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# GRASER: A Kinetics Code for Study of Neutron-Pumped Gamma-Ray Laser Systems 

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GRASER: A KINETICS CODE FOR STUDY OF NEUTRON-PUMPED
GAMMA-RAY LASER SYSTEMS
by
John W. Pettit and George C. Baldwin


#### Abstract

Description, listing, sample plots and operating instructions are given of a computer code for the CDC -6600 which calculates the time-dependence of populations of isomeric nuclear states and the time- and space-dependences of the vector potential of a plane wave of recoilless gama radiation initiated by spontaneous emission and amplified by stimulated emission in a medium of specified properties. The code is based upon a continuousfunction approximation of the neutron flux arising from a fast source burst of user-specified intensity in an infinite hydrogenous moderator. A variety of properties of the nuclear transition and of the medium may be specified by the user, including single-resonance and $1 / v$ capture parameters of the parent isotope; statistical weight factors, isomer inversion ratio and lifetimes of the graser levels; and degree of line broadening, Debye-Waller factor and nonresonant absorption coefficient of the medium.




## I. INTRODUCTION

GRASER is a computer code that solves the Kinetics equations of the type 1 , directly pumped gamma-ray lasers that are described in the documents, "Kinetics of Stimulated Emission in Neutron-Pumped Nuclear Laser Systems," by G. C. Baldwin and "Notes on Graser Seminars," by J. W. Pettit et al. GRASER calculates the development of the wave vector potential as a function of two dimensions: $X$, distance along the axis of the graser body, and time, $t$. The wave vector potential is that initiated by a single spontaneously emitted gamma ray at $\mathrm{X}=0$. GRASER generates a family of plots that describe the pumping as well as the development of the wave vector potential. These plots are placed on separate
subplot areas, one above the other, that have a common time scale so that relationships between points on the two plots can be easily ascertained. Copies of sample plots are included to clarify this description.

## II. DATA INPUT TO GRASER

There are twenty-four variables that GRASER reads in to evaluate the graser kinetics of a particular transition in a solid of specified properties. These variables are stored on an indirect access permanent file called DATA. The variables in DATA can be changed to any value by the person operating program GRASER. A call to execute program GRASER first executes program GHANGE, which has the job of reading in all variables on DATA, asking the operator which variable he desires to change and then inputting the new value of that variable. This procedure is repeated until the operator signals that he desires that program GRASER be executed at which time program GHANGE places all the changed variables into DATA and GHANGE terminates. Program GHANGE will verify all of the changes made by the operator by outputting to the operator the values as they are being written onto DATA. Program GRASER is then executed. First it reads the current contents of DATA as input, then begins analyzing the kinetics of the transition given by DATA. In program GRASER, the variables read in from DATA are assigned meanings according to the order in which they are read in. The inputted variables are first read into array XDAT(I) and program GRASER prints out the variables as they are read in so that the operator may ascertain that the variables have their desired values before proceeding with the plotting. The order in which the variables are read in, the meaning assigned to each, the required units and input format are given in Table I.

## III. METHOD OF COMPUTATION

Program GRASER first computes a number of parameters from the data read in from DATA. These are:
$\lambda_{2}=1 / \tau_{2}$, decay constant of upper graser level:
$\lambda_{1}=1 / \tau_{1}$, decay constant of lower graser leve1;
$\mathrm{G}=\left(2 \mathrm{I}_{2}+1\right)\left(2 \mathrm{I}_{1}+1\right)$, statistical weight factor;
$R=5.37 \times 10^{-4} * \mathrm{E}_{\gamma}{ }^{2} / \mathrm{A}$, recoil energy in eV ;
$\mathrm{f}=\operatorname{Exp}(-2 / 3 * \mathrm{R} / \mathrm{K}(\operatorname{D})$, Mössbauer fraction at $\mathrm{T}=\emptyset \mathrm{K}$;
$\sigma_{\gamma}=\left(2.45 \times 10^{-15} / \mathrm{E}_{\gamma}{ }^{2}\right) * \mathrm{G} * \mathrm{f} * \tau_{1} /(1+\alpha) * \Gamma *\left(\tau_{1}+\tau_{2}\right)$, asymptotic value of the resonant absorption or stimulated emission cross section, $\mathrm{cm}^{2}$;
$\Delta \Gamma=\left(\lambda_{1}+\lambda_{2}\right)(\Gamma-1.0) / 2.0$, excess half-breadth of recoilless line;
$\mu_{h}=\mu_{h}$ (barns) $\times 1.0 \times 10^{-24} \mathrm{~cm}^{2}$, host absorption cross section, $\mathrm{cm}^{2}$; $\mu_{p}=\mu_{p}$ (barns) $\times 1.0 \times 10^{-24} \mathrm{~cm}^{2}$, parent absorption cross section, $\mathrm{cm}^{2}$;
$\mu=\left(N_{h}-N_{p}\right) \mu_{h}+N_{p} \mu_{p}$, if $N_{h} \neq 0 \mid$ nonresonant absorption
$=N_{\mathrm{p}} \mu_{\mathrm{p}}$, if $\left.\mathrm{N}_{\mathrm{h}}=0 \quad\right\} \quad$ coefficient, $\mathrm{cm}^{-1}$;
$\left.\begin{array}{l}\mathrm{x}_{\text {max }}=\mathrm{X}_{\text {end }} / \mu \\ \mathrm{X}_{\text {min }}=\mathrm{x}_{\text {start }} / \mu \\ \mathrm{t}_{\text {max }}=2.4 * \tau_{2},\end{array}\right\}$
$t_{\max }=2.4 * \tau_{2}$, maximum time in seconds at which pumping and vector potential are calculated

Program GRASER now solves the four first-order, coupled differential equations which describe the pumping. The solutions are given at twenty-six values of time between zero and $t_{\text {max. }}$. The equations are

$$
\begin{align*}
& \stackrel{\circ}{N}_{0}=-R(t) \quad N_{p}(t),  \tag{1}\\
& \stackrel{\circ}{N}_{2}=\xi \eta R(t) N_{p}(t)-\lambda_{2} N_{2}(t),  \tag{2}\\
& \stackrel{\circ}{N}_{1}=\xi(1-\eta) R(t) N_{p}(t)+\lambda_{2} N_{2}(t)-\lambda_{1} N_{1}(t) \text {, }  \tag{3}\\
& \stackrel{\circ}{Q}=N_{2}(t)-G N_{1}(t) \text {. } \tag{4}
\end{align*}
$$

The symbols have the following meanings:
$N_{p}(t)$ is the parent nuclide number density as a function of time. This is included to allow for depletion of the parent.
$N_{2}(t)$ is the number density of the upper graser level as a function of time.
$N_{1}(t)$ is the number density of the lower graser level as a function of time.
$Q(t)$ is the time-integral of the inversion density, $N^{*}(t)$, given by $N^{*}(t)=N_{2}(t)-G N_{1}(t)$, where $G$ is the statistical weight factor.
The rate function $R(t)$ is defined as

$$
R(t)=\int_{0}^{\infty} \sigma_{c a p}(V) \Phi(V, t) d V e^{-t / t_{n}}
$$

where $V$ is the velocity of the neutrons, $\sigma_{c a p}(V)$ is the velocity-dependent neutron capture cross section of the parent nuclide and $\Phi(V, t)$ is the time- and velocity-dependent neutron flux per unit velocity, given by

$$
\Phi(V, t)=S\left(V \Sigma_{s} t\right)^{2} e^{-\left(V \Sigma_{s} t\right)}
$$

The above expression for the neutron flux per unit velocity is strictly valid only for an infinite homogeneous hydrogenous moderator, so we attach a leakage term $e^{-t / t_{n}}$ to allow for the loss of neutrons out of the sample. $t_{n}$ is the neutron lifetime, $\Sigma_{s}$ is the macroscopic scattering cross section of the hydrogeneous moderator and $S$ is the number of fast neutrons injected by the neutron source burst at $t=0$. The neutron capture cross section is described by a single effective neutron capture resonance at energy $E_{0}$ with resonance integral $I_{\gamma}$ and a $1 / V$ contribution whose thermal capture cross section is $\sigma_{\text {th }}$. The capture rate at a time $t$ is thus given by $R(t) N_{p}(t)$. The formation of the graser isomeric levels from neutron capture and subsequent decay of the compound nucleus is described by the variables $\xi$ and $\eta$.

$\xi$ is the fraction of all captures that go to either graser level in a time short compared to the lifetime of the graser level. ( $1-\xi$ ) is the fraction of all captures that go to other levels. $\eta$ is the fraction, of those captures that go to either graser level, which go to the upper graser level. ( $1-n$ ) is the fraction of $\xi$ that go to the lower level. This essentially gives two degrees of freedom to describe decay processes that may be quite complex. To clarify these concepts, consider as an example the nuclide ${ }^{82} \mathrm{Kr}$ which goes to ${ }^{83} \mathrm{Kr}$ upon neutron capture and has a Mössbauer transition, between a $9.2-\mathrm{keV}$ level and the ground state, of lifetime $2 \times 10^{-7}$ seconds. Measurements of activation cross sections indicate that two-thirds of all captures go to an isomeric level above the $9.2-\mathrm{keV}$ Mössbauer level. This capture level has a Iifetime of 1.85 hours, so that it is useless for feeding the Mössbauer level, although all decays eventually proceed through the upper Mössbauer level. So in this case $\xi=0.33$ and $\eta=1.0$ since all captures that do not get stuck in the 1.85 -hour level do go to the upper isomeric level and the ground state is not fed directly by pumping.

GRASER calls a library-supplied ordinary differential equation solver subroutine named ODE (D204A ODE in PIM-2) with absolute and relative errors of 0.000001 and will print out a flag if it cannot solve the equations to the specified tolerances. This situation has never arisen over the few months that GRASER has been used to date, but if it does, ODE will calculate the solution as accurately as it can in 500 steps and then continue, so that a fatal execution error is avolded.

GRASER next computes the vector potential as a function of time, holding $X$ constant. This is done for five equally spaced values of $X$ between the ranges of $X$ supplied by the program operator as input. These computations are stored to be plotted later. The equation used to evaluate the vector potential, $A(x, t)$, is

$$
A(x, t)=e^{-\frac{\left(\lambda_{2} t+\mu X\right)}{2}}\left[1.0+e^{-\Delta \Gamma t}(\text { BESSL }-1.0)\right],
$$

where BESSL $=I_{0}\{2 \sqrt{Q(t) X}\}$ if $Q(t) X>0$,

$$
=J_{0}\{2 \sqrt{Q(t) X}\} \text { if } Q(t) X<0,
$$

and $\quad \Delta \Gamma=\left(\lambda_{1}+\lambda_{2}\right)(\Gamma-1.0) / 2.0$.
This completes the computational portion of GRASER. The remainder of GRASER is devoted to plotting the output.

## IV. OUTPUT SECTION OF GRASER

The finished output consists of two subplots on a single page. The lower plot gives $N_{p}(t), N_{1}(t), N_{2}(t)$ and $Q(t)$, and the upper plot gives $A(x, t)$ vs $t$ for five values of $X$ within the ranges specified by the user. The time scale is normalized to units of $\lambda_{2} t$. In order to convert the scale to absolute time units, one multiplies by $\tau_{2}$. Similarly, for labeling of the distance $X$, it is given in units of absorption lengths (i.e., $\mu \mathrm{x}=3, \mu \mathrm{x}=6$, etc); in order to convert to centimeters, one divides by $\mu$, the absorption coefficient. A number of other parameters are also listed to the right of the plots. Sample copies of the output are appended for illustration.

GRASER uses the graphics package DISSPLA to generate the plots. The output may be sent either to a Tektronics terminal, to a Zeta plotter or to the FR80 microfiche by specifying the value of the last input variable IPLOT.

```
IPLOT = 1, output sent to Tektronics terminal,
IPLOT = 2, output sent to Zeta plotter,
IPLOT = 3, output sent to FR80 microfiche.
```


## V. OPERATING DETAILS

GRASER is the name of a procedure file that does all of the necessary file manipulations and operations. There are four files associated with the graser program. A list of these is:

1. GRASER: A procedure file
2. TEST2 : The name of the program that does the computation
3. DATA : A data file
4. GHANGE: A program that is used to change the data on DATA interactively
5. DAT : A temporary working storage file used by GHANGE

These files and programs are set up for operation on the KRONOS operating system and reside on machine zero.

To use GRASER, one must first sign on machine zero and enter the BATCH subsystem. Then one gets file GRASER with the control statement GET, GRASER CR*. To execute the procedure file GRASER, one types in -GRASER CR). This will cause the proper files to be retrieved and the DISSPLA graphics package to be attached to the working files. Program GHANGE is first executed. It reads in the file DATA, outputs it to the terminal and asks the program operator what variable he desires to change. Table I defines each variable and gives its ordinal number. When the integer number corresponding to one datum is entered, program GHANGE then asks for the new value of that variable. This must be entered with the format indicated on Table $I$. When it is entered, GHANGE again asks for a variable to be changed and this procedure is repeated as often as the program operator desires. When the program operator is satisfied that the data file contains the proper values for a run, he enters zero when GHANGE next asks what variable is to be changed. This causes GHANGE to print out the amended data list, write it back on to DATA and store it.

Program TEST2 is then executed with no additional interaction with the program operator. Program TEST2 performs all of the computation and plotting described in the previous section. TEST2 first prints out the data as it has been read in from DATA and also outputs a number of parameters that have been calculated. TEST2 then prints a message that plotting is commencing and asks the operator to enter line speed and term type when executing the program from a Tektronics terminal. At this point, while TEST2 is waiting for input before plotting, the program operator may take the time to make a hard copy of the

This indicates carriage return. The characters to be typed in are underlined. This is the same convention as in the NOS manuals.
data and parameters to be associated with the plot if he is using the Tektronix terminal. One may also type in a message explaining what variable has been changed or what one is looking for, before making the hard copy. When it is desired to produce the plot, one enters $120,3 \mathrm{CR}$.

When it is desired to output to the microfiche or plot on the Zeta plotter, the procedure is slightly different. First of all, IPLOT on the data file must be set to its proper value for the desired output device. This is done as if one were changing any other variable on DATA, as described above. To send the output file to be processed on microfiche, one executes GRASER in the usual manner as described above, but the program will terminate without asking for the line speed and term type (as it does when outputting to the Tektronics terminal). The following control card must be executed in order to write the output to the microfiche processor: PFICHE, FR80,FR80.N $\varnothing$ S FR-80 FORMAT TEST CB. The response from the computer is FICHE COMPLETE. This is described in Chap. 8 of the LASL Guide to NOS, PIM-4, p. 8-4 next to DISSPLA File.

When one is operating at a terminal which has a Zeta plotter, the output can be plotted by setting IPLOT equal to 2. The output will be on a file called ZETA and, after the program has stopped, one executes the following control cards to commence plotting on the Zeta:
REWIND, ZETA
TERM, TTYD (CR LIST, $\mathrm{F}=\mathrm{ZETA}$ (CB).

When the plotting on a Tektronics terminal is completed it is necessary to press the carriage return and enter STOP © one or more times to rapidly terminate the program. In the other cases, the program terminates rapidly. To execute the program again, simply enter -GRASER © $\mathbb{C R}$, make any changes desired when it is indicated to do so, enter 0 to terminate GHANGE and execute TEST2 and so forth. To sign off, enter BYE CR.

The next several pages illustrate several examples of the use of GRASER.

SIGN-ON EXAMPLE (User inputs are underlined, carriage return follows input)

```
    M00RKER STATUS: L.02 M-01 N-72 R-09 5.02
    76/08/25. 12.48.26
```



```
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    TERMINAL,SYSTEM: BATCH
    RECOUER'SYSTEM: BATCH
    GRFL50000.
1,GET,GRASER
    this IS the present contents of dath
```

```
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```

2. XDAT (1) =2.0000000E+22 I = 1
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M,
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XDAT(4): 2.0000e00E-0
xDAT(I):10 1:.56
xDAT(I):10 1:.56
XDATII):7110 I - T
XDATII):7110 I - T
XDAT(I)=9.2000日e I - 8
XDAT(I)=9.2000日e I - 8
XDAT(I)=5.500000 1 = %
XDAT(I)=5.500000 1 = %
XDAT(I):4.500000 1 = 10
XDAT(I):4.500000 1 = 10
XDAT(I):1, \30000-11 I - 12
XDAT(I):1, \30000-11 I - 12
XDATII:O 40 1-13-1
XDATII:O 40 1-13-1
XDATII):200 I - 14
XDATII):200 I - 14
XDATII':45 I. 15
XDATII':45 I. 15
XDGT(I): E.EOUNAM 16 - 17
```
    XDGT(I): E.EOUNAM 16 - 17
```




```
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```

    XDAT(I): IA I I = 19
    XDAT(I): i I - 20
    XDAT(I): i I - 20
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    XDATII)=1.4UROOR I , 2e
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    IDAT(23) =6.0NCROCOE-08 1 - E3
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    ENTEP THE NUMBER OF THE !!mRIGELE TO RE EHAlliged
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    2 1
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    ENTER THE NEL MALUE
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    5.OE+22
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3.% ENTER THE mumger of the Uariagle to ee chamged
4.TME CONTENTS OF DATA IS NOL

```
4.TME CONTENTS OF DATA IS NOL
```



```
1. This executes GRASER
2. Look to Table I for the meaning of each entry
3. This terminates GHANGE and causes TEST2 to be executed
4. GHANGE verifies the changes by outputting the data while writing to DATA
5. Message written by program operator. Be sure to hit the ESC key after writing each line!
```

－GRASER

THIS IS THE PRESENT CONTENTS OF DATA

```
XDAT(1)=2.0000000E+21 I = 
XDAT(3) = 2.0000000E-07 I = 
XDAT(4)=2.0000000EE-07 I = 4
XDAT(5) = 0.00 I = 5
XUAT(I) = 10 I -G
YDAT(I) = 71 19000
XDAT(I) = 9.200000 I =? 
XDAT(I)=3.500000 I = O
XXDAT(I) = 4.500000 11
XDGTII: - 330日00 I - 12
XDAT(I)=40 I = 13
XDAT(II)=200 I= 144
XDAT(II)=45 I= I=15
```



```
XHAT(I)=83 I = 18
XINGTIIN = 10 I = 20
XDATIII = O I = 20
XIATII, - 1.40900e I - 2E
```



```
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```


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ENTER THE NEG UHLUE
? 18
Enter the mumber of the uariable to be ihanged
THE CONTENTS GF DATA IS NOW

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|  |  |  |
| XDAT（3） | －2．0000000E－07 |  |
| XDAT（I） | －2．0080000E－07 |  |
| XDAT（I） | 0 I－5 |  |
| XDAT（I） | 1 1． 6 |  |
| XDAT（I） | 71.18000 I | 7 |
| XDAT（I） | 9.200000 I |  |
| XDAT（I） | 3.500000 I |  |









```
OINTI: \(=5\) I - 23
XDATII - 18 I I 21 - 21.4000001 - 22
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```
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                                    by program operator
```

PRIGGRAM GROSER MOW BEING EIECUTED
THE IMTH READ IH APE

```
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KJATICI=5.0000600E+2L
```



```
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\(\because D A T I=10\)
```



```
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:\{DMTII - 4.500000
:DATI: - 1
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XidTII \(=200\)
(0)TII) \(=200\)
\(\begin{array}{ll}\text { KDHTIII }=45 \\ \text { XIATIII } & 450\end{array}\)
XIATII \(=450\)
\(\therefore\) DATII \(2.300000 ~\)
詋れTI: 23
```



```
:DATI: \(=6\)
K「ウT (I) - 18
```




```
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```






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                                    PLOTTING COMMENCING
Ni. OF FIRST PLOT 0
```

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2 l2e．3 This causes plotting to begin on the Tektronics

## THIRD EXAMPLE SHOWING HOW TO OUTPUT TO MICROFICHE

## program graser nol being executed

the data read in are

```
XDAT(1) - 5.0000000E+22
XDAT(2) = 5.0000000E+2己
XDAT(3): 2.0000000E-37
XDAT(4): 2.0808000E-07
XDAT(5):0
XDAT(I): 10
XDAT(I) - }711
XDATI) = 9.200000
XDAT(I) = 3.50000&
XDATII = 4.500000
xDAT(I),:4
*:DAT(I): - 33000*
XEAT(I) - 40
<<LAT(I): 200
YOHT(I): 45
<DAT!I:-45
XDGT(I,: 2.Seve00
XDAT!I): &j
XDATIII=10
XUGTII;:5
XMAT(I)=18
XDGTC23).6.00reribee-as
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HORIZ. AXIS LINEAR
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## $\mathrm{g}_{\mathrm{O}} \mathrm{FITEQ}$ THE IUMEEP CH THE UAPIMELE TO RE CHAIGEIO

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    -DAT141 - 2.d\30000E-OT
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OI.ATII) = 3.500000
IHTII - 4.500000
```



```
{[HTTI) = .33Ne*0
\thereforeL.GTI I) = +000
#[FTMI) = 200
<(DAT:I) = 45
YDH-1, = = 450
IFTIII= 2.820^100
{[mmTI) - 83
<<HT!|l. 10
"[HT!IM=1.200M@4
```



```
    #LH\mp@subsup{M}{}{+1}
```




```
-27
#MII = इ37553 DTH = 45* HLFHM = E.8000000
```



```
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## 15T0P STOP STOP <br> GTERMINATED:

TO START GRASER AGAIN. ENTER: -GRASER

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STOPPED GR TERMIHATED BEFORE E:YECUTIHU STOPPED GR TERMIHATED BEFORE E: ECUTIIU
GRASER AGAIN.
 $-:$

TABLE I
ORDER OF INPUT, DEFINITIONS, UNITS AND FORMAT FOR VARIABLES IN FILE DATA

| INPUT ORDE |  | VARIABLE |  | FORMAT |
| :---: | :---: | :---: | :---: | :---: |
| XDAT (1) | $\rightarrow$ |  | (Number of fast neutrons injected at $t=0, \mathrm{~cm}^{-3}$ ) | E7.1 |
| XDAT (2) | $\rightarrow$ | $\mathrm{N}_{\mathrm{p}}$ | (Number density of parent nuclei at $\mathrm{t}=0, \mathrm{~cm}^{-3}$ ) | E7. |
| XDAT (3) | $\rightarrow$ | $\tau_{2}$ | (Lifetime of the upper graser level, seconds) | E7.1 |
| XDAT (4) | $\rightarrow$ | $\tau_{1}$ | (Lifetime of the lower graser level, seconds) | E7.1 |
| XDAT (5) | $\rightarrow$ | $\mathrm{N}_{\mathrm{h}}$ | (Number density of the host, $\mathrm{cm}^{-3}$ ) | E7.1 |
| XDAT (6) | $\rightarrow$ | $\mu_{h}$ | (Microscopic nonresonant absorption cross section of the host, barns) | F10.4 |
| XDAT (7) | $\rightarrow$ | $\mu_{p}$ | (Microscopic nonresonant absorption cross. section of the parent, barns) | F10.4 |
| XDAT (8) | $\rightarrow$ | ${ }^{\text {E }}$ Y | (Energy of the gamma transition, keV ) | F10.4 |
| XDAT (9) | $\rightarrow$ | $\mathrm{I}_{2}$ | (Spin of the upper graser level, dimensionless) | F10.4 |
| XDAT (10) | $\rightarrow$ | $\mathrm{I}_{1}$ | (Spin of the lower graser level, dimensionless) | F10.4 |
| XDAT (11) | $\rightarrow$ | $\eta$ | (Fraction of all upper graser levels formed by neutron capture in the parent, or isomer ratio, dimensionless) | F10.4 |
| XDAT (12) | $\rightarrow$ | $\xi$ | (Fraction of all captures which form either graser level, dimensionless) | F10.4 |
| XDAT (13) | $\rightarrow$ | $\mathrm{E}_{0}$ | (Effective energy of a single neutron capture resonance in the parent nuclide, eV) | F10.4 |
| XDAT (14) | + | $\mathrm{I}_{\gamma}$ | (Resonance integral of the capture resonance in the parent, barns) | F10.4 |
| XDAT (15) | $\rightarrow$ | $\sigma_{\text {th }}$ | (Thermal neutron capture cross section of the parent nuclide, barns) | F10.4 |
| XDAT (16) |  | (17) | (Effective Debye temperature of the hostparent system, ${ }^{\circ} \mathrm{K}$ ) | F10.4 |
| XDAT (17) | $\rightarrow$ | $\alpha$ | (Internal conversion coefficient of the graser isomer, dimensionless) | F10.4 |
| XDAT (18) | $\rightarrow$ | A | (Atomic mass number of the graser isomer, dimensionless) | F10.4 |
| XDAT (19) | $\rightarrow$ | $\Gamma$ | (Factor by which the graser gamma line is inhomogeneously broadened, dimensionless) | F10.4 |
| XDAT (20) | $\rightarrow$ | $\mathrm{X}_{\text {start }}$ | (Distance in absorption lengths at which it is desired that GRASER start calculating the vector potential, dimensionless) | F10.4 |

TABLE I - Continued


## COMPLETE PROGRAM LISTING

LASL Identification：LP－0712．

```
LIST:F=SRASER
GET(TESTZ, DRT, DRTR,जMHNIGE)
REIJIND (DRTR ; DRT,IFHPNNIE)
RETURM(LGZ)
FIJY(5:I=İHRNGE)
RE!INDSDRTR :DRT)
REPLRCE (DRT=DRTA)
RFL(55000)
GET (DRTR)
RTTRCH(DISSPLR-IJN=LI BRPRRY)
IIBRRRY(DISSPLR)
REININD(TESTE)
RETIIRM(LGO)
FIJN(5:I=TESTE)
RERD'Y.
LIST:F=TESTコ
    PRDGRRM GRRミER (INPUT,GITPIJT:DATA,TRPEZ=nRTR)
S
C
    E%TERNRL F
```






```
O
C
    PRINT MESSRIGE THAT GRREER IS BEINIG EXECIJTED
        PRINT 50n
    E00 FIPMPT (%, PRRIGRAM GRASER NDW BEING E:<ELIJTED*:<)
        PRINT 5こ?
    Sこ7 FGRMRT (4THE DRTR RERD IN RRE*.>)
C
```

```
C RERD IN DATA
C
    RERD(2.555) <DAT(1)
    RERD(2,555) < (DAT(2)
    PEAD(2,666) : \DAT (3)
    READ(2.565) : \DAT(4)
    READ(2,655) :\DAT(5)
    I!ITPUT,:'DAT(1)
    ZITPIUT :<DAT (2)
    \squareITPIJT :XDAT (3)
    \squareITPIJT,:KDRT (4)
    ZITPIJT,:DDAT(5)
    SSS FORMAT(EP.1)
    Dロ 13 I=5,こ2
    READ(2.55?) :<DAT(I)
557 FDRMAT(F10.4)
    \squareITPIJT, :RDRT(I)
    13 CDNTINJE
    RERD(2,565) <DAT(23)
    I!JTPIIT :XDAT (23)
    READ(2,568) IPLDT
    ZIJTPIJT,IPLDT
668 FIRMAT(I1)
    S='xDAT (1)
    XNP=:SDAT (2)
    TRIJ=:<DRT (3)
    TRIJ1= XDAT (4)
    XNH=\DAT (5)
    'JH='xDAT (6)
    IJP={DAT(?)
    EG=:XDAT(3)
    S!J=xDAT (9)
    SL=%DAT (10)
    ETA=XDAT (11)
    SI='RDAT (12)
    ED=KDAT(13)
    RESINT=:KDRT (14)
    T:SSECT=:XDAT(15)
    DTH=XDRT (15)
    ALPHA=%DAT (17)
    AMAS=XDAT (1:3)
    FLIN=XDAT (19)
    JST=.XDAT (20)
    IJND='XDRT (21)
    ES={DAT (23)
    TNL=1.0%XDAT(23)
```

r.

CALCILATE INITIRL VRLUES

```
NEQ=4
IFLRG=1
RELERR=0.000001
ABSERR=0.000001
T=0.0
TMT=0.0
DEC=1.0.TRIJ
DEC1=1.0/TAIS1
I`1=SL*2.0
IS2=3リ*2.0
G=(<2.0*SU)+1.0)<(<2.0*SL)+1.0)
SIG=2.45E-15/(EIG**2)*5*(1.0/(1.0+RLPHA))
RECDIL =5.37E-4*(EG**2)-AMAS
FM:X=EXP(-<3.0/2.0)*REC口IL)(3.51PE-5*DTH))
SIGM=SIG/FLIN*FMO*TRII1* (1.0/(TADI+TAIJ))
DELGAM=(DEC+DEE1)*(FLIN-1.0)/2.0
ABH=IJH*1, DE-24
ABP=1JP* 1. DE-24
XDIF=XNH-XNNP
IF(XDIF .LT, 0.0) KDIF=0.0
ABSCD=((XDIF)*ABH)+(XNP*ABP)
XMASK=IJND/ABSCD
KMIN=UST/ABSCD
TMA, }=2.4*TAI
XE=TXSECT*1.0E-24*220000.0
XNPT(1)=XNP
x (1)=0.0
x1(1)=0.0
TC(1)=0.0
Q(1)=0.0
QB<1)=0.0
Y(1)=XNP
T(2)=0.0
r(3)=0.0
Y(4)=0.0
M,
ZUITPIT,:SIGM,SIJ,SL,FMX,T'XSECT,RESINT,IPLIT, ES
EALIULATE DENSITIES FGR TUENTY SIX YALIJES DF TIME
#0 10 I=2,25
TOUT=TםIST+TMAX.25.0
TC(I)=T\IT
CALL GDE(F,NEQ,Y:T,TOUT,RELERR,ABSERR,IFLRG,NDRK, INORK)
XNPT (I)=Y(1)
XZ(I)=Y(3)
X1(T)=Y(3)
```

```
        Q(I)=Y(4)*SIGM/4.0*DELGRM
        QB(I)=Q(I)&1.NE+19
        T=T||\T
        IF(IFLRG .EQ. こ) 50 TD 10
        \squareIJTPIIT:IFLRG
        10 EDNTINUE
        PRINT 150
    150 FIRMAT (5X, CRLCIJLRTING VECTOR PDTENTIRL*)
C
E CRLCIJLRTE YECTDR PDTENTIAL FDR FIWE YRLUES DF X RND
C
C
    7口 30 I=1,25
    Dロ 30 . = 1:5
    XX=((XMRX-XMIN)/4,D*(.J-1))+XMIM
    XLC(.J)=SX*RBSCD
    TIM=TC(I)
    RRGR={(I) © X:X
    IF(PRGA .LT, 0.0) FD TD O5
    RRG=2, D*SQRT (Qr.I)* XX)
    BESSL=FI 0 (RRG) - EXP (PRRG)
    G口 T\ 26
    25 RRGR=-Q(I) *ixM
    ARG=2 , D*SQRT (PRGR)
    BESSL=F.JD(PRPG)
    25 VECT (I,J)=EXP(-0.5*((TIM/TRII)+(RBSCD*XX)))*
    1(1.0+(EXP(-DELGAM*TIM)* (BESSL-1,0)))
    UECT(I,J)=RBS(YECT(I,J))
30 SDNTINIJE
C
C
C
40 TE(I)=TC(I)*DEC
C
C
C
    TDP=RNP
    'YSTP=TDP-5.0
    ज口 TD <100,200,300):IPLDT
100 EPLL TEKTRN
    50 TD 400
    200 EALL ZETR
    50 TD 400
300 ERLL FR80(3)
400 CDNTINIJE
    ERLL BGNPL(0)
    ERLL PH'r'SOR(1,0,1,0)
```

CALL BASALF（SHSTANDPRD）
CRLL MIXRLF（GHL－CSTD）
CRLL MX3RLF（5HGREEK；1HE）
ERLL MX4RLF（3HL EGREEK，1H＋）
CALL TITLE（1H ：195H＋L（T），5：7HDENSITY，7．5．0．4．0）
CRLL GRAF（0．0，0．2，2．5．0．0．＇अSTP，TOP）
CRLL CIJRYE（TC，9＇2，26，5）
CRLL CURVE（TC，：X1，26，5）
CRLL CURVE（TC，QR：26，5）
CRLL CIJRVE（TC，XNPT，26．5）
CRLL LINES（12HUPPER LEYELS，IPAK，1）
CRLL LINES（12HLDUER LEYELS，IPAK，2）
CRLL LINES（16HINTEGRAL DF INVF，IPAK，3）
CRLL LINES（15HPARENT DENSITYS，IPAK：4）
CRLL LEGEND（IPAK，5，5．0．2．0）
CRLL MESSRG（5H8G＋T＝，5，5．0．4．75）
CALL RERLND（FLIN，2，4HABUT，4HABHT）
CALL MESSA5（5H＋S $=9.5,5.0,4.5)$
CALL RERLND（TXSECT，1，4HABUT，4HRBIJT）
ERLL MESSRG（4H（TH），4，5．1，4．46）
CRLL MESSA5（3HEQ＝，3，5．0．4．25）
CRLL RERLND（DTH，1，4HRBIJT，4HABHJT）
CRLL MESSAS（ $4 \mathrm{H}(F)=, 4,5.0,4.0)$
ERLL RERLND（FMX，2，4HRBUT，4HRBIJT）
CRLL ENDGR（1）
CALL PHYSOR（1．0．6．0）
CRLL TITLE（7HYP YS T，7．5H＋L（T），5，5HLDG YP．6．5．0．4．0）
$T \square P=0.0$
Dロ $50 \mathrm{~J}=1.5$
D $50 \mathrm{I}=1$ ．25
50 TDP＝RMRX1（YECT（I g．J）：TDP）
TDP＝RLDG10 ©TDP）
$T D P=T D P+0.5$
ITDP＝TDP
TAP＝ITAP
CRLL जRPF（0．0，0．2，2．5，－3．0，1．0，TDP）
Dロ $70 . J=1,5$
吅 $50 \mathrm{I}=1$ ，25
IF（YECT（Ig．J）．LT，0．กी1）YECT（I，J）＝0．001
$50 \mathrm{R}(\mathrm{I})=\mathrm{RLDG10}(\mathrm{YECT}(I, 1))$
CRLL CURYE（TL，R，26：5）
70 CINTINIJE
JDIJM＝L INE．ST（IPRK，80，8）
CALL LINES（ $7 \mathrm{H}+\mathrm{M}(\mathrm{X}=\mathrm{S}=\mathrm{IPRK}, 1$ ）
CRLL LINES（ $7 H+M(x=5$, IPRK． 2 ）
CRLL LINES（ $7 H+M(x=5, I P R K, 3)$
CRLL LINES（ $84+M(X=5$, IPAK， 4$)$
CRLL LINES（8H＋M（X＝SYIPAK，5）

```
    CALL LEGEND(IPAK,5,5,0,2,95)
    CRLL RERLND(XLC(1),4,5.6,3.75)
    CALL REALNO(XLC(2),4,5.6,3.55)
    CALL REALND(XLC(3),4,5.5,3.35)
    CALL REALND(XLC(4),4,5.5,3.15)
    CALL REALNO(XLC(5),4,5.6,2,95)
    CRLL MESSA5(2HS=,2,5,0,2,7)
    CALL RERLND(S,-1,4HABUT,4HABLIT)
    CALL MESSAG(3HN=,2,5,0,2,45)
    CALL REALND(XNP,-2,4HABIJT,4HABUT)
    CALL MESSAG( }3\textrm{H}+\textrm{T}=,3,5,0,2,2
    CALL REPLND(TAU,--2,4HABIJT,4HABUT)
    CALL MESSAG(3H+C=,3,5.0,1.95)
    CRLL RERLNO(ETR,2,4HABUT,4HABIJT)
    CALL MESSAG(3H+M=,3,5.0,1.7)
    CALL RERLND(ABSCD,-2,4HABUT,4HABIJT)
    CALL MESSAG ( }3\textrm{H}+\textrm{X}=,3,5.0,1.4.5
    CALL REALND(SI,2,4HABIJT,4HABUT)
    CALL MESSA5(4H+S =,4,5,0,1.2)
    CRLL REALND(SIGM,-2,4HABUT,4HABIJT)
    CALL MESSAG(2H+5,2,5.1,1.1)
    CALL MESSAG(3HI =,3,5.0,0.95)
    CALL REALND(RESINT,1,4HABIT,4HABIJT)
    CALL MESSAG(2H+5,2,5,1,0.86)
    CALL MESSAG(4HE+D=,4,5.0,0.7)
    CALL REALMD(ED,1,4HRBUT,4HAPUT)
    CALL MESSAG(4HE+G=,4,5.0,0.45)
    CALL REALND(EG,1,4HABUT,4HABUT)
    CALL MESSAG(3HI1=,3,5.0,0.2)
    CRLL INTND(IS1,4HABIJT,4HABIJT)
    CALL MESSAG(2H/2,2,4HABUIT,4HARUT)
    CALL MESSAG(3HI2=,3,5.0,0.0)
    CALL INTND(IS2,4HABIST,4HRBUT)
    CALL MESSAG(2H}/2,2,4HABUIT,4HABIJT
    CRLL ENDGR(2)
    CRLL LASLDGO(2.0,6.5.1.0)
    CALL ENDPL(0)
    CALL DONEPL
    STIP S END
C
SIJBROITINE F(T,'Y,YP)
CIMMIN X,XE,XNP,ETR,DEC1,G:RESINT,ED,TNL,ES,S,DEC,SI
DIMENSIDN Y(4),'YP(4)
'YP(1)=-RATE (T)-Y(1)
Y'P(2)=(ETR*RATE (T)*Y(1)*SI)-DEC*Y(2)
YP(3)=(1, D-ETR)*RATE (T)*Y(1)*SI+DEC*Y(2)-DEE1*Y(3)
YP(4)=Y(2)-5*'Y(3)
RETIJRN
END
C
```

```
C
            FUNCTIDN RATE(TY)
            CDMMIN X,XE,XNP,ETR,DEC1,F,RESINT,ED,TNL,ES,S,DEC,SI
            F=RATFUN\TY \
            RATE=EXP(-TY*THL)* (XE+F)*S
            RETURN $ END
C
            FUNETIDN RATFUN(TY)
            CDMMIN X,XE,XNP,ETR,DECI,E,RESINT,ED,TNL,ES,S,DEC,SI
            EX=EO&1.60209E-12
            XM=1.65976E-24
            V=SQRT (2.0*EX/XM)
            FLUX=( (Y*ES*TV)** ) * EXP (-V*ES S TV)
            ARER=RESINT*1.0E-24*4
            RRTFIJN=FLUX*FAREA
            RETURN $ END
C
```

```
            FIINCTIDN FIO(ZP)
```

            FIINCTIDN FIO(ZP)
                C342
                C342
    ********\&+******************************************************************** C342

* FIO(X) CDMPUTES THE REFL BESSEL FUNCTIDN ID TIMES EXP(-X) DF THE - C342
* RRGuMENT * .ET. I
- C342

```

```

    DIMENSIDN P(9,2),贝(3,2) C342
    DIMENSIDN PD(5,2):QO(4,2) C:342
    EQUIYALENCE (EYIO,EYEIO,FID) C342
    DATA (P(J),J=1,9), C342
    *.3306413389260115E+22, [342
    *.792908:3985978161E+21, C342
    *.4340939205795706E+20, [342
    ..9506389969703280E+18, C342
    . .1032250768917613E+17, [342
    ..5124926562275096E+14, E.342
    *.2042613182306772E+12, [342
    *.3651524854074652E+09, [342
    *.2787285947599744E+06% E.342
    DRTR (Q(J),J=1,8), C342
    *.3306413889260115E+22, C342
    *-.3369507371721258E+20, C342
    . .1704434675708268E+18, C342
    ```
*-.5618158600403229E+15, ..... C342
-. \(1326178904074606 \mathrm{E}+13\), ..... C342
- \(-2305132440239370 \mathrm{E}+10\), ..... C342
- .2889856220077479E+87, ..... C342
-. \(2392135609522520 E+04 /\) ..... C342
DATA (P(I),I=10,18), ..... C. 342
-. \(1590162083763072 \mathrm{E}+17\), ..... C342. \(.5368395855470032 \mathrm{E}+16\),-. \(3756135827519507 E+15\),-. \(9422080573862922 E+13\),
. . \(9718863641273663 E+11\),-. \(4165980320912641 \mathrm{E}+09\),
. \(.6879907643492760 \mathrm{E}+06\),-. .3536566189687649E+03,
C342C342C342C342
C342
C342
C342
-. \(2963656768308448 \mathrm{E}-01\)
C342
DRTR (Q(I) \(, \mathrm{I}=9,16) 1\)
DATA (Q(I) \(I=9,16) /\)
\(+\quad .2606708705529648 E+17\),
-. \(2022142175869257 E+17\).
. . \(1980645892386831 \mathrm{E}+16\),
-. \(6358669883569537 E+14\),
-. \(8204440573998663 \mathrm{E}+12\),
-. \(4413044733863003 \mathrm{E}+10\),
-. \(7394714900641401 E+07\),
-. \(6697052546975880 \mathrm{E}+04 /\)
    DATA ( \(\mathrm{PO}(\mathrm{J}), \mathrm{J}=1,5)\),
-. \(7064621469033392 E-13\).
-- \(1436279642653691 \mathrm{E}-08\),
-. \(5286489105163732 \mathrm{E}-05\),
*-. \(3830439714639074 E-02\),
-.2829406075894839E+00r C342
    DRTA (QD(J), J=1,4),
-. 1770837992384417E-12,
--. \(3606859805023185 E-08\),
-. 133852024714781 DE-04,
- . \(1007723338776333 \mathrm{E}-01\),
DATA (PO(I),I \(=6,10\) )
-. \(2069343093741415 E-12\),
C342
C342
C342
C342
C342
C342
C342
C342
C342
C342
C342
C342
C342
C342
--.4422252452216457E-08,
C342
-. \(1366441906147109 E-04\),
C342
```

    --7387885439863839E-02, C342
    *.3710722095990018E+00/ C342
        DATR (QO(I),I=5,8)/ C342
    *.5187073908684608E-12. C342
    *-.1108727721754090E-07, C342
    *.3430127364212944E-04, C342
    *-.1866802289017835E-01/ C342
        I=1
        X=ZP
        Z=X-X
        IF\X .GT. 16.)\GD TD 1
        IF(X .GT. 8.) I=2
        EYEI 0= (P(1,I) +Z*(P(2,I) +Z* (P(3,I) +Z*(P(4,I) +Z*(P(5,I) +Z*(P(6,I)+Z C342
    * - (P(7,I)+Z*(P(8,I)+Z*P(9,I)) ) ) ) ) ) ) )
    - (Q(1,I)+Z*(Q(2,I)+Z*(Q(3,I)+Z*(Q(4,I)+Z*(Q(5,I)+Z*(Q(6,I)+Z
                -(Q(7,I)+Z*(Q(8,I)+Z)))))>))
    IF(I .EQ. 1) EYEIO=EXP(-X) EYEIO C342
    O-OC342
    1 z=1./(64*Z)
    Q01=\langleP0(1,1)+Z*(P0(2,1)+Z*(P0(3,1)+Z*(P0(4,1)+Z4P0(5,1)))))
    - (QO<1,1)+Z*(QO(2,1)+Z*(Q0(3,1)+Z*(QO(4,1)+Z))))
        001=001/(8*X)
        P01=(P0(1,2)+Z*(P0(2,2)+Z*(P0(3,2)+Z*(P0(4,2)+Z*P0(5,2)))))/ C342
    - (QO(1,2)+Z*(QO(2,2)+Z*(QO(3,2)+Z*(QO(4,2)+Z)))) C342
        EYEID=(P01+Q01)/SQRT(X) C342
        C342
        C342
    END FTIDN FJO(ZP)
    C340A
    ```

```

* F.jO(X) CDMPUTES THE REPL BESSEL FUMCTIOM JO DF THE REPL ARGUHENT - C340A
* X .GT . 0 C340R

```

```

    DIMENSIDN P(9,2),Q(8,2)
    C340A
DIMENSIIN PO( 5,2),QO(4,2) C340R
EQUIVALENCE (EYJO,EYEJO,FJO) C340R
C340A
DATA (P(J),J=1,9)/
C340A
*-.1030790592800841E+21, C340A

* .2305050589779804E+19,
C340A
C340A

```
    -. \(1608225312767766 E+15\),
    -. \(5864983055305724 E+12\),
    *. \(1247014316352538 E+10\),
    - \(-1441160259923904 E+07\),
    -. \(7057781986067161 \mathrm{E}+03 \rho\)
    DATA (Q( \(J\) ) \(, J=1,8\) ),
    -.1947930043950693E+22,
    -. \(1866656846683426 E+20\),
    -. \(8988812598699360 E+17\),
    -.2872923345367091E+15;
    - . \(6757621507401545 \mathrm{E}+12\),
    -. \(1218915111066339 E+10\),
    -. \(1685448234198584 E+07\),
    -. \(1690305128256799 E+04\)
    DATA ( \(\mathrm{P}(\mathrm{I}\) ) \(, \mathrm{I}=10,18\) ),
    -. \(1915735987569625 E+21\),
    -. \(1001781172709201 \mathrm{E}+20\),
    - .2205602059805950E+18,
    \(-.2402516341734763 E+16\),
- . \(1445553026998197 \mathrm{E}+14\),
-. \(5012886478578140 \mathrm{E}+11\)
-. \(9974512187863315 E+08\),
-. \(1058363049975556 E+06\),
-. 465316955954 0574E+02
    DATA ( \(\mathrm{Q}(\mathrm{I}\) ) \(\mathrm{I}=9\),16)
-. \(1915744022256219 E+21\)
-. \(1955478121458678 E+19\)
-. \(1019029152817659 E+17\)
-. \(3594650.569271279 E+14\),
-. \(9693226280485690 \mathrm{E}+11\),
-. \(2020934854546515 E+09\)
-. \(3977520908299590 €+06\).
-. \(3951153319317984 E+03\)
DATA ( \(\mathrm{PO}(J), \mathrm{J}=1,5\) ),
--.2669230889166635E-12,
-. \(3487301310346338 \mathrm{E}-08\),
-. \(1420614795808099 \mathrm{E}-04\),
-. \(8789741021455747 E-02\),
-. \(5423439.570936309 E+00\) ر
DATA (QO (J), J=1,4),
C340A C340R C340A C340A C340A C 340 A C340A C340A C340 C340 C340A C340A C 340 A C340A C340A C340A C340日 C340A C340A C340A C340 C 340 A C340A \begin{tabular}{l}
C 340 A \\
\hline
\end{tabular} C340 C340 C340A C340A C340A C340R C340A C340A C340R C340A C340A C340A C 340 A C340R C340A C340A
*-.3345384807898387E-12,
```

    *.4358138840301680E-08,
    ..1797068587349931E-04,
    -.1165656249458522E-01/
    DATR (PO(I),1=6,10)/
    *-.1616796790064454E-11% C340A
    *. .1538702516195051E-07,
    *.4.373398193154472E-04, C340R
    *. .1812080215474507E-01,
    * .7331365490421742E+00/
        COCOA
        *-.2026354274154102E-11, C340R
        * .1927565757246875E-07. C340R
    +..5490008915137954E-04,
    * .2294894906253812E-01/
    C
DRTA T=PI/4.
DATA T/.7853981633974831/
I=1
X=ZP
C
Z=X*X
Z=X\bulletX C340R
IF(X .GT. 14.)GO TD 1
IF(X .GT. 9.5) I=2
EYEJO=(P(1,I)+Z*(P(2,I)+Z*(P(3,I)+Z*<P(4,I)+Z*(P(5,I)+Z*(P(6,I)+Z C340A
- -(P(7,I)+Z*(P(8,I)+Z*P(9,I))))>))))
- (Q(1,I)+Z*(Q(2,I)+Z*(Q(3,I)+Z*(Q(4,I)+Z*(Q(5,I)+Z*(Q<6,I)+Z
-(Q(7,I)+Z*(Q(8,I)+Z)))) ) ) )
EYEJO=(1.-EYEJO\bulletZ/4.) C340R
RETIJRN
1 Z=1./(64*Z)
Q01= (P0(1,1) +Z*(P0(2,1)+Z-(P0(3,1)+Z-(P0(4,1)+Z*P0(5,1)))))/ C340R
- (Q0(1,1)+Z*(Q0(2,1)+Z*(Q0(3,1)+Z*(Q0(4,1)+Z)))) C340R
Q01=Q01/(8\&X) C340R
P01=(P0(1,2)+Z*(PO(2,2)+Z*(P0(3,2)+Z*(PO(4,2)+Z*PO(5,2)))))
- (Q0(1,2)+Z-(Q0< 2, 2)+Z*(Q0(3,2)+Z*(Q0(4,2)+Z)))) C340A
EYEJO= (P01*COS (X-T)+Q01*SIM(X-T) )/SQRT(X) C340R
RETIRNN
RETIJRN
-END DF FILE-
? END
END TEXT EDITIMG.
READY.

```
        C340A
        C340R
        C340R
        C340
        C340A
C340A
        C340R
C340R
C. 340 R
C.340A
C340A
C340A
C340A
C340A
C340R
C340A
C340A
        C340A
C340A
C340R
C340A```

