 7.0E-07.
 KF(68) = 2.E-16.
 KF(10) = 9.0E-19.
 KF(11) = 3.E-18.
 KF(12) = 1.6E-18.
 KF(13) = 6.6E-18\$
 1965.
 105.
 4.5
 11.5
 13.5
 15.8
 9.9
 11.5
 14.4
 .01
 6.5
 5.0
 9.5
 8.2
 13.0
 11.8
 5.0
 4.0
 12.4
 3.0
 8.8

KR(10) = 9.0E-19.
 KR(12) = 1.6E-18.
 40.
 84.
 38.

1234567890123456789012345678901234567890123456789012345678901234567890

Figure 7

SUMMARY OF UPDATED RATES FOR INPUT REACTION SCHEME OF SYNTHETIC KINETICS CODE GENERATED
 BY WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY CENTER, HAWTHORNE, CALIFORNIA

I	REACTION(I)	KF(I)	KR(I)	REFERENCES OR COMMENTS
1	AR * E * AR * E			***** THE ORIGINAL RATE HAS BEEN MODIFIED *****
2	KR * E * KR * E			***** THE ORIGINAL RATE HAS BEEN MODIFIED *****
3	KR * E * KR * * E			***** THE ORIGINAL RATE HAS BEEN MODIFIED *****
4	AR * E * AR * * E			***** THE ORIGINAL RATE HAS BEEN MODIFIED *****
5	AR * E * AR(*) * E * E			***** THE ORIGINAL RATE HAS BEEN MODIFIED *****
6	KR * E * KR(*) * E * E			***** THE ORIGINAL RATE HAS BEEN MODIFIED *****
7	F2 * E * F * F~	1.0000E-07		***** THE ORIGINAL RATE HAS BEEN MODIFIED *****
8	AR2 * E * AR * AR * E	1.0000E-07		
9	KR2 * E * KR * KR * E	1.0000E-07		
10	AR * HE- * AR * HE-	9.0000E-19	9.0000E-19	***** THE ORIGINAL RATE HAS BEEN MODIFIED *****
11	AR * HE- * AR(*) * HE- * E	3.3000E-18		***** THE ORIGINAL RATE HAS BEEN MODIFIED *****
12	KR * HE- * KR * HE-	1.6000E-18	1.6000E-18	***** THE ORIGINAL RATE HAS BEEN MODIFIED *****
13	KR * HE- * KR(*) * HE- * E	6.6000E-18		***** THE ORIGINAL RATE HAS BEEN MODIFIED *****
14	AR(*) * AH * M * AR2(*) * M	2.5000E-31		
15	AR(*) * KR * M * AHKR(*) * M	2.5000E-31		
16	KR(*) * KR * M * KR2(*) * M	3.0000E-31		
17	KR(*) * AR * M * AKKR(*) * M	1.0000E-31		
18	AR(*) * KR * AH * KR(*)	3.0000E-11	X E(-E/KT)	
19	AR2(*) * KR * KR(*) * AR * AR	7.5000E-10		BOHME ET AL, J. CHEM. PHYS. 52, 5094 (1970)
20	AHKR(*) * KR * KR2(*) * AH	3.2000E-10	X E(-E/KT)	BOHME ET AL, J. CHEM. PHYS. 52, 5094 (1970)
21	KR2(*) * E * KR * KR	2.0000E-07		***** THE ORIGINAL RATE HAS BEEN MODIFIED *****
22	AR2(*) * E * AR * AR	7.0000E-07		***** THE ORIGINAL RATE HAS BEEN MODIFIED *****
23	AR * AR * M * AR2 * M	1.0000E-32		HILL, GUTCHECK, HUESTIS, ET AL, SRI REPORT, 1974.
24	AR * KR * M * AKKR * M	1.0000E-32		
25	KR * KR * M * KR2 * M	5.5000E-32		HUGHES LASL ASPEN 9/76

* THE ORIGINAL RATE CONSTANT(S) HAVE BEEN MODIFIED

Figure 8

SUMMARY OF UPDATED RATES FOR INPUT REACTION SCHEME OF SYNTHETIC KINETICS CODE GENERATED
BY WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY CENTER, HAWTHORNE, CALIFORNIA

I	REACTION(I)	KF(I)	KR(I)	REFERENCES OR COMMENTS
26	KR* + AR + M + ARK* + H	1.0000E-12		
27	ARKR* + KR + KR2* + AR	1.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976
28	AR2(*) + F- + ARF* + AR	1.0000E-06	X E(-E/KT)	
29	AR2(*) + F- + AR2F*	1.0000E-06		
30	AR(*) + F- + ARF*	1.0000E-06		
31	KR2(*) + F- + KRF* + KR	1.0000E-06	X E(-E/KT)	
32	KR2(*) + F- + KR2F*	1.0000E-06		
33	KR(*) + F- + KRF*	1.0000E-06		
34	ARKR(*) + F- + KRF* + AR	1.0000E-06	X E(-E/KT)	
35	ARKR(*) + F- + ARKRF*	1.0000E-06		
36	KR* + F2 + KRF* + F	7.2000E-10	X E(-E/KT)	VELAZCO, KOLTS, SETSER, JCP 65, 3469 (1976)
37	AR* + F2 + ARF* + F	7.5000E-10	X E(-E/KT)	VELAZCO, KOLTS, SETSER, JCP 65, 3469 (1976)
38	AR* + KR + AR + KM*	6.2000E-12	X E(-E/KT)	PIPER, SETSER, CLYNE, JCP 6, 4018 (1975)
39	AR + KRF* + M + ARKRF* + M	4.0000E-33		SRI REPORT NO. MP 76-99, DEC., 1976
40	AR2* + KR + AK + AK + KR*	8.0000E-11		ZAMJR (PRIV. COMMUN. TO SRI)
41	AR2* + AR2* + AR2(*) + AR + AR + E	3.0000E-10		
42	ARF* + KR + KRF* + AR	1.5000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976
43	AR2* + F + ARF* + AR	3.0000E-10	X E(-E/KT)	
44	KR2* + F + KRF* + KR	3.0000E-10	X E(-E/KT)	
45	AR2* + F2 + AR2F* + F	2.5000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976
46	ARKR* + F2 + KRF* + AR + F	6.0000E-10		SRI REPORT NO. MP 76-99, DEC., 1976
47	ARKR* + F2 + ARKRF* + F	3.0000E-10	X E(-E/KT)	
48	KR2* + F2 + KR2F* + F	3.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976
49	AR2F* + F2 + AR + AR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976
50	ARKRF* + F2 + AR + KR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976

Figure 8 (Continued)

SUMMARY OF UPDATED RATES FOR INPUT REACTION SCHEME OF SYNTHETIC KINETICS CODE GENERATED
WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY CENTER, Hawthorne, California

I	REACTION(I)	KF(I)	KR(I)	REFERENCES OR COMMENTS
51	KR2F • F2 • KR • KR • F • F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976
52	KRF • KR • AR • KR2F • AR	2.0000E-33		SRI REPORT NO. MP 76-99, DEC., 1976
53	ARF • AR • AR • AR2F • AR	2.0000E-33		SRI REPORT NO. MP 76-99, DEC., 1976
54	AKRF • KR • KR2F • AR	1.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976
55	KRF • F2 • KR • F • F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976
56	ARF • F2 • AR • F • F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976
57	AR2F • KR • KRF • AR • AR	1.0000E-10		
58	AR • M • AR • M	1.0000E-10	X E(-E/KT)	
59	KR • M • KR • M	1.0000E-10	X E(-E/KT)	
60	ARF • AR • F	3.3000E+07		SRI REPORT NO. MP 76-99, DEC., 1976
61	AR2 • AR • AR	3.8000E+06		SRI REPORT NO. MP 76-99, DEC., 1976
62	ARKR • AR • KR	3.0000E+06		
63	KR2 • KR • KR	3.3000E+06		SRI REPORT NO. MP 76-99, DEC., 1976
64	AR2F • AR • AR • F	2.0000E-08		SRI REPORT NO. MP 76-99, DEC., 1976
65	AKRF • AR • KR • F	5.0000E+07		SRI REPORT NO. MP 76-99, DEC., 1976
66	KR2F • KR • KR • F	6.7000E+07		SRI REPORT NO. MP 76-99, DEC., 1976
67	KRF • KR • F • HNU	1.6000E+08		HAY, DUNNING (6 NS LIFETIME)
68	KRF • RAD • KR • F • RAD	2.0000E-16		***** THE ORIGINAL RATE HAS BEEN MODIFIED *****
69	F2 • RAD • F • F	1.5000E-20		
70	F • RAD • F • E	5.4000E-18		A. MANDL, PHYS REV A3, 251 (1971)
71	AR2(*) • RAD • AR • AR(*)	1.5000E-17		STEVENS (PARK CITY CONFERENCE)
72	KR2(*) • RAD • KR • KR(*)	1.0000E-17		ESTIMATED

* THE ORIGINAL RATE CONSTANT(S) HAVE BEEN MODIFIED

Figure 8 (Continued)

where it has been assumed that $\Delta\tilde{\nu} \sim 600 \text{ cm}^{-1}$, and $\tau \sim 6.7 \text{ ns}$. It should be noted, of course, that comparison of gain predictions with experimental data depend directly upon this cross section. The value assumed, $2.0 \times 10^{-16} \text{ cm}^2$, provides very good agreement with the experimentally measured value. Current estimates of the stimulated emission cross section range from $1.0 - 2.5 \times 10^{-16} \text{ cm}^2$, so the present choice is not unreasonable. The pulse shape of the e-beam was found to be peaked at about 500 A/cm^2 , with a full-width at half maximum of about 20 ns , so a Gaussian shape was used in the analysis as shown in Figure 9. Figure 10 and 11 show the predicted values of laser gain, internal absorption in the medium, and the resulting net gain coefficient. Figure 12 shows results of the analysis for the population densities for the various species included in the excited mixture.

In order to provide some quantitative assessment of the sensitivity of the various reactions included in the kinetic scheme, the computer code generates, according to input requests, tables such as those presented in Figure 13. These tables summarize the numerical value of the contribution each reaction makes (at a given time) to each species in the system, expressed for each species as a percentage of the maximum rate contribution for that species. Those reactions which never contribute more than a specified percentage are flagged with an asterisk, and are summarized at the conclusion of the analysis. Thus, after a variety of calculations have been made for different conditions and parameters, it is possible to determine whether any given reaction may be considered to be unimportant and deleted from the scheme.

For KrF^* , for example, it can be seen from Figure 13 that spontaneous emission, fluorine quenching, ArF^* displacement, ion-ion

recombination, metastable production, and trimer formation of ArKrF^* all contribute. The relative importance of these mechanisms changes in an electric discharge excitation, where there is more metastable production, and less F^- for ion-ion recombination processes. From Figure 13 it is possible to get a quantitative feeling for the importance of each reaction. Figure 14 presents a schematic representation of the principal reactions involved in KrF^* production and loss.

In conclusion, the dominant reactions involved in the krypton fluoride laser operation are identified. The results of the small signal gain measurement agree quite well with those predicted by the code, thereby supporting the proposed reactions and their rate constants. However, uncertainties regarding some of these rates still remain to be resolved. For example, estimates of the stimulated emission cross section, the electron attachment rate for F_2 , and ion-ion recombination rates appear to vary by at least a factor of two. Parameters such as the electron energy deposition profile and the three-body quenching of KrF^* by Ar present even more uncertainty. Some of these rates are expected to be refined in the near future as a result of continuing investigations at several laboratories. These updated rates will be most useful for scaling predictions. However, the basic mechanisms for the KrF laser operation, identified in this investigation, are not expected to change significantly.

E-BEAM CURRENT DENSITY (AMP/CM²) AS A FUNCTION OF TIME

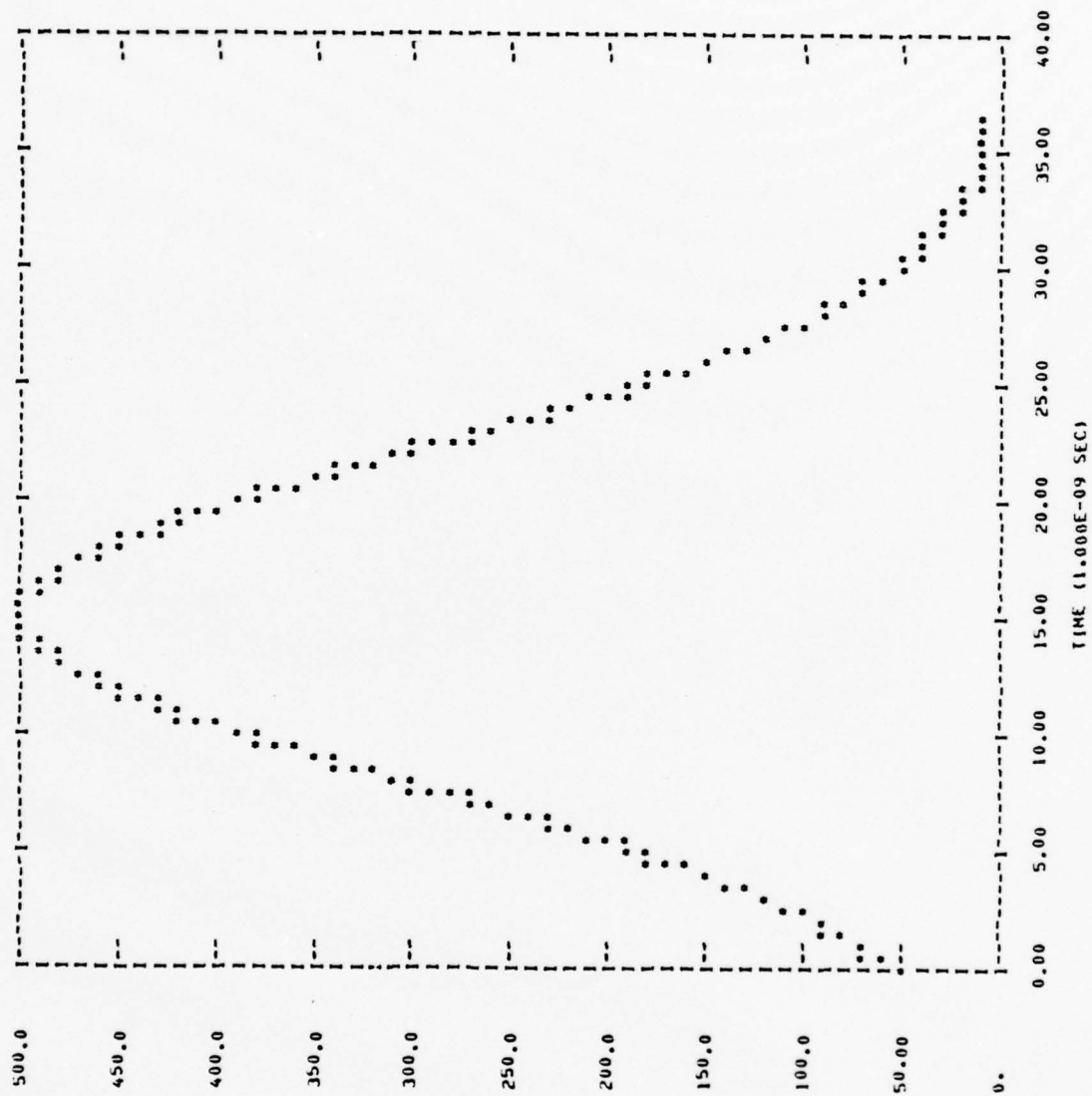


Figure 9

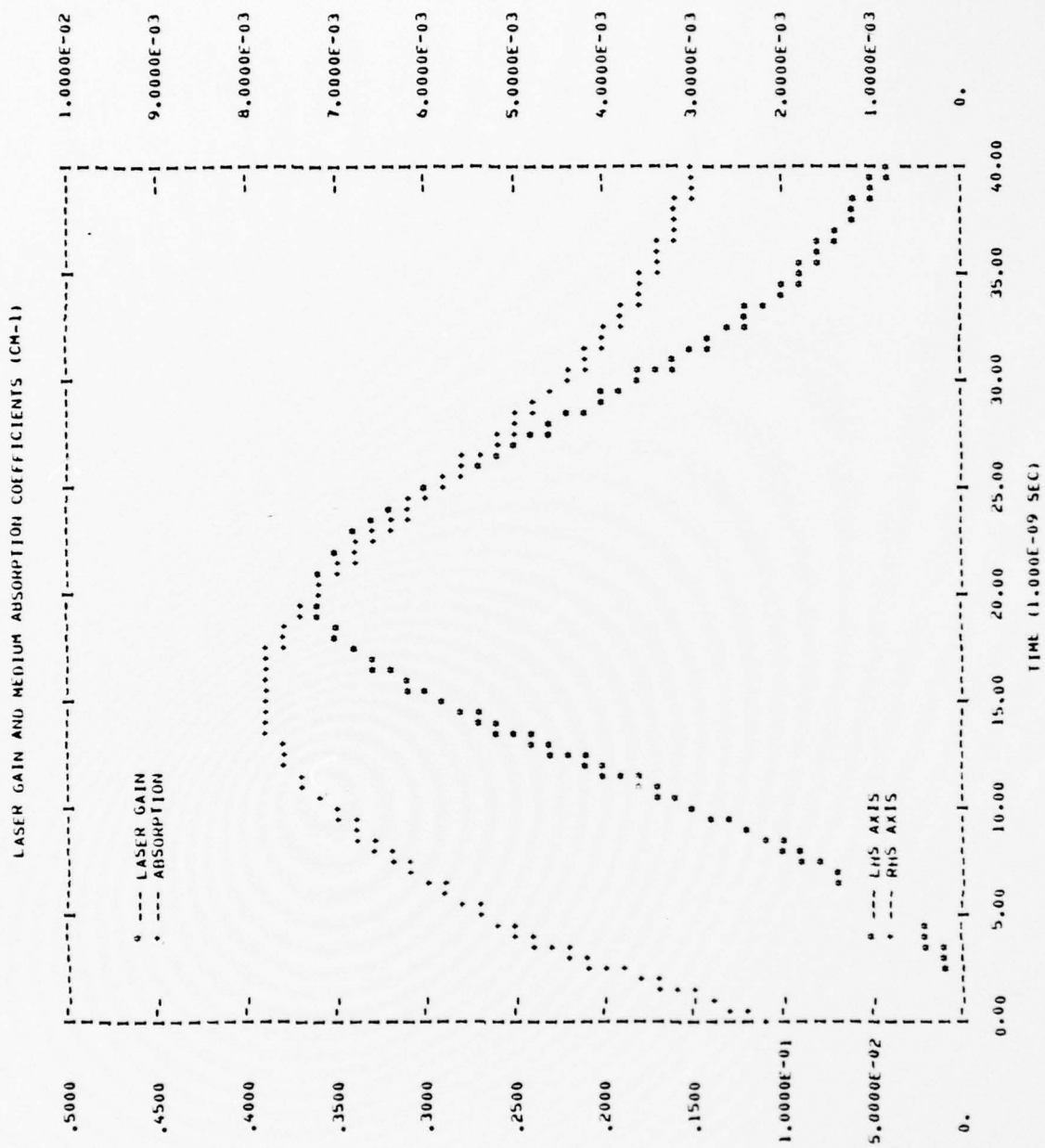


Figure 10

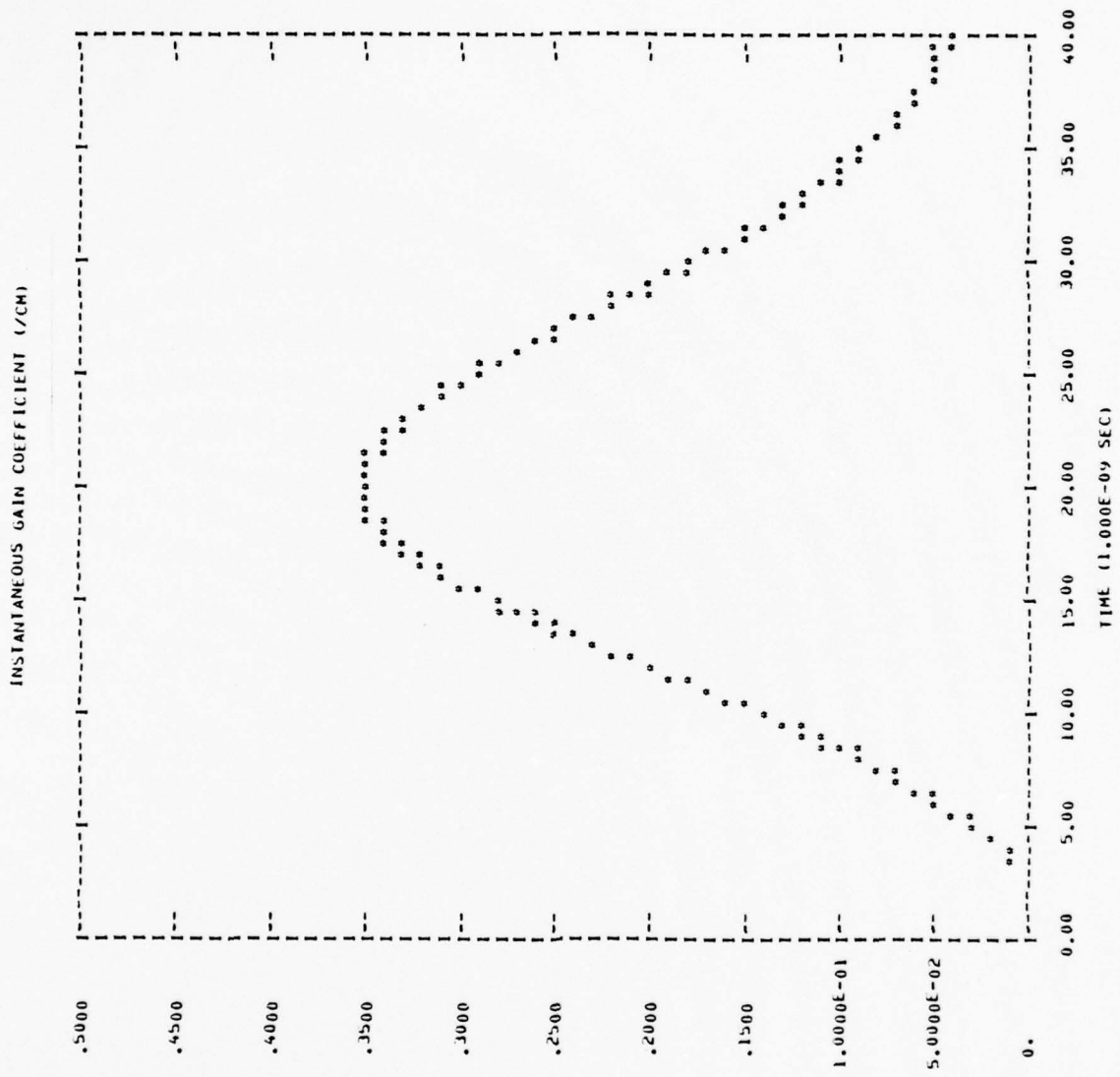


Figure 11

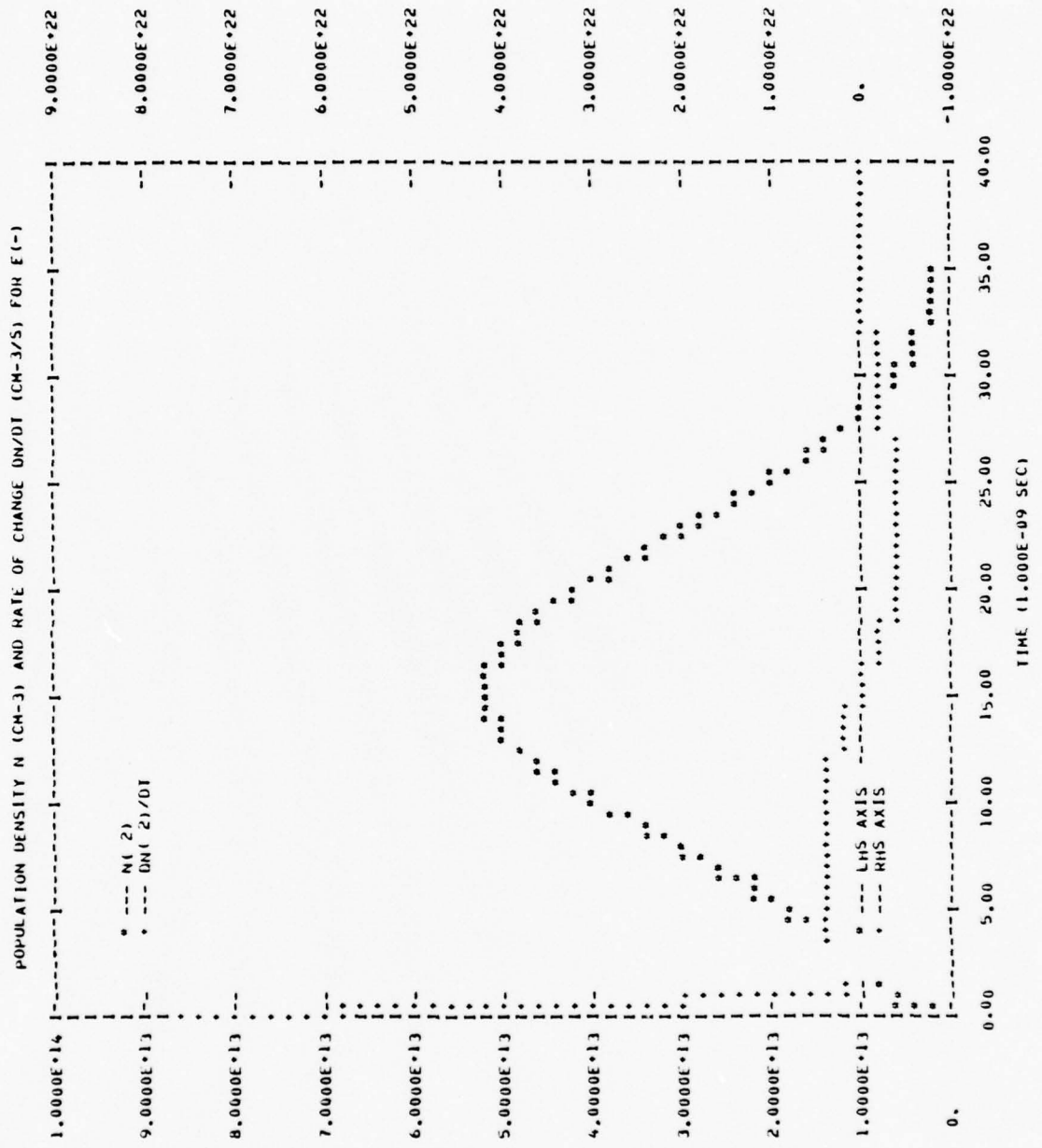


Figure 12

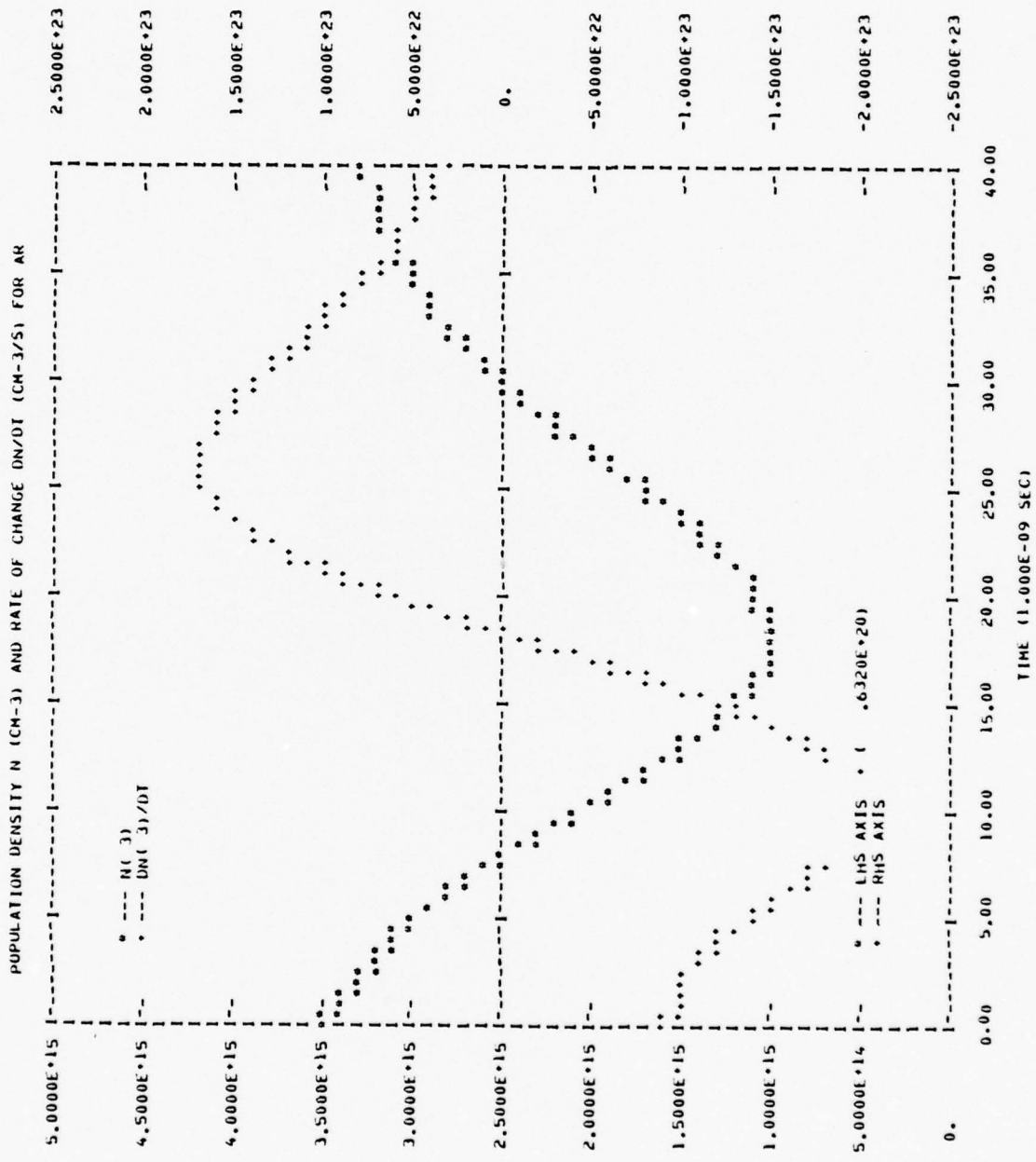


Figure 12 (Continued)

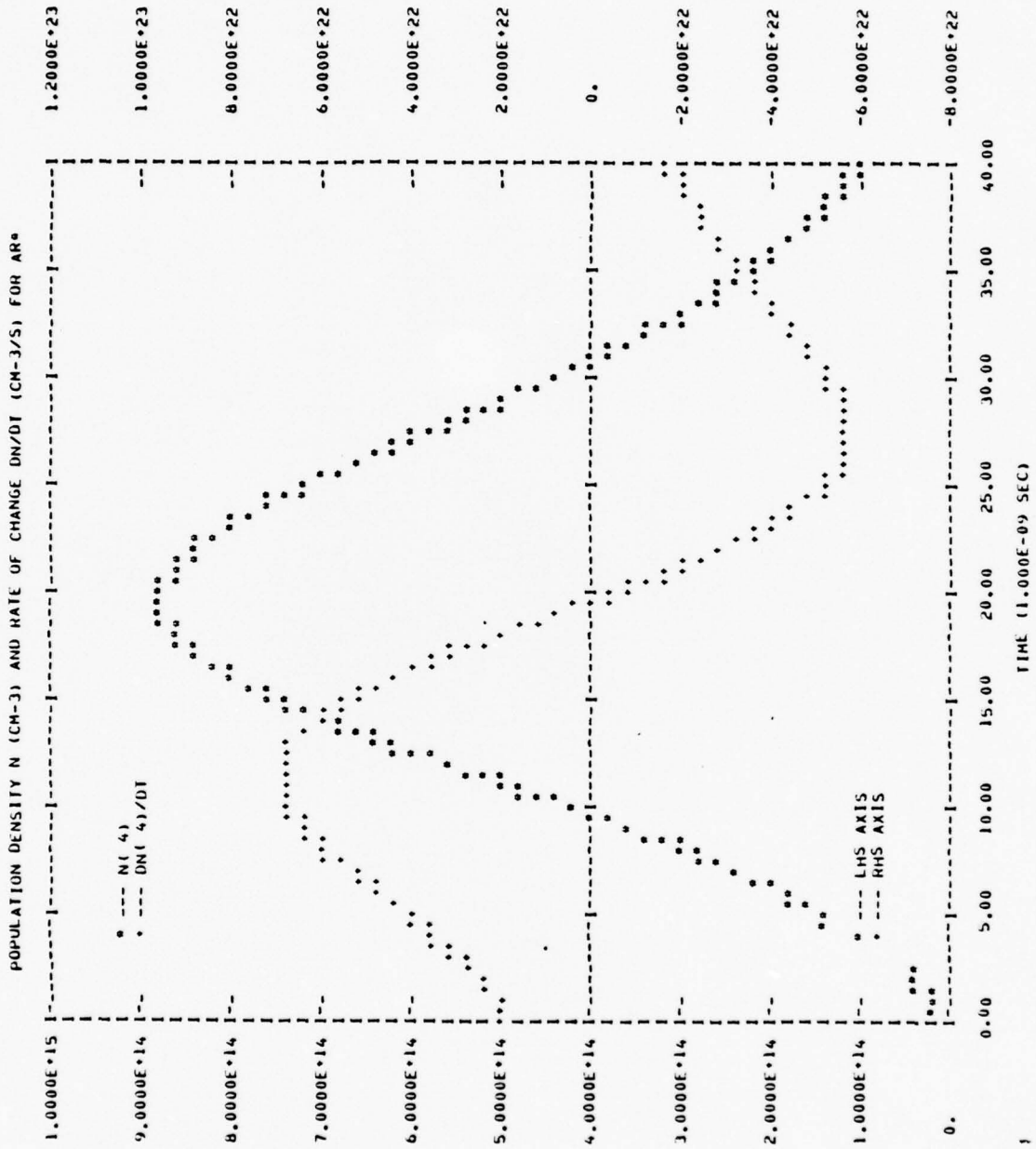


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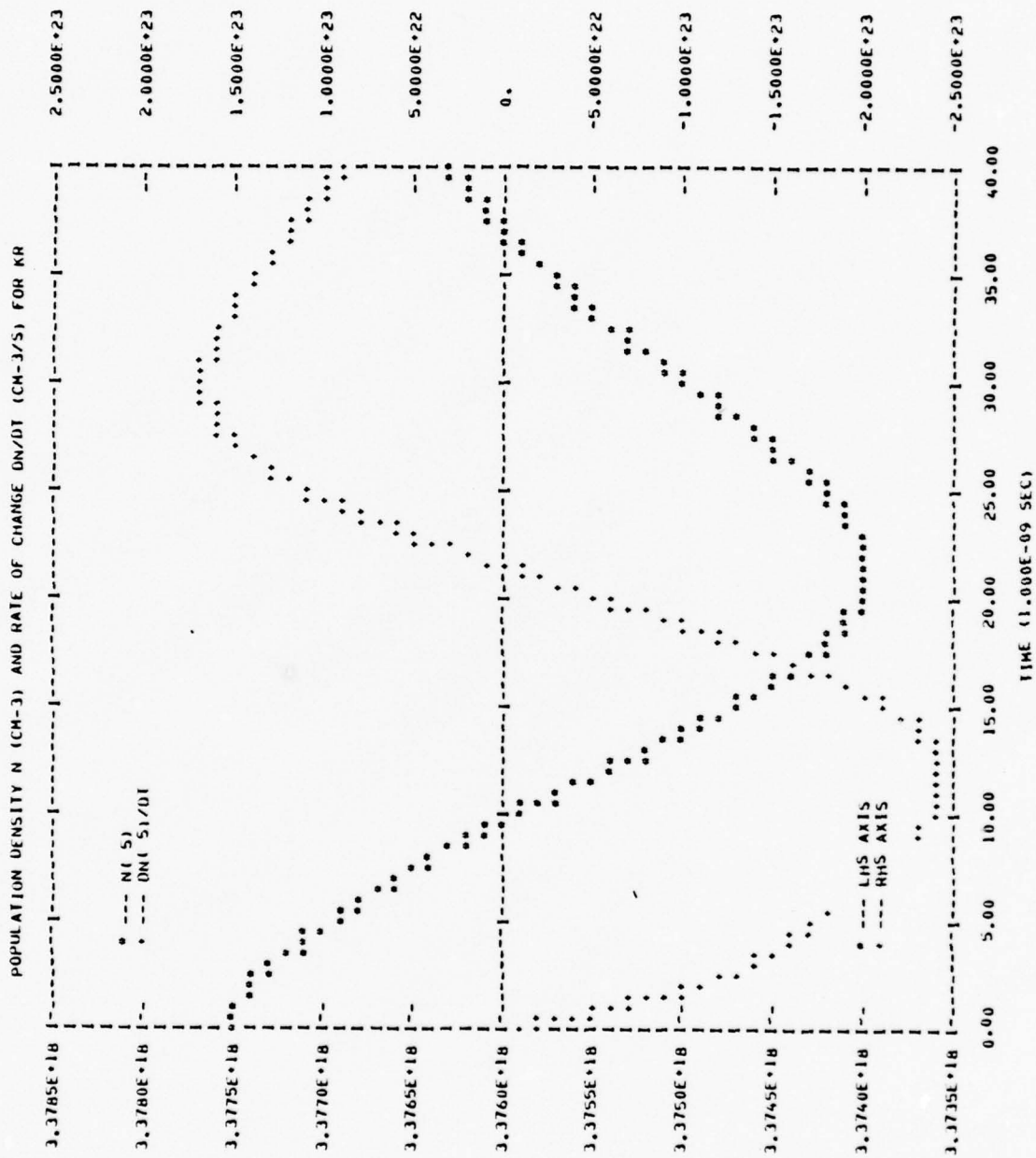


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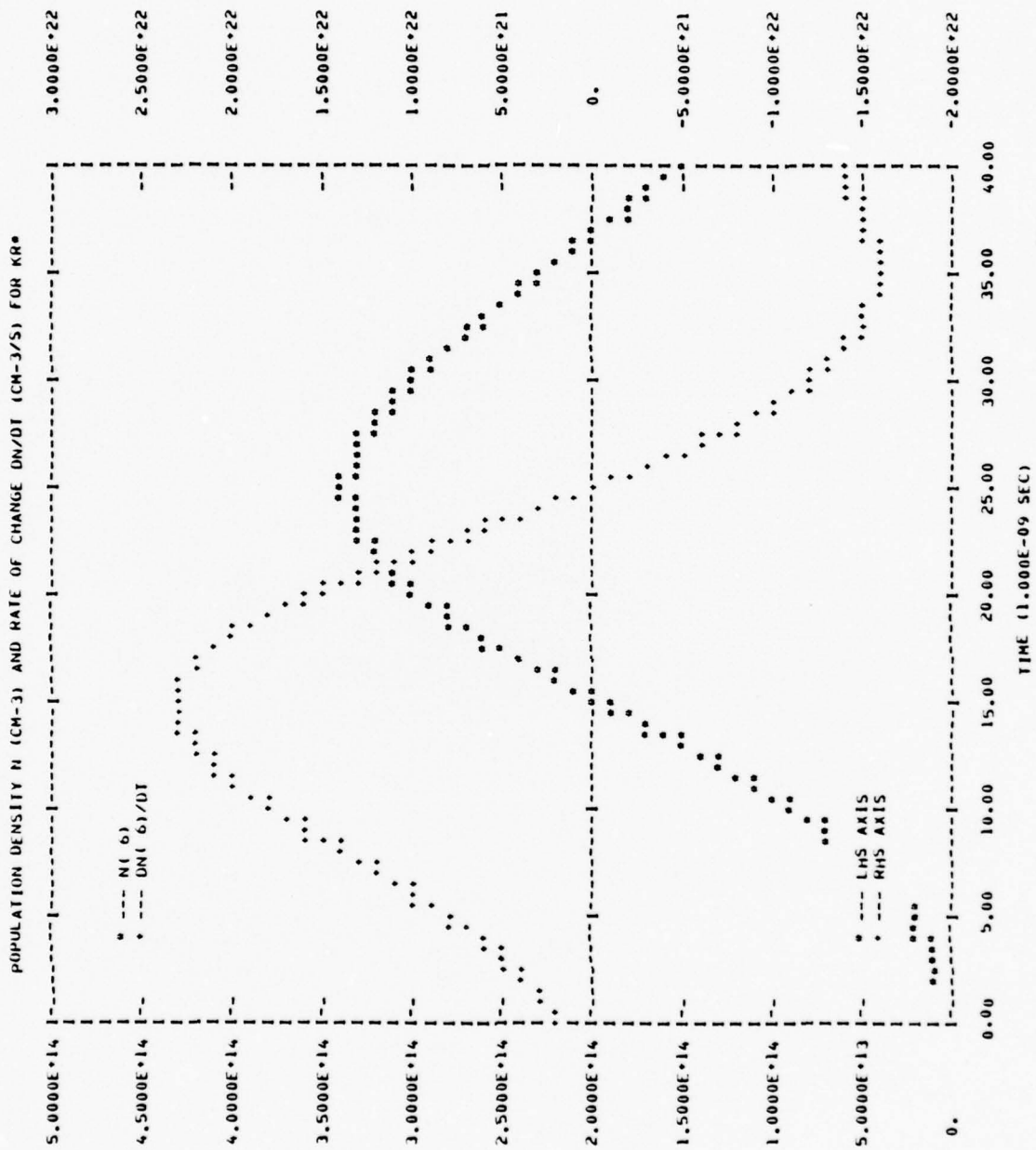


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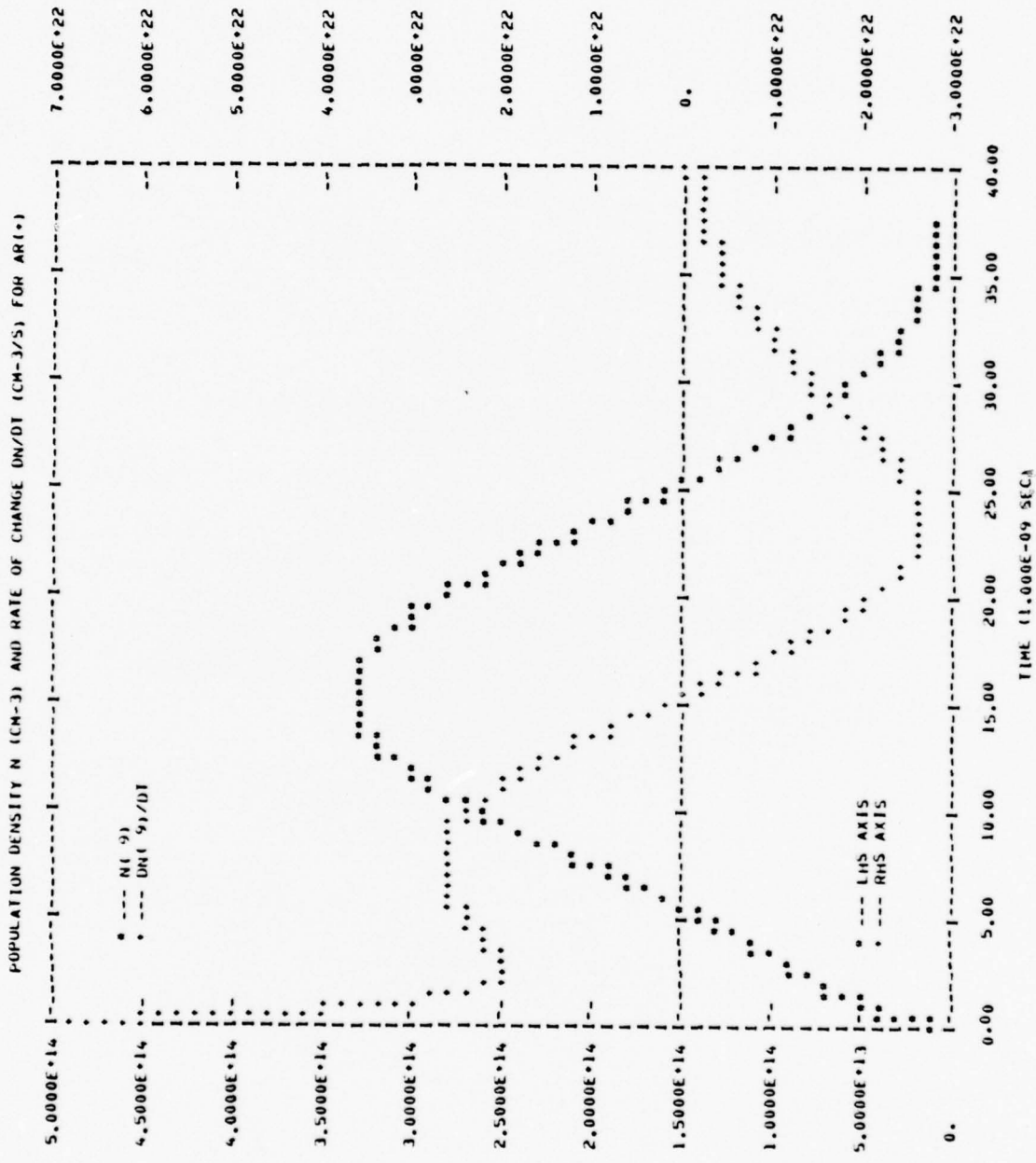


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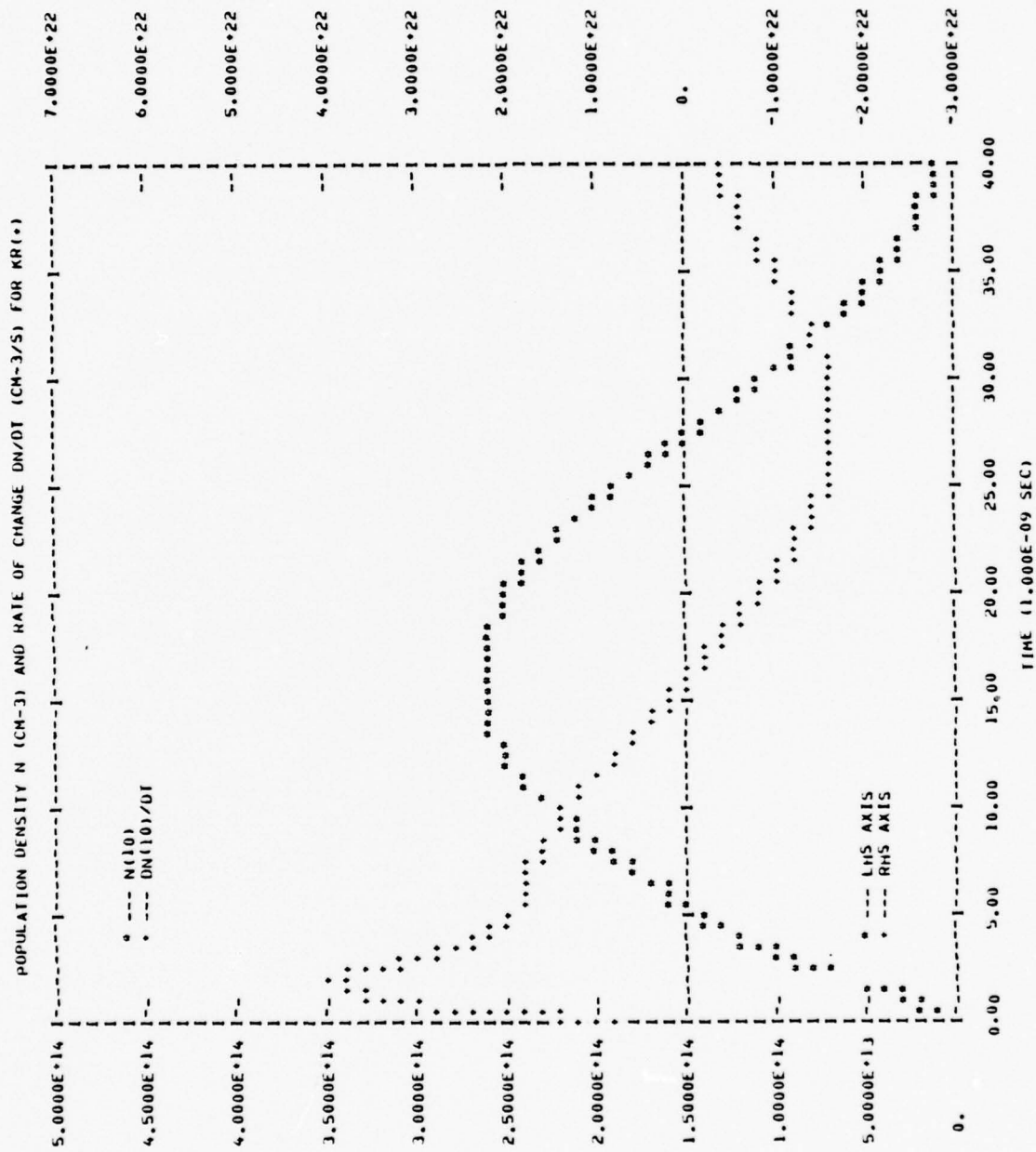


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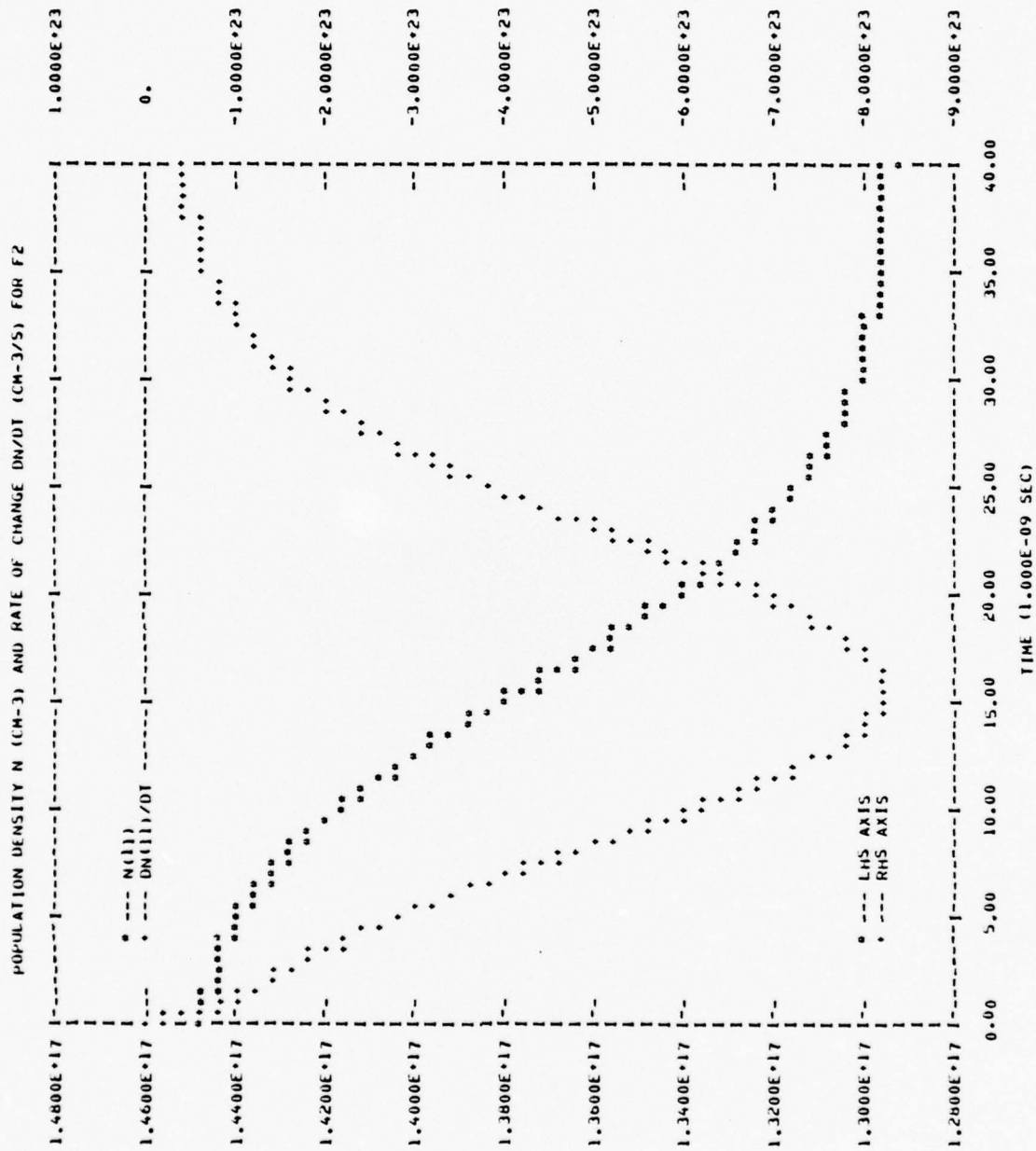


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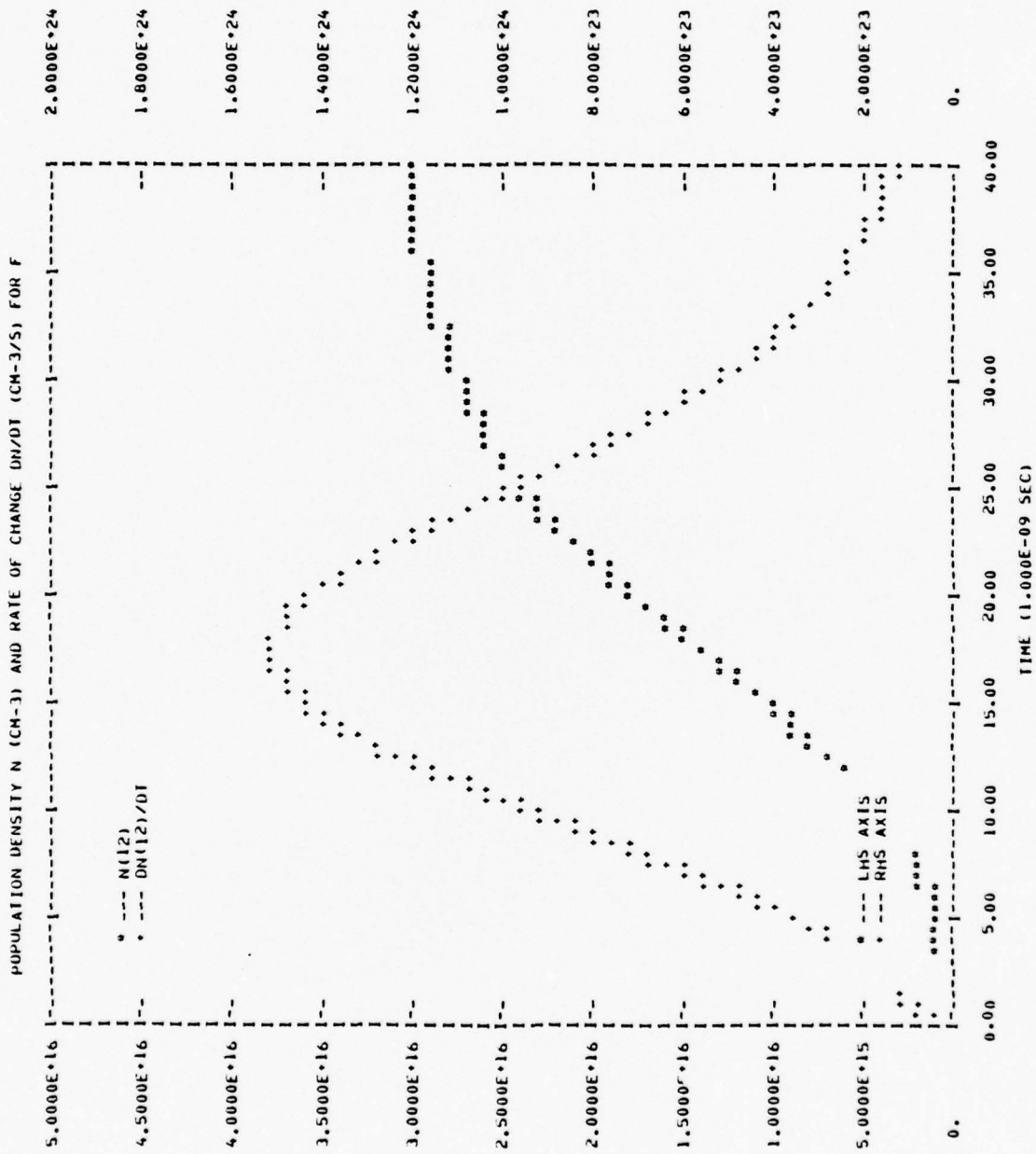


Figure 12 (Continued)

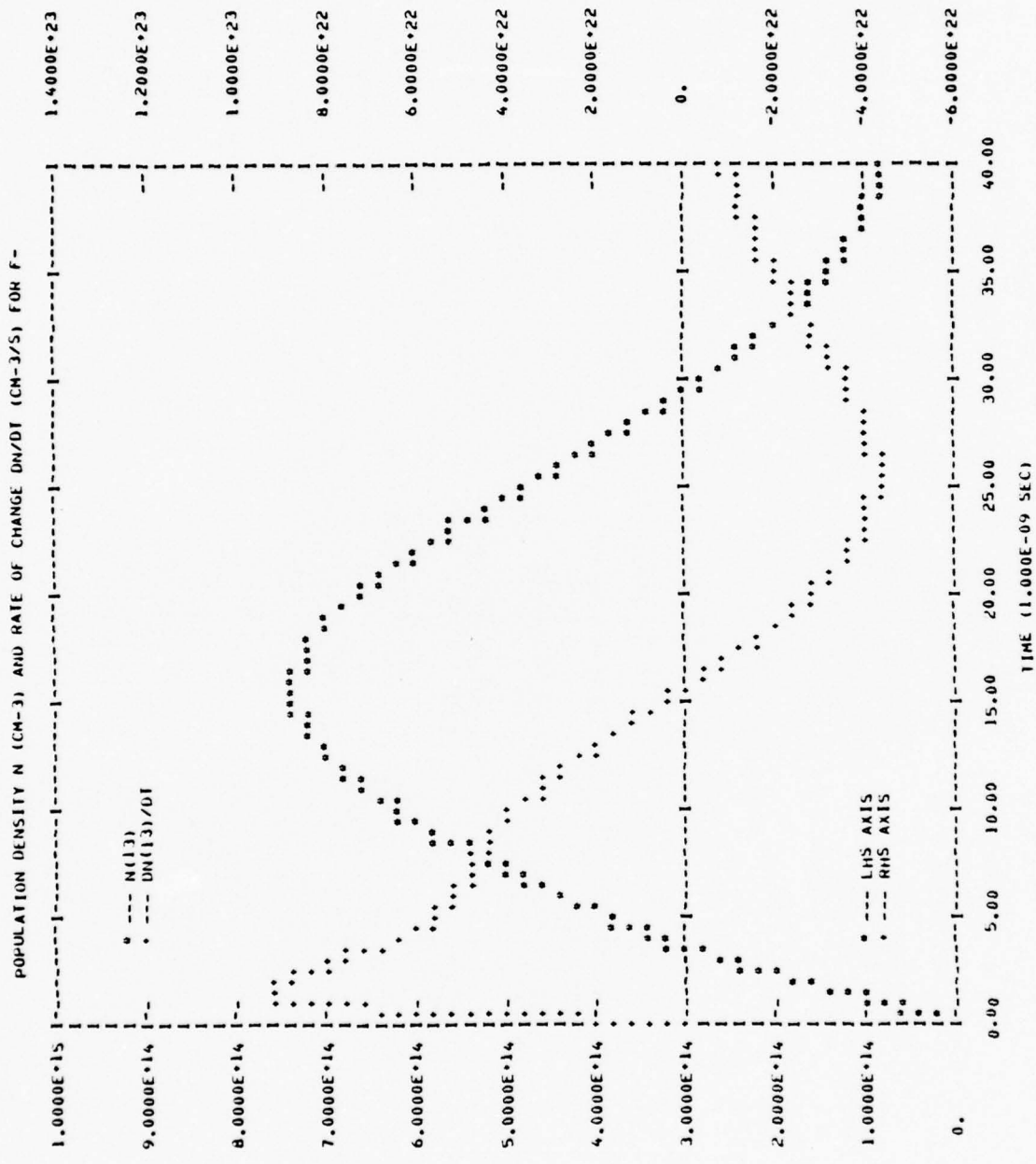


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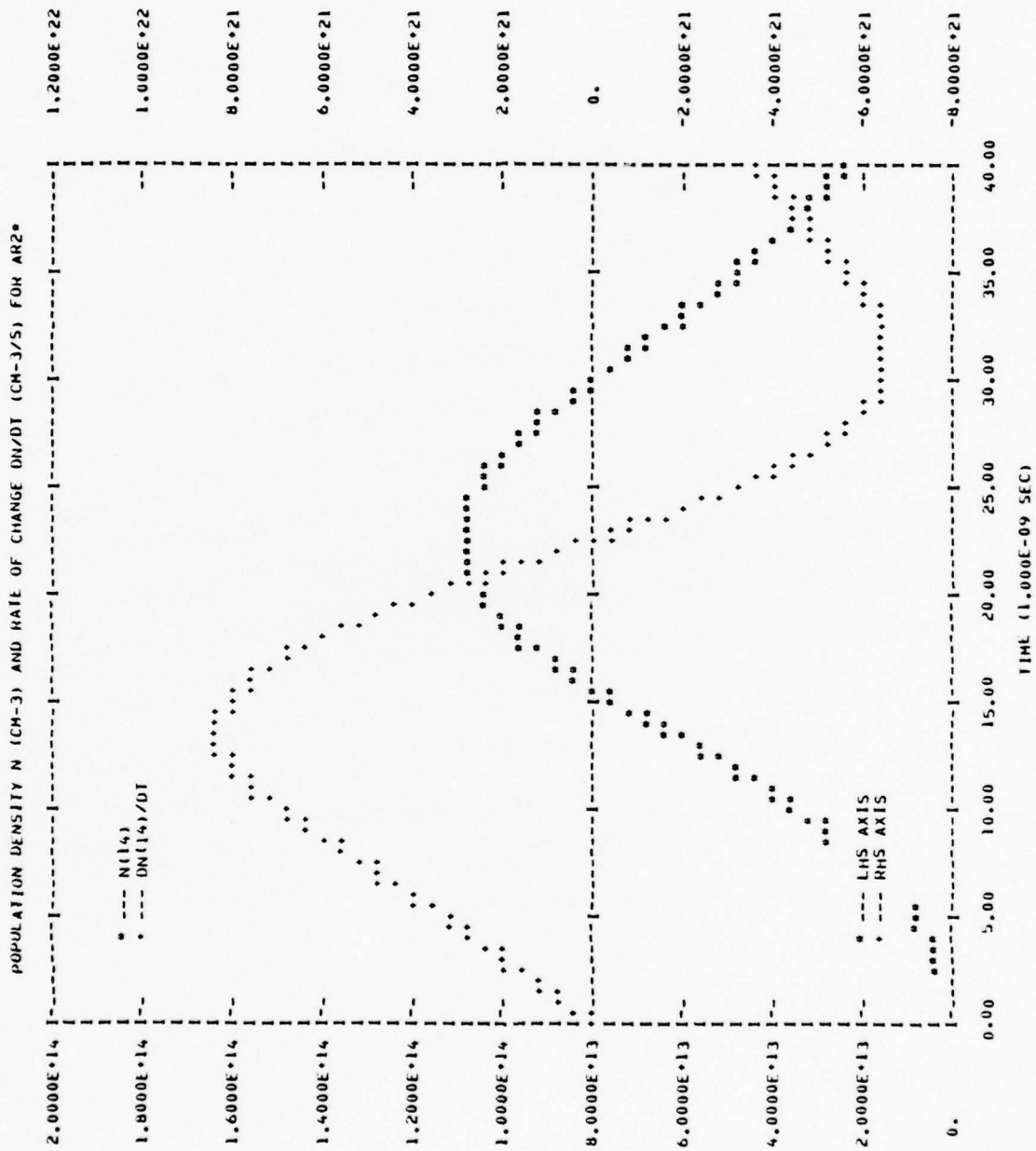


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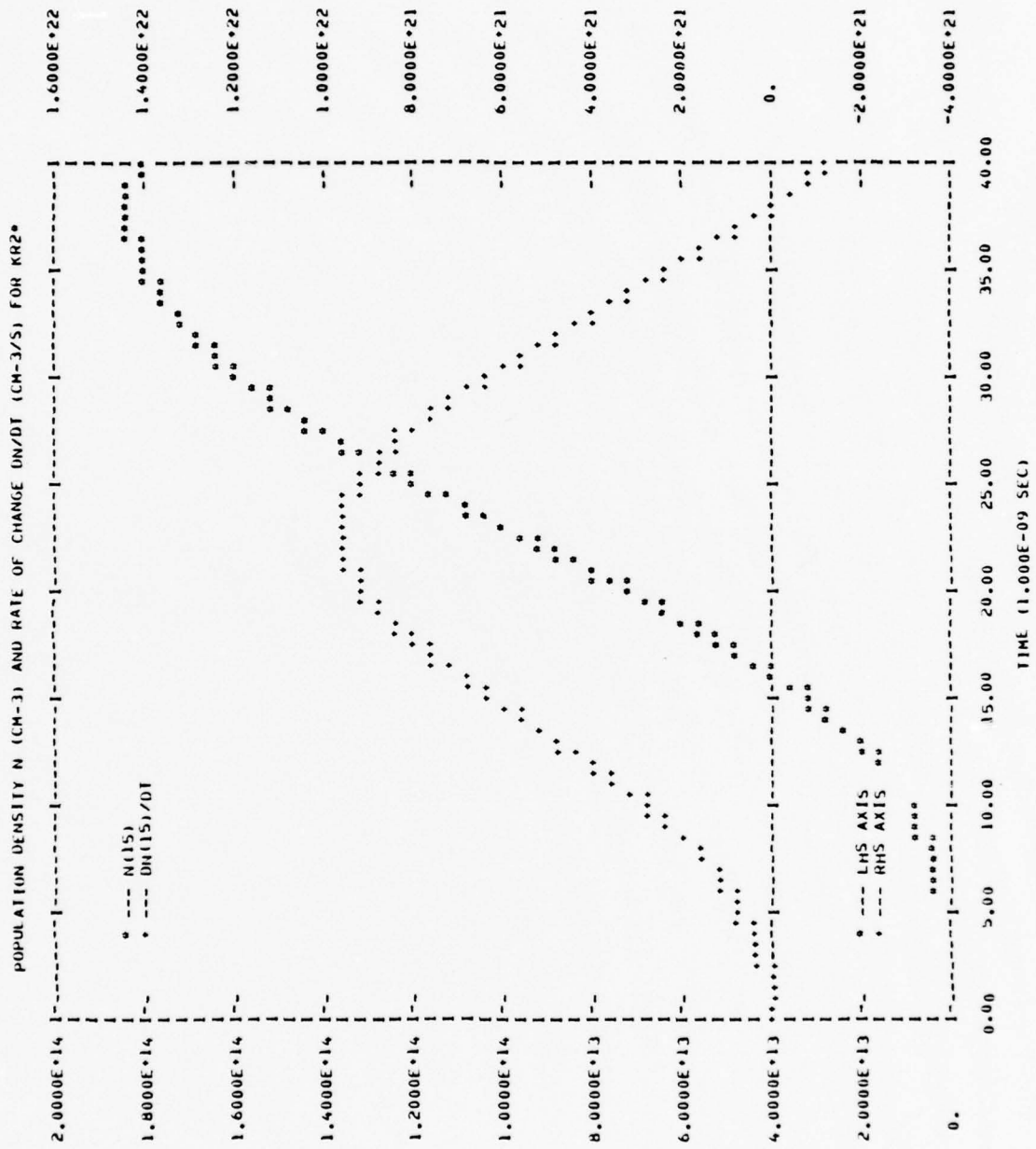


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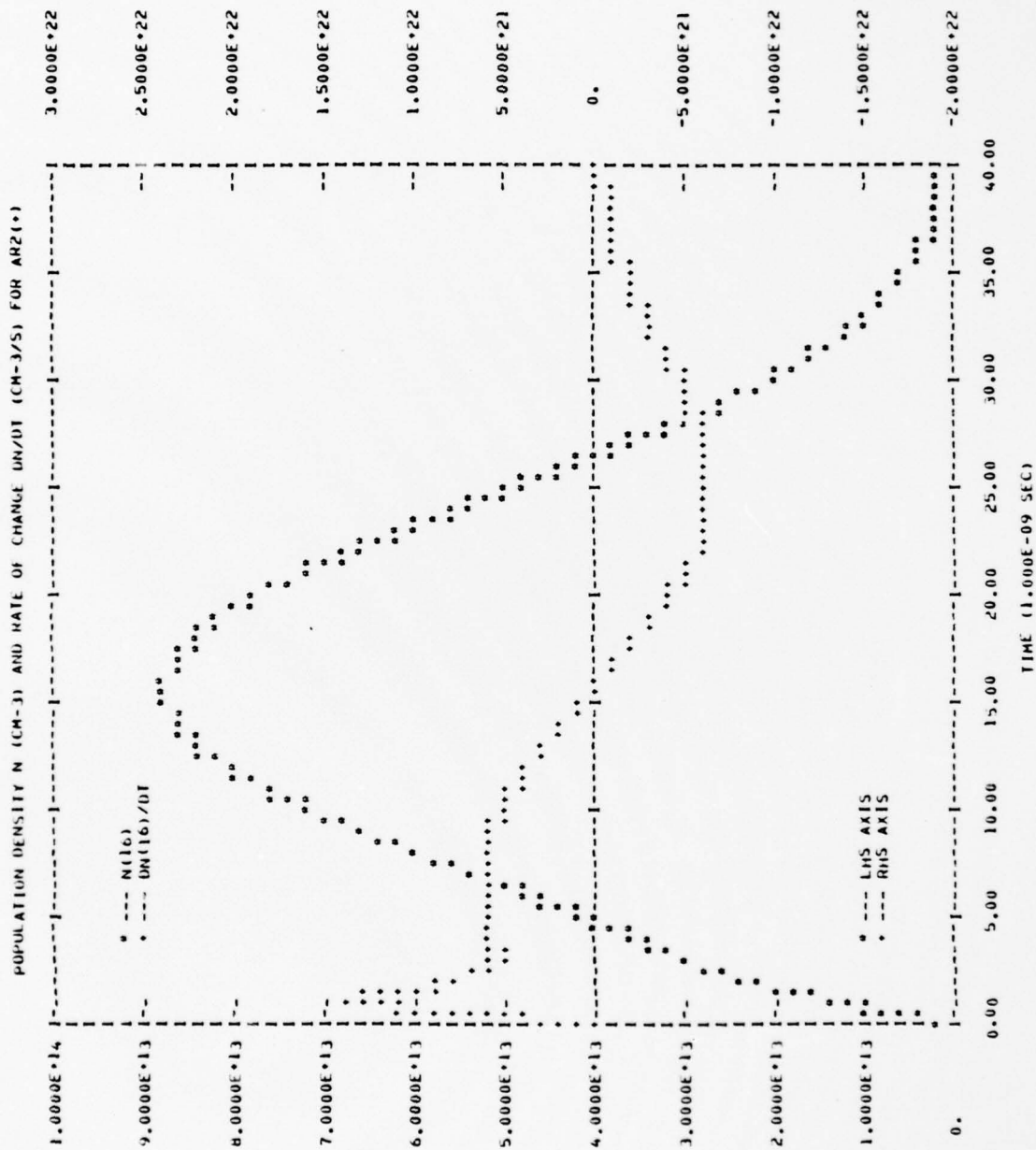


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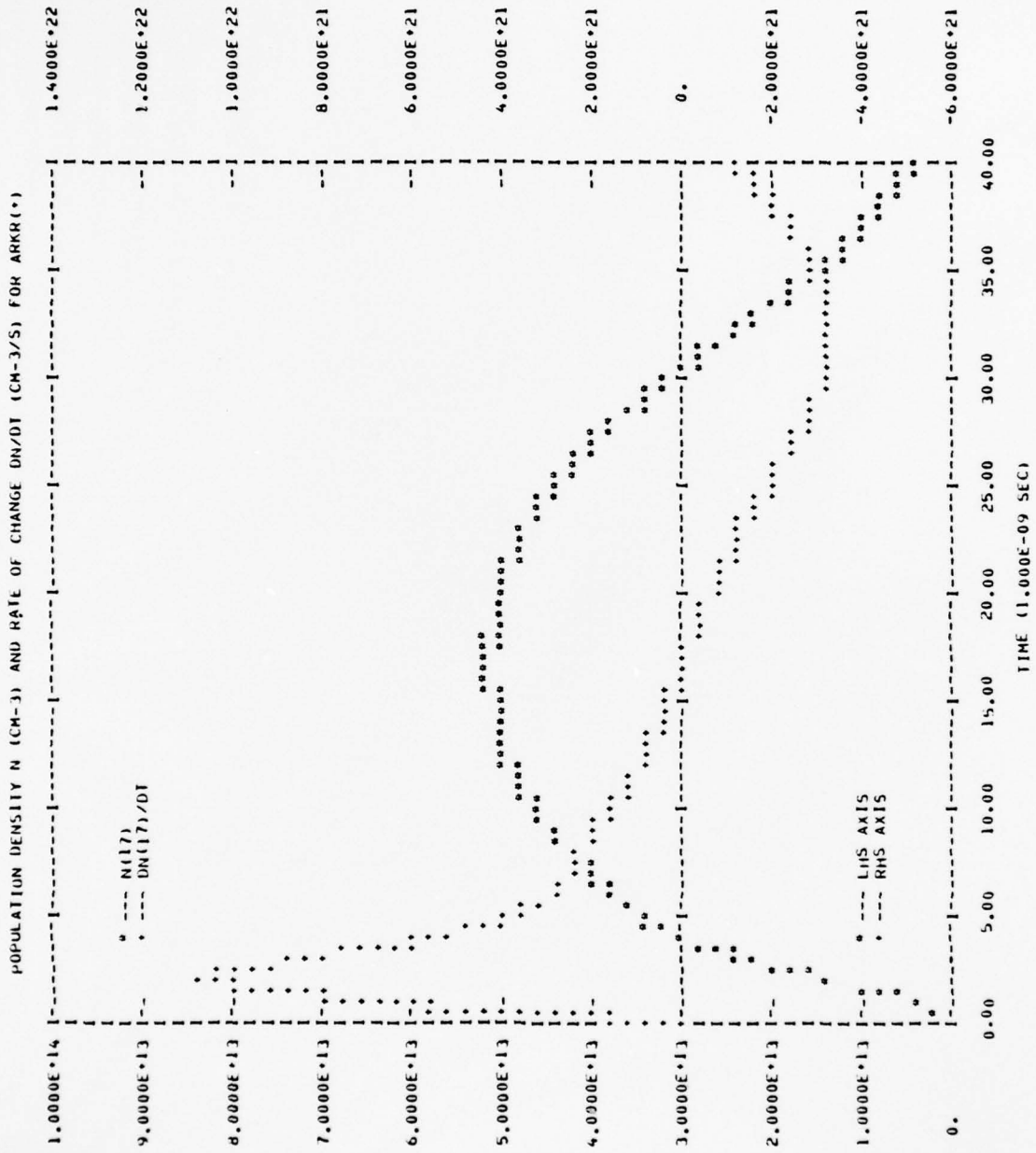


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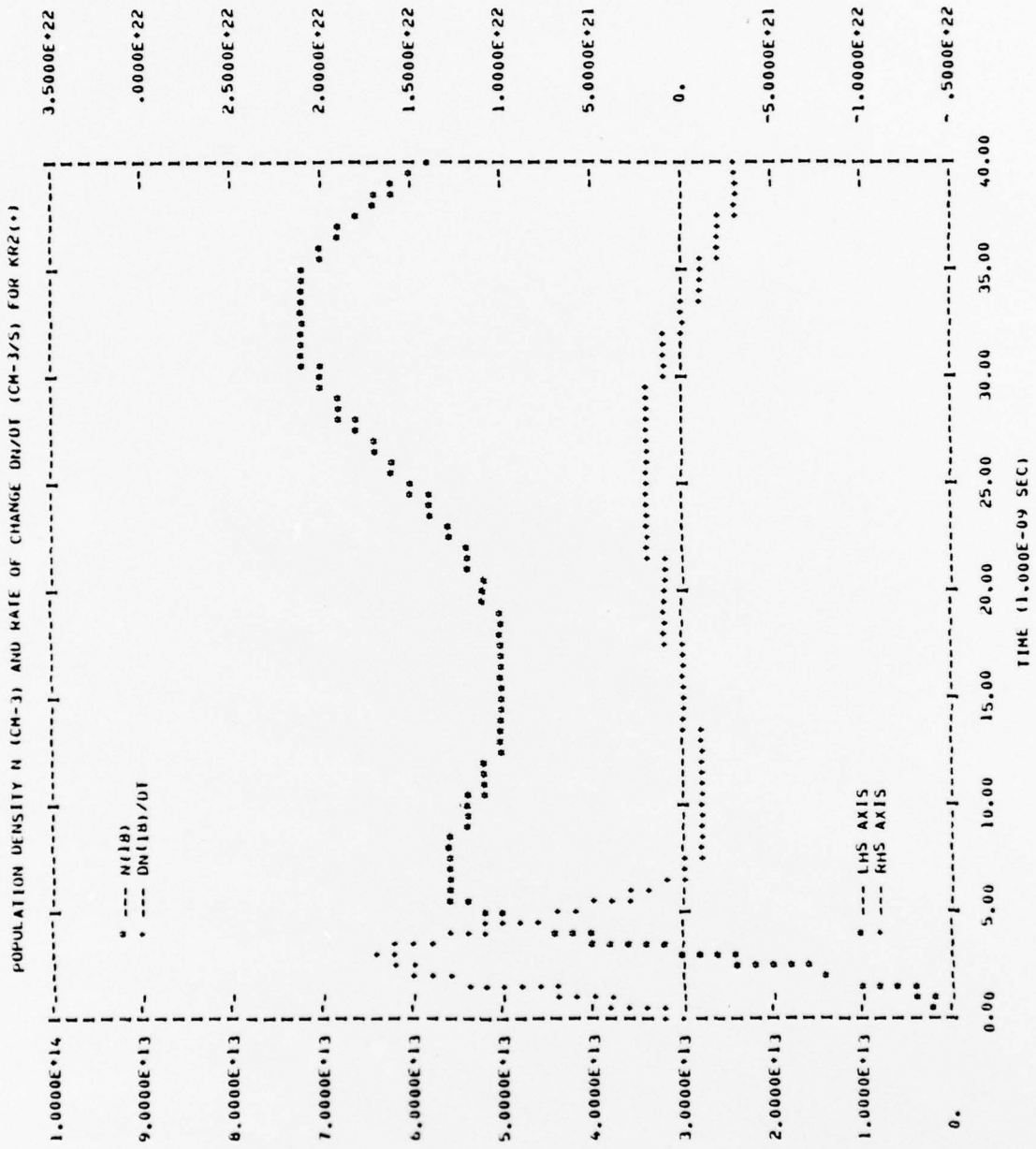


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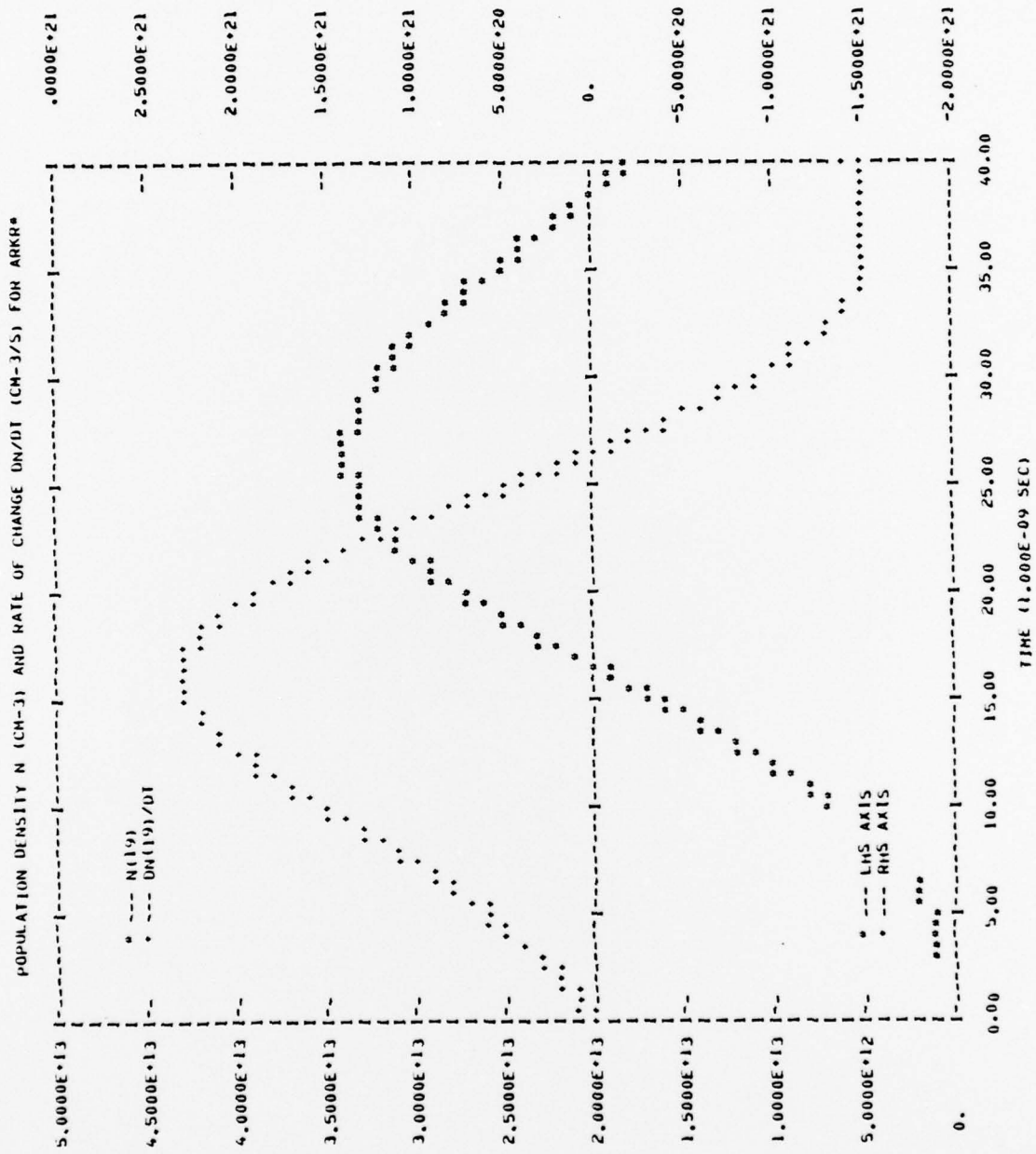


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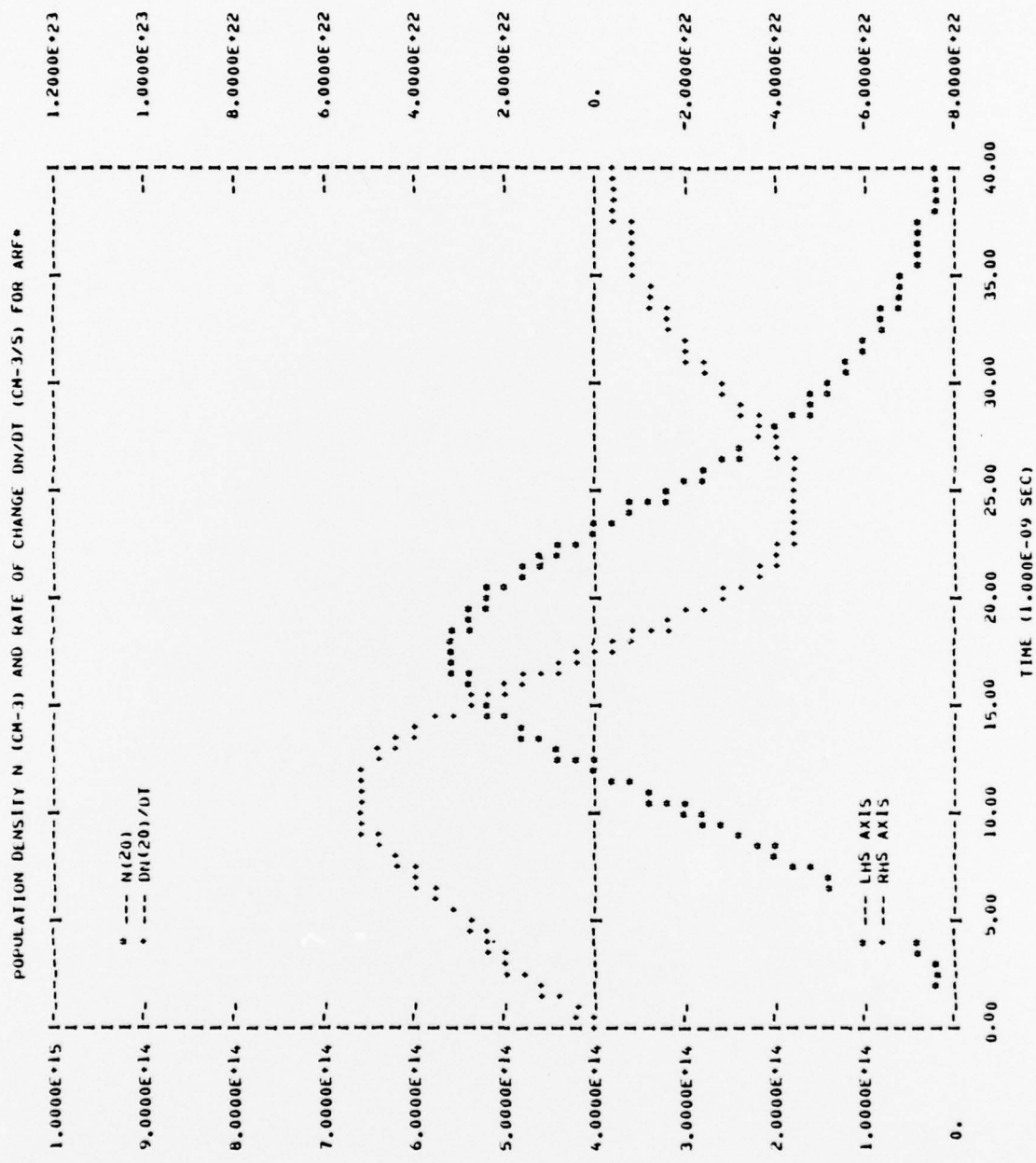


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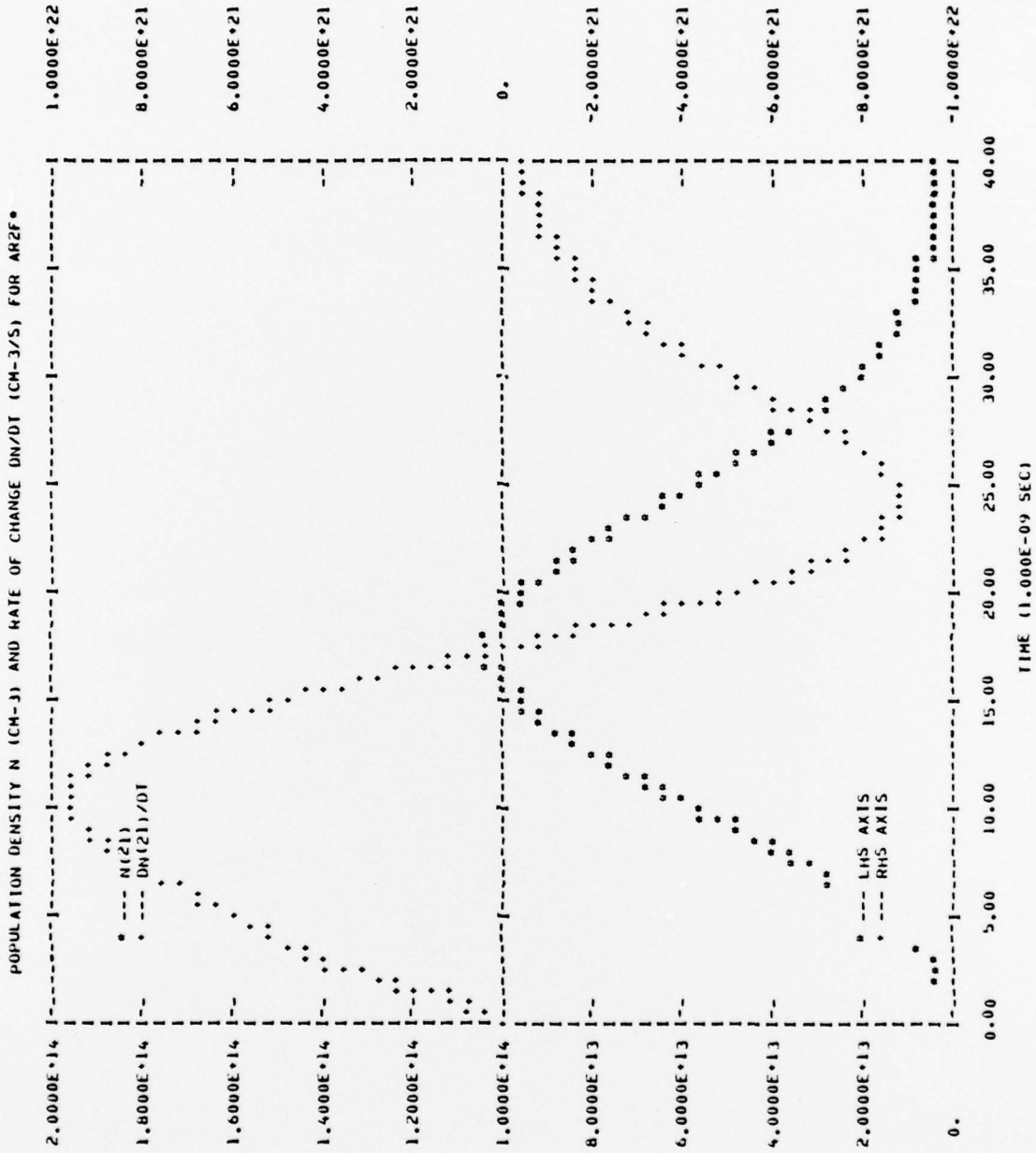


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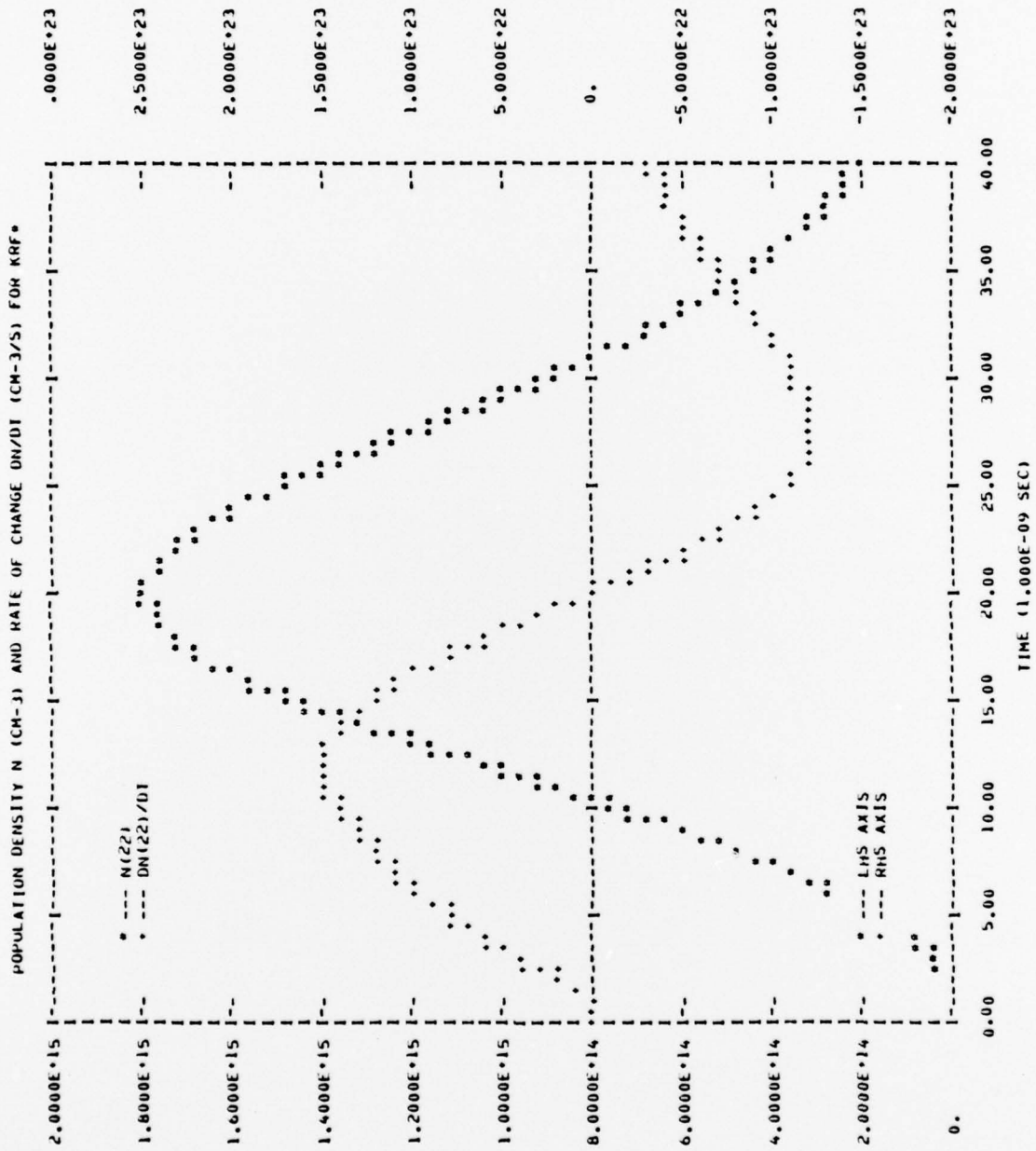


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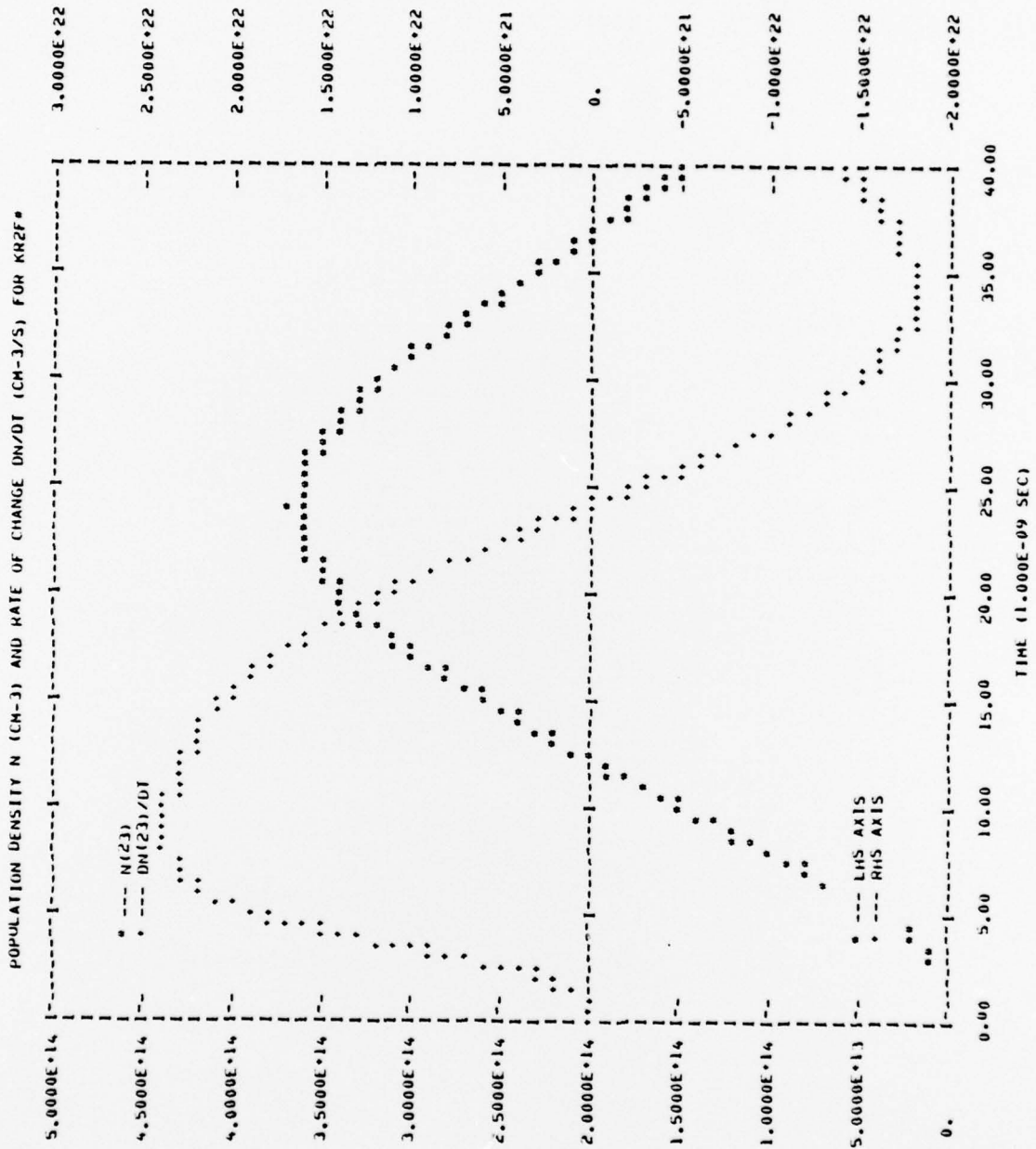


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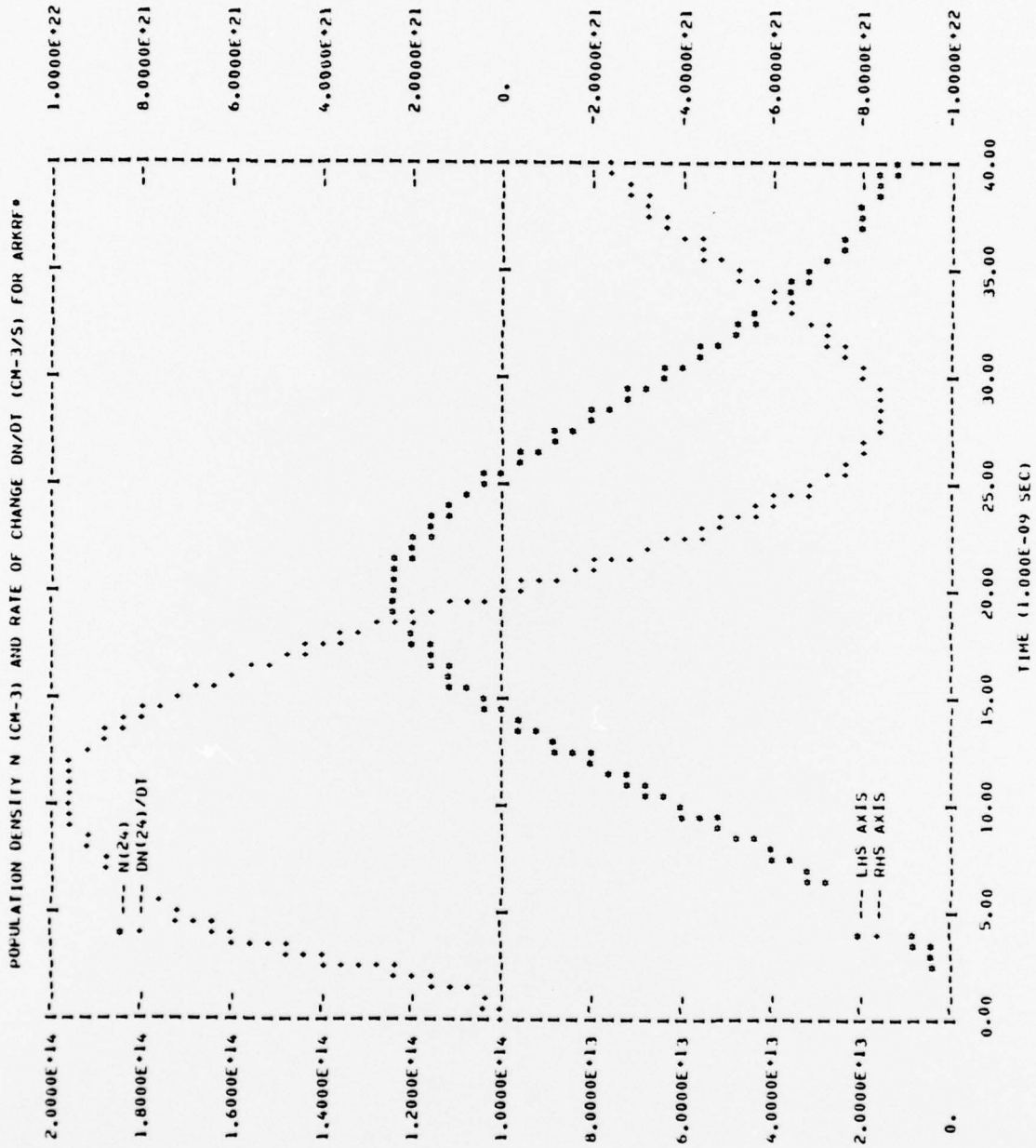


Figure 12 (Continued)

TIME T = 2.500E-08 SEC
 PERCENTAGE CONTRIBUTION OF REACTION K TO DN(I)/DT, EXPRESSED (FOR EACH SPECIES)
 AS A PERCENTAGE OF THE MAXIMUM RATE OCCURRING FOR ALL REACTIONS INCLUDED

K	RATE(K)	MAX %	RAD	E(-)	AR	AR*	KR	KR*	KR**	AR**	AR(+)	KR(+)
• 51	4.781E+22	100.0					40.126					
• 52	6.352E+20	1.3					-.267					
• 53	2.527E+21	10.8			-1.018							
• 54	3.535E+22	100.0			14.244		-14.837					
• 55	1.958E+23	82.2					82.158					
• 56	4.158E+22	26.0			16.752							
• 57	1.921E+22	82.1			15.480		-8.062					
• 58	1.240E+11	100.0				.000						
• 59	-5.228E-07	100.0										
• 60	1.044E+22	6.5			4.206							
• 61	4.018E+20	1.3			.324							
• 62	1.000E+20	.7			.040							
• 63	3.919E+20	3.5										
• 64	1.139E+22	48.7			9.176		.042					
• 65	5.239E+21	14.8			2.111		.329					
• 66	2.437E+22	51.0					2.199					
• 67	2.383E+23	100.0					20.452					
• 68	0.	0.0					100.000					
• 69	0.	0.0										
• 70	0.	0.0										
• 71	0.	0.0										
• 72	0.	0.0										

• THIS REACTION CONTRIBUTES LESS THAN 5. % TO ALL SPECIES THROUGHOUT THE ENTIRE CALCULATION SO FAR

PERCENTAGE CONTRIBUTION OF REACTION K TO $\frac{dN_i}{dt}$, EXPRESSED (FOR EACH SPECIES) AS A PERCENTAGE OF THE MAXIMUM RATE OCCURRING FOR ALL REACTIONS INCLUDED

TIME $t = 2.500E-08$ SEC

K	RATE (K)	MAX %	AR2F*	KRF*	KR2F*	ARRKF*
1	0.	0.0				
2	0.	0.0				
3	0.	0.0				
4	0.	0.0				
5	0.	0.0				
6	0.	0.0				
7	2.680E+23	100.0				
8	2.156E+20	.7				
9	2.422E+20	2.2				
10	6.531E+22	92.5				
11	2.395E+23	100.0				
12	6.198E+21	19.5				
13	2.557E+22	20.6				
14	1.652E+23	100.0				
15	8.821E+21	11.2				
16	1.264E+22	26.6				
17	7.890E+22	100.0				
18	1.586E+22	12.8				
19	1.241E+23	100.0				
20	4.756E+22	100.0				
21	2.471E+20	.8				
22	6.999E+20	1.0				
23	3.022E+22	100.0				
24	1.613E+21	11.4				
25	4.153E+21	36.9				
26	1.415E+22	100.0				
27	1.125E+22	100.0				
28	2.339E+22	14.6				
29	2.339E+22	100.0	100.000			
30	7.475E+22	46.7				
31	2.891E+22	60.8		12.132	60.468	
32	2.891E+22	60.8		37.451		
33	8.924E+22	71.9		8.818		59.433
34	2.101E+22	26.6				
35	2.101E+22	59.4		13.321		
36	3.174E+22	100.0				
37	7.064E+22	100.0				
38	1.499E+22	47.2				
39	2.513E+22	71.1		-10.544		71.067
40	2.654E+22	94.5				
41	3.354E+18	.0				
42	1.601E+23	100.0		67.185		
43	7.546E+20	2.5				
44	8.475E+20	7.5		.356		
45	3.475E+21	14.9	14.854			
46	2.610E+21	18.6		1.104		
47	1.315E+21	9.3				
48	4.683E+21	41.6			9.797	3.720
49	7.484E+21	32.0	-31.992			
50	1.377E+22	39.0				-38.958

* THIS REACTION CONTRIBUTES LESS THAN 5. % TO ALL SPECIES THROUGHOUT THE ENTIRE CALCULATION SO FAR

Figure 13 (Continued)

TIME $t = 2.500E-08$ SEC
 PERCENTAGE CONTRIBUTION OF REACTION k TO $dn(i)/dt$, EXPRESSED (FOR EACH SPECIES)
 AS A PERCENTAGE OF THE MAXIMUM RATE OCCURRING FOR ALL REACTIONS INCLUDED

K	RATE(K)	MAX %	ARZF*	KRF*	ARRHF*
51	4.781E+22	100.0		-100.000	
52	6.352E+20	1.3		1.329	
53	2.527E+21	10.8	10.803		
54	3.535E+22	100.0		73.952	-100.000
55	1.958E+23	82.2		-82.158	
56	4.158E+22	26.0			
57	1.921E+22	82.1			
58	1.240E+11	100.0	-82.120		8.062
59	-5.228E-07	100.0			
60	1.044E+22	6.5			
61	4.018E+20	1.3			
62	1.000E+20	.7			
63	3.919E+20	3.5			
64	1.139E+22	48.7			
65	5.239E+21	14.8	-48.675		
66	2.437E+22	51.0			
67	2.383E+23	100.0		-100.000	
68	0.	0.0			
69	0.	0.0			
70	0.	0.0			
71	0.	0.0			
72	0.	0.0			
				-50.969	-14.818

* THIS REACTION CONTRIBUTES LESS THAN 5. % TO ALL SPECIES THROUGHOUT THE ENTIRE CALCULATION SO FAR

Figure 13 (Continued)

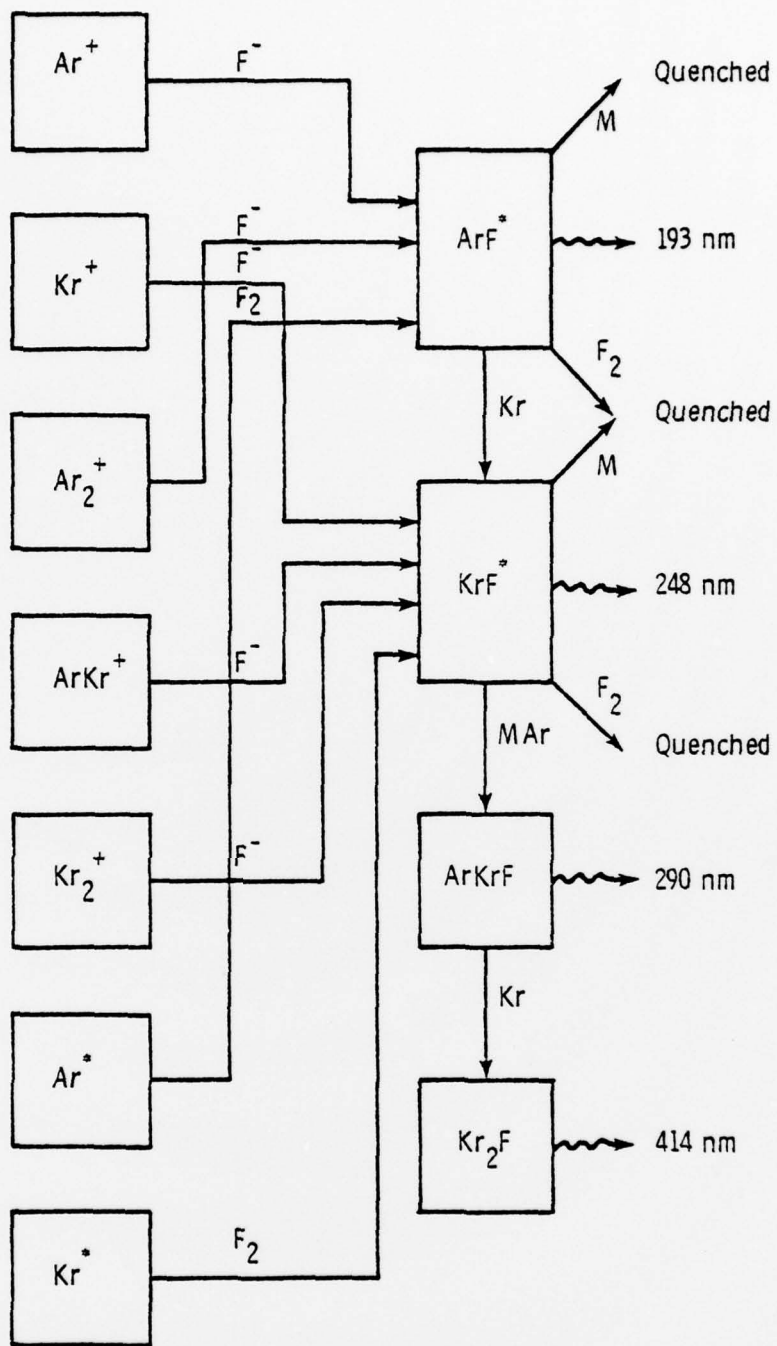


Figure 14 Schematic Representation of the Principal Reactions Involved in KrF^* Production and Loss