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A COMPUTER PROGRAM FOR THE KINETIC TREATMENT OF RADIATION-INDUCED SIMULTANEOUS CHEMICAL REACTIONS: A REVISED VERSION IN FORTRAN IV

by

Klaus H. Schmidt

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Chemistry

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Chemistry Division

March 1970

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ABSTRACT

WR20, a program written in OS/360 FORTRAN IV for an IBM-360/75 digital-computer system, calculates, as a function of time, the concentrations of all chemical species in a set of radiation-induced chemical reactions with homogeneous kinetics. It also calculates the concomitant changes in electrical conductivity and optical absorbance. As data, the program essentially requires the chemical reaction equations with rate constants, a list of the chemical species with their radiation yields, initial concentrations, equivalent conductances, absorptivities, etc., and the dose rate as a function of time. The program is an improved version of one described in an earlier report (ANL-7199, April 1966) written for a CDC-3600 system. The new features of the revised program, in particular, the possibility to treat reaction systems involving chain reactions and to study the effect of repetitive radiation pulses, are described, and detailed instructions are given for the use of the program. This report also describes two plotting programs to be used in connection with WR20. One creates a plot on a 780-Calcomp plotter, the other a plot on the printer.

1. INTRODUCTION

In an earlier report,* I described a program written in 3600-FORTRAN for a CDC-3600 digital-computer system which allows one to construct kinetic models for the behavior of a chemical system exposed to ionizing radiation. One enters as data the reaction equations with rate constants, a list of the chemical species involved with their radiation yields, initial concentrations, equivalent conductances, absorptivities, etc.,

*K. H. Schmidt, A Computer Program for the Kinetic Treatment of Radiation-induced Simultaneous Chemical Reactions, ANL-7199 (April 1966).

the dose rate as a function of time, and some additional instructions controlling the calculation. The program then calculates the concentrations of all species as functions of time and the changes in electrical conductivity and optical absorbance.

The original program, WR16, has been used successfully at this laboratory for several years, for the evaluation of pulse-radiolysis experiments. It was later adapted to the Laboratory's IBM-360/75 system for the following reasons: (1) Problems run two to three times faster on this machine; (2) the latter system accepts FORTRAN IV, so that the new version of the program, which is written in this language, is now much more readily adaptable to other computer systems.

During the adaptation and more recently, the program was improved in a number of ways. The Ionic Equilibrium Subroutine, which calculates the dissociation equilibrium of ionic species, was completely rewritten and is now applicable over a much wider pH range. The Steady State Subroutine, which computes the concentrations of species that have reached a steady state was also extensively modified to improve its convergence and to make it capable of calculating the equilibrium of species involved in a chain reaction. Another new option allows one to study the effect of repetitive radiation pulses. Some further modifications will be mentioned later.

This report describes the new features of the program in its present form (new name: WR20) and gives detailed instructions for its use. Reference to the previous report (ANL-7199) will be made in a few cases. Thus, the mathematical method of the main program as described in Sections 3.1-3.3 and 3.4.1 of ANL-7199 has not been changed and is therefore not described in the present report. The options of "Skipping of Species and Reactions" (Sections 4.1 and 4.2 of ANL-7199) have remained in a somewhat modified form; it is, for example, now possible to cancel skipping instructions. Furthermore, the suggestions regarding the use of the program in special cases (Section 6.1 of ANL-7199) are still valid. With these exceptions, the present report is independent of the previous one.

2. ALGORITHM OF THE NEW EQUILIBRIUM SUBROUTINES

2.1 The Ionic Equilibrium Subroutine

The Ionic Equilibrium Subroutine (named IONIC) has two entries: EQUIL1 and EQUIL2. EQUIL1 is invoked once at the beginning of a run. It reads from the data dissociation equations of the form

$$H^+ \cdot HA_i^- = H_2A_i \cdot K_{1i} \tag{1a}$$

$$H^+ \cdot A_i^= = HA_i^- \cdot K_{2i} \tag{1b}$$

or similar equations in the basic form (beginning with OH^-), with $i = 1, 2, \ldots, n_{eq}$, n_{eq} being the total number of equations. (Pairs such as 1a and 1b count as one equation.) The routine then labels those reactions that produce the above equilibrium. If, for example, it encounters Eq. 1a, it labels the reaction equations 2a and 2b, or the same reactions written in their basic form, 3a and 3b.

$$H^+ + HA_i^- \rightarrow H_2A_i \tag{2a}$$

$$\text{DUMMY} + H_2A_i \rightarrow HA_i^- + H^+ \tag{2b}$$

$$OH^- + H_2A_i \rightarrow HA_i^- + H_2O \tag{3a}$$

$$H_2O + HA_i^- \rightarrow H_2A_i + OH^-, \tag{3b}$$

DUMMY denoting a dummy species with the concentration 1 M. The reactions thus labeled* are automatically skipped by the main program when subroutine IONIC is used.

EQUIL2 is called after every 20th cycle of the main integrating algorithm and calculates the dissociation equilibrium by the following method:

$$T_{i0} = [H_2A_i]_0 + [HA_i^-]_0 + [A_i^=]_0; \tag{4}$$

$$[HA_i^-] = \frac{K_{1i}[H^+]T_{i0}}{[H^+]^2 + K_{1i}[H^+] + K_{1i}K_{2i}}; \tag{5}$$

$$[A_i^=] = \frac{K_{1i}K_{2i}T_{i0}}{[H^+]^2 + K_{1i}[H^+] + K_{1i}K_{2i}}, \tag{6}$$

where the subscript $_0$ refers to the (unreadjusted) values encountered when EQUIL2 is called.

The concentrations of all species taking part in the equilibrium can thus be expressed as functions of $[H^+]$, those of the remaining species being regarded as known constants. To maintain balance of charge, the following equation must hold:

$$F([H^+]) = \sum_{j=1}^{n_c} q_j c_j = 0, \tag{7}$$

*For more details, see Section 4.1.7.g.

n_c being the total number of species, and q_j the charge of the jth species. Equation 7 is solved by Newton's method. One obtains a fast-converging series with the recursive formula

$$[H^+]_{n+1} = [H^+]_n - F([H^+]_n)/F'([H^+]_n). \tag{8}$$

$F'([H^+]_n) = dF([H^+]_n)/d[H^+]_n$ can easily be derived from Eqs. 5 and 6. It can be shown that $F'(x) > 0$ for all $x \geq 0$, and that the series $D_n = |[H^+]_n - [H^+]_e| \leq \{A([H^+]_0 - [H^+]_e)^2\}^n$, $[H^+]_e$ being the exact solution of Eq. 7, A being a constant. After $[H^+]_e$ is obtained with sufficient accuracy, the remaining concentrations are calculated using Eqs. 5, 6, and 9.

$$[H_2A_i] = T_{i0} - [HA_i^-] - [A_i^=]. \tag{9}$$

2.2 The Steady State Subroutine

The Steady State Subroutine (named STEADY) performs a function similar to that of subroutine EQUIL3 in program WR16 (described in ANL-7199). It is used when the net rates of change of the concentrations of one or several chemical species are small compared to the actual rates of formation and disappearance. The subroutine has two options.

Option 1 is applied if the concentration of one or several species have reached a quasi-steady state, i.e., if the concentration of each species is the result of an equilibrium between its rate of formation and its rate of disappearance, and if these species are relatively independent of each other.

Option 2 goes into effect if a quasi-equilibrium exists between the concentrations of a group of species. This is the case if these species are converted into each other by a chain of fast reactions, with the sum of their concentrations changing relatively slow, either because they have reached a quasi-steady state or because the chain-terminating reactions are much slower than the chain-propagating reactions. Both options are based on the approximation.

$$\frac{dc_j}{dt} = g_j + \sum_i \alpha_{ji} k_i c'_{i1} c'_{i2} = 0, \tag{10}$$

c_j being the concentration of the jth species processed by the subroutine, c'_{i1} and c'_{i2} the concentrations of the first and second species on the left side of the ith reaction, α_{ji} the net formation of the jth species in the ith reaction, and k_i the rate constant.

Equation 10 is solved for c_j in the manner described on page 16 of ANL-7199. The result can be written in the form

$$^2c_1 = F_1(^1c_2, {}^1c_3, {}^1c_4, \ldots),$$

the upper indices 1 and 2 referring to the old and the new value of the c's, respectively. This procedure is carried through for the remaining species

$$^{2}c_2 = F_2(^{2}c_1, {}^{1}c_3, {}^{1}c_4, \ldots),$$

$$^{2}c_3 = F_3(^{2}c_1, {}^{2}c_2, {}^{1}c_4, \ldots),$$

$$^{2}c_4 = F_4(^{2}c_1, {}^{2}c_2, {}^{2}c_3, \ldots), \text{ etc.},$$

until all c's have the upper index 2. By periodic repetition of this cycle, one obtains for each species a series $^{n}c_j$ with the recursive formula

$$^{n+1}c_j = \Phi_j(^{n}c_1, {}^{n}c_2, {}^{n}c_3, \ldots), \tag{11}$$

the functions Φ_j representing the result of one entire cycle.

It can be shown that the series $^{n}c_j$ are convergent in a region around the true values c_j if, in this region,

$$\left| \frac{\partial \Phi_j}{\partial {}^{n}c_j} \right| < 1, \quad \text{i.e.,} \quad \left| \sum_{k=1}^{j-1} \frac{\partial F_j}{\partial c_k} \frac{dF_k}{dc_j} \right| < 1.$$

This is, however, equivalent to the condition that the concentrations of the species are not too strongly interdependent.

Option 1 of subroutine STEADY uses the functions Φ_j to create a faster converging series $^{m}c_j^*$ with the following recursive procedures:

$$^{1}X_j = {}^{m}c_j^*;$$

$$^{2}X_j = \Phi_j(^{1}X_1, {}^{1}X_2, \ldots);$$

$$^{3}X_j = \Phi_j(^{2}X_1, {}^{2}X_2, \ldots);$$

and

$$^{m+1}c_j^* = \frac{\left(^{2}X_j\right)^2 - {}^{1}X_j {}^{3}X_j}{2\,^{2}X_j - {}^{1}X_j - {}^{3}X_j}.$$

Option 2 uses directly the following modified version of Eq. 11:

$$^{n+1}c_j = \Phi_j(^nc_1, {}^nc_2, \ldots) \frac{\sum_{m=1}^{m_g} {}^1c_m}{\sum_{m=1}^{m_g} \Phi_m(^nc_1, {}^nc_2, \ldots)} . \tag{11'}$$

In this way,

$$\sum_{m=1}^{m_g} {}^nc_m = \sum_{m=1}^{m_g} {}^1c_m \text{ for all } n \geq 1,$$

m_g being the number of species in the respective group of interdependent species; i.e., the routine readjusts only the relative values of their concentrations while keeping their sum constant.

A further slight modification was incorporated into the subroutine: The sequence in which it processes the species is reversed after every second cycle. This does not affect the performance of Option 1. In Option 2, the modification eliminates a small error that occurs in some cases, the sign of the error depending on the sequence of the species in a group.

A rigid proof of convergence for the final algorithms of the two options was not attempted. Test runs showed, however, that both series converge fast under normal conditions. If convergence is poor, a warning message is printed.

3. INPUT AND OUTPUT

3.1 Data Cards

The program WR20 requires the following data cards:

3.1.1 One "Run Number Card" with

a: NORUN, a four-digit number assigned to the run.

Col. 2-5, FORMAT: I4

b: LIMT, the time limit in minutes allotted to the run. Default value 2.

Col. 7-8, FORMAT: I2

c: IPUNCH, a plot index. Enter 1 if a plot is desired; otherwise, leave blank.

Col. 10, FORMAT: I1

d: KOMENT, any comment that is to appear in the output.

Col. 11-65

e: MORE, the number of additional comment cards, up to nine.

Col. 66, FORMAT: I1

3.1.2 COMENT, further comments on zero to nine additional comment cards.

Col. 2-80

3.1.3 One to 50 "Reaction Cards" with

a: A(I,1) and A(I,2), the names of exactly two reacting species.

Col. 1-5 and 7-11, FORMAT: A5

b: A(I,3) - A(I,6), the names of zero to four product species.

Col. 13-17, 19-23, 25-29, and 31-35, FORMAT: A5

c: B(I,4) - B(I,6), + or - signs in Col. 18, 24, and 30 (default = +).*

d: RK, the second-order rate constant in $M^{-1}sec^{-1}$.

Col. 36-45, FORMAT: E10.3

3.1.4 One blank card, indicating the end of the List of Reactions.

3.1.5 One to 27 "Species Cards" with

a: AC, the name of the species.

Col. 1-5, FORMAT: A5

b: CHARGE, the charge of the species. In case of default, the charge is determined from the number of + or - signs in the name. For example, CO3--: charge = -2.

Col. 6-10, FORMAT: I4

c: G, the G value, i.e., the radiation yield in particles per 100 eV.

Col. 11-20, FORMAT: E10.3

*These signs will be treated by the computer as such. Example: 02- + HO2 = H2O2 - H+. However, any character in Col. 6 is treated as +.

d: S, the rate of spontaneous (thermal) formation in M sec^{-1}. Example: H^+ or OH^- from H_2O.*

Col. 21-30, FORMAT: E10.3

e: CI, the initial molar concentration.

Col. 31-40, FORMAT: E10.3

f: EQCO, the equivalent conductance in mho cm^2eq^{-1}.

Col. 41-50, FORMAT: E10.3

g: EXT, the molar absorptivity in $cm^{-1}M^{-1}$.

Col. 51-60, FORMAT: E10.3

The remaining columns may be used for identification purposes.

3.1.6 One blank card, indicating the end of the List of Species.

3.1.7 One to 50 "Time Cards" for successive time intervals, with

a: T, the end of the time interval in sec, as measured from the beginning of the first time interval.

Col. 1-10, FORMAT: E10.3

b: DR, the mean dose rate in eV $\ell^{-1}sec^{-1}$ during this time interval. (1 rad/min = 1.04×10^{15} eV $\ell^{-1}sec^{-1}$ in water.)

Col. 11-20, FORMAT: E10.3

c: SPSK(1,K) and SPSK(2,K), the names of zero to two species that are to be "skipped or labeled." The effect of listing such species depends on further instructions given on the same card. Normally the species are "skipped;" i.e., their concentrations are not changed by the integrating algorithm during this and subsequent time intervals. If IUN = -1 (see h below), the opposite effect is achieved; namely, any previous skipping instruction for these species is canceled. If IST = 1 (see f below), the species are labeled for processing by the Steady State Subroutine, Option 1, and at the same time "skipped." If IST ≥ 2, the species are labeled for Option 2 of the same subroutine, but not skipped.

Col. 21-25 and 26-30, FORMAT: 2A5

d: CSK(1,K) and CSK(2,K), the concentrations to be used for the skipped species until the skipping instruction is canceled. These values

*S cannot be used if subroutine IONIC is invoked during the run. Instead, the reaction DUMMY + H2O = OH- + H+ must be entered.

need be entered only if IUN ≥ 0 and IST = 0. In this case, CSK overrides any previously defined concentration value. Otherwise, CSK is ignored.

Col. 31-40 and 41-50, FORMAT: 2E10.3

e: NRS(1,K) - NRS(5,K), the numbers of up to five reactions that are to be "skipped," i.e., taken out of the integrating algorithm. The numbers refer to the sequential position of these reactions in the List of Reactions. As for species, previous skipping instructions for reactions may be canceled by inserting here the numbers of reactions to be "unskipped" and entering the Unskipping Instruction IUN = -1. Skipping instructions for reactions are valid until canceled, except for such instructions entered on cards with IST ≥ 1; the latter are automatically canceled by the first subsequent card with IST = 0.

Col. 52-53, 55-56, 58-59, 61-62, and 64-65, FORMAT: 5I3

f: IST, the Steady State Instruction. If IST = 0, subroutine STEADY is not invoked during the specified time interval. IST ≥ 1 invokes the subroutine for all species listed as "skipped or labeled" on this card or previous cards with IST ≥ 1.

For species labeled with IST = 1 (Option 1), the steady state (i.e., the equilibrium concentration determined by the total rate of formation and the total rate of disappearance of those species at this time) is periodically readjusted. At the same time, these species are skipped by the integrating algorithm.

If 2 ≤ IST ≤ 5 for a group of species (Option 2), the equilibrium ratio between the concentrations of these species is periodically readjusted, while the sum of their concentrations is kept constant and equal to the value encountered when STEADY is called. Species in such groups are <u>not</u> skipped by the program. It is therefore necessary to skip the <u>reactions</u> that determine their equilibrium, i.e., those that propagate the chain. Groups with different IST are treated independently of each other.

The Steady State Instruction and the labels attached to the species by the value of IST are only valid during time intervals defined by cards with IST ≥ 1; i.e., the instruction and the labels are canceled by the first subsequent card with IST = 0.

Col. 67, FORMAT: I1

g: ION, the Ionic Equilibrium Instruction. If ION = 0, subroutine IONIC is not invoked during the specified time interval. ION ≥ 1 invokes the subroutine, which then periodically adjusts the ionic equilibrium as determined by the dissociation equations listed under Eq. 10. The reactions that determined the equilibrium before are automatically skipped by the integrating algorithm. Example: When IONIC processes the dissociation equation (see 3.1.10 below).

$$[H^+] \cdot [A^-] = [HA] \cdot K,$$

the two reactions

$$DUMMY + HA \rightarrow A^- + H^+$$

and

$$H^+ + A^- \rightarrow HA$$

are skipped.

A reaction is labeled for skipping, if and only if the two species A^- and HA (or an analogous pair) in the dissociation equation also occur in the reaction equation and are located on the immediate left and right of the = sign (which stands in place of the arrow). If some other reaction containing the same pair of species is not to be skipped, it is sufficient to locate one of the species away from the = sign.

Subroutine IONIC may not be used during time intervals in which there is any nonnegligible formation or decay of the first species in the equilibrium equations (H^+ or OH^-) other than from the ionic dissociation or recombination reactions.

Col. 68, FORMAT: I1

h: IUN, an "Unskipping Instruction" for canceling skipping instructions, if this is desired. As mentioned under c and e above, IUN = -1 "unskips" all species and/or reactions listed on the same card in the columns for skipped species or reactions; IUN = -2 automatically cancels all previous skipping instructions.

Any value of IUN $\neq$ 0 causes the program to start the specified time interval with the Minimum Time Increment DTMIN. Whenever skipping instructions are canceled, either explicitly or automatically, the program is likely to require a much smaller time increment than before. Unless IUN < 0, it is therefore advisable to specify IUN = +1 on cards that cancel the use of one or both of the subroutines IONIC and STEADY.

Col. 69-70, FORMAT: I2

i: MREP, Repetition Factor. The repetition factor $2 \leq$ MREP $\leq$ 9999 on one (and only one) Time Card, say the Mth card with the time T(M), has the effect that the entire computation procedure up to the time T(M) is executed MREP times. After each cycle, the time values T(1), T(2), ..., T(M) are automatically incremented by the initial value

of T(M), and the concentrations reached are used as initial values for the next cycle. Note that the times T(M + 1), T(M + 2), ..., are not incremented. Therefore, one has to make sure that $T(M+1) \geq MREP \cdot T(M)$. Skipping instructions are not automatically canceled at the beginning of a new cycle, nor is DT reset to DTMIN. It may therefore be necessary to set IUN = -2 or +1 on the first Time Card.

Col. 72-75, FORMAT: I5

3.1.8 One blank card, indicating the end of the Time Cards.

3.1.9 One Parameter Card, with

a: ACCFAC, the Accuracy Factor. The Accuracy Factor determines the accuracy* of the integrating algorithm and (inversely) the computation time. The time increments chosen by the program are proportional to ACCFAC. Default values: ACCFAC = 0.1, if none of the subroutines IONIC and STEADY are invoked; otherwise, ACCFAC = 0.05.

Col. 1-10, FORMAT: E10.3

b: DTPMIN, the Minimum Print Interval. The Minimum Print Interval is the minimum (model) time interval between two printed lines of concentrations. In case of default, the value is chosen so that one obtains one page of printed results per group of six species, with the time values approximately equally spaced. Irrespective of the spacing, the times on the Time Cards are always printed.

Col. 11-20, FORMAT: E10.3

c: DTMIN, the Minimum Time Increment. This is the Minimum Time Increment to be used by the integrating algorithm. The algorithm starts with this value and adjusts it after every 20 cycles of computation. The default value is T(NT1)/50000, T(NT1) being the beginning of the first time interval in which one of the subroutines STEADY and IONIC is invoked, or, if this is not the case, the end of the last time interval.

Col. 21-30, FORMAT: E10.3

d: DTMAX, the Maximum Time Increment. The Maximum Time Increment sets an upper limit to the time increment DT that can be chosen by the program. Default value: T(NT)/2000, if none of the subroutines STEADY and IONIC are invoked, T(NT)/5000 otherwise, T(NT) being the end of the last time interval.

Col. 31-40, FORMAT: E10.3

*For details, see Section 3.3 of ANL-7199.

3.1.10 Zero to 10 Equilibrium Cards with dissociation equations for subroutine IONIC

The equations must be written in the form

$$H+ * A- = HA * K_a$$

or

$$OH- * B+ = BOH * K_b,$$

the K's being dissociation constants. If there are two stages of dissociation, the equation for the first stage must come first, and the two equations may not be separated:

$$H+ * HA- = H2A * K_1$$

$$H+ * A-- = HA- * K_2.$$

All equations must begin with the same species, i.e., either H+ of OH-; in other words, equations in the acid form and equations in the basic form may not be mixed.

Species (AE(1,K) - AE(3,K)): Col. 1-5, 7-11, and 13-17
Dissociation Constant (EQ): Col. 21-30

3.1.11 One blank card, indicating the end of the Equilibrium Cards (or their absence)

Any number of runs (complete data decks as described above) can be stacked for one ASP job. Normally, the time limit specified on the Job Card should equal the sum of the time limits set for the individual runs, plus 1 min. This will allow sufficient time for all ASP operations, for printing the results, and for plotting (see Chapter 5).

3.2 Example of a Computer Run

The example presented here uses essentially all features and options of program WR20. It is a kinetic model for the irradiation of a hydrogen-saturated, aqueous solution of 1 m<u>M</u> NaOH at 25°C, with three successive pulses of electrons from a linear acclerator, with a pulse duration of 6 μsec and a repetition rate of 720/sec. Most of the data used for this run are based on literature values, a few values are based on my measurements, and a few are estimates. No literature references will be given here as this would go beyond the scope of this report.

Figure 1 shows a printout of the data cards. The output obtained with these data is reproduced on pages 22-29. In the following discussion of the input data, the card numbers mentioned refer to the numbering of the Reaction, Species, and Time Cards appearing in the printed output.

3.2.1 Run Number Card

The data on this card are self-explanatory. The 1 in column 66 indicates one additional Comment Card.

3.2.2 Comment Card

No explanation is required.

3.2.3 Reaction Cards

The reaction $e^- + H_2O_2 = OH + OH^-$ has been split up into the reactions 8 and 9. Reaction 8 converts e^- into OH but does not affect H_2O_2. It will later be skipped when the reaction chain $e^- - OH - H - e^-$ is processed by subroutine STEADY. Reaction 9 removes H_2O_2 and produces OH^- without affecting e^-. Therefore it has essentially no influence on the automatically determined time increments, as opposed to reaction 8. Reactions 12 and 13 represent the dissociation equilibrium $H^+ + OH^- \rightleftharpoons H_2O$, reactions 21 and 22 the equilibrium $H^+ + O_2^- \rightleftharpoons HO_2$. The equilibrium between HO_2^- and H_2O_2 is here represented by reactions 28 and 29.* Reaction 13 can be omitted in runs that do not use subroutine IONIC, if S = 1.450E-03 is entered on the Species Cards for H^+ and OH^-.

3.2.4 Species Cards

Because no charge values were entered, they are determined by subroutine SCAN from the number of + or - signs in the names of the species. An initial concentration CI = 4.9×10^{-7} M for O_2 is assumed; this approximate level of contamination is frequently encountered. The species Na^+ is listed only for the purpose of achieving balance of charge so that subroutine IONIC can work properly. The molar absorbance (EXT) entered for e^- is for λ = 715 nm, at which wavelength no other species absorbs appreciably.

3.2.5 Time Cards

The Time Cards constitute the "time table" for the entire calculation and require particular consideration. We will therefore discuss them one by one. Before doing this, we have to establish criteria governing the

*I consider this representation more realistic under the given circumstances (pH, etc.) than the conventional form.

```
 7199    1 FORMATION OF H2O2 IN ALKALINE, H2-SATURATED H2O BY     1
 SUCCESSIVE ELECTRON PULSES FROM A LINEAR ACCELERATOR.
E-    +E-    =OH-   +OH-   +H2                5.000E+09
E-    +OH    =OH-                             3.000E+10
OH    +OH    =H2O2                            4.500E+09
OH    +O2-   =O2    +OH-                      1.200E+10
OH-   +H     =E-    +H2O                      2.000E+07
E-    +H+    =H                               2.400E+10
E-    +H     =OH-   +H2                       2.500E+10
E-    +H2O2  =OH    +H2O2                     1.300E+10
E-    +H2O2  =OH-   +E-                       1.300E+10
E-    +HO2-  =OH    +OH-   +OH-   -H2O         3.500E+09
E-    +H2O   =H     +OH-                      1.600E+01
H+    +OH-   =H2O                             1.430E+11
DUMMY+H2O    =OH-   +H+                       2.599E-05
H     +H     =H2                              8.000E+09
H     +OH    =H2O                             2.000E+10
OH    +H2    =H     +H2O                      4.500E+07
OH    +H2O2  =H2O   +HO2                      2.300E+07
H     +H2O2  =OH    +H2O                      0.900E+08
E-    +O2    =O2-                             1.900E+10
H     +O2    =HO2                             1.900E+10
DUMMY+HO2    =O2-   +H+                       8.000E+05
H+    +O2-   =HO2                             5.000E+10
HO2   +O2-   =O2    +HO2-                     7.900E+07
H     +HO2   =H2O2                            2.000E+10
H     +O2-   =HO2-                            2.000E+10
E-    +HO2   =HO2-                            2.000E+10
E-    +O2-   =HO2- -H2O   +OH-                1.000E+10
OH-   +H2O2  =HO2- +H2O                       1.000E+08
H2O   +HO2-  =H2O2 +OH-                       1.022E+04

E-          2.8                                   1.900E+02 1.850E+04
H+          2.9                       1.006E-11 3.498E+02
OH-         0.1                       1.000E-03 1.976E+02
OH          2.7
H           0.48
H2          0.45                      7.000E-04
H2O2        0.7
HO2-                                              4.450E+01
HO2         0.02
O2-                                               6.500E+01
O2                                    4.900E-07
H2O                                   5.535E+01
DUMMY                                 1.
NA+                                   1.000E-03 5.011E+01

 1.000E-08 1.000E+25H2O  DUMMY 5.535E+01 1.                                1
 5.000E-08 1.000E+25NA+  H2    1.000E-03 7.000E-04
 2.000E-06 1.000E+25H+                                                  1
 4.000E-06 1.000E+25                                                    1
 6.000E-06 1.000E+25                                                    1
 6.050E-06                                                                1
 2.000E-05          H+                                                  1
 4.000E-05                                                               1
 3.000E-04                                                               1
 3.000E-04          OH   H                          5  6  8 11 16 21
 1.389E-03          E-                                                  21        3
 5.000E-03                                                              11

            4.000E-05 1.000E-10 5.000E-06
H+   *OH-  =H2O    * 1.818E-16
H+   *O2-  =HO2    * 1.600E-05
H+   *HO2- =H2O2   * 1.780E-12
```

Fig. 1. Data Cards for Test Run 7199

use of the subroutines IONIC and STEADY. As a rule of thumb, none of these subroutines should be invoked before at least seven relaxation times of all species processed by the particular subroutine have elapsed since the last major change in dose rate. The relaxation time τ is defined here as the time during which the (small) difference between the actual concentration of a species and its (quasi-) steady-state or equilibrium concentration has decreased to the fraction $1/e$. Upper limits for the relaxation times can easily be derived from the fastest reactions in which a species is involved, as the following examples illustrate:

If an essentially independent species X disappears by first or pseudo-first order by the reaction: $X + S \rightarrow$ products (rate constant k_{XS}), $\tau = 1/(k_{XS}[S])$. For a purely second-order disappearance of the form: $X + X \rightarrow$ products (k_{XX}), $\tau = 1/(4k_{XX}[X]_0)$, $[X]_0$ being the estimated steady state value. For two species X and Y involved in a chain reaction: $X + S_1 \rightarrow Y + \ldots$ (k_1), $Y + S_2 \rightarrow X + \ldots$ (k_2), one obtains $\tau = 1/(k_1S_1 + k_2S_2)$. The case of three and more species is more complicated, but one can always obtain an upper limit for τ by disregarding some of the reactions and thus simplifying the system. For example, if three species are involved in a "triangular" chain reaction: $X + S_1 \rightarrow Y + \ldots$ (k_1), $Y + S_2 \rightarrow Z + \ldots$ (k_2), $Z + S_3 \rightarrow X + \ldots$ (k_3), with $k_3[S_3]$ being the greatest of the three products $k_i[S_i]$, one can arrive at a reasonable estimate for τ by using the greater of the two values

$$\tau' = \frac{2}{k_1[S_1] + k_2[S_2] + k_3[S_3]}$$

and

$$\tau'' = \frac{1}{k_1[S_1] + k_2[S_2]}.$$

Table I lists the species in our model with fast turnover rates, together with their estimated relaxation times, and the reactions on which these estimates are based. With the information contained in Table I, we can now discuss the Time Cards.

TABLE I. Species with Fast Turnover Rates in Run 7199 with Fastest Reactions and Relaxation Times

(Group of) Species	Fastest Reaction(s)	Relaxation Time τ, sec	7τ, sec
H^+	12	7×10^{-9}	5×10^{-8}
H_2O_2, HO_2^-	28, 29	1.5×10^{-6}	1×10^{-5}
HO_2, O_2^-	21, 22	1.25×10^{-6}	9×10^{-6}
e^-, OH, H	8,[a] 16, 5	3.8×10^{-5}	3×10^{-4}

[a] $H_2O_2 = 3 \times 10^{-7}$ M estimated from trial run.

Card 1 is used to skip permanently the species H_2O and DUMMY, starting from time zero, and determines their (constant) concentration. It further contains the instruction IUN = +1, which causes the program to reset the time increment DT to DTMIN each time it cycles back from card 11 to card 1. (The latter instruction would not be necessary for the first cycle.)

Card 2 skips Na^+ after 10^{-9} sec.* Although it would be desirable to skip this species from the beginning, this is not possible since only two species can be skipped on each card. As a compromise, we specified on card 1 a short time of only a few time increments (zero is not allowed).

Card 3 invokes subroutine STEADY for H^+, starting after 5×10^{-8} sec (see Table I).

Card 4 forces a printout of concentration values at the time specified.

Card 5 marks the end of the irradiation pulse.

Card 6 cancels the use of subroutine STEADY for H^+ at the end of the pulse by setting IST = 0, and causes the program to reset DT to DTMIN by specifying IUN = 1.

Card 7 reinvokes STEADY for H^+, starting at the time specified on card 6, i.e., 5×10^{-8} sec after the end of the pulse.

Card 8 cancels subroutine STEADY for H^+ and at the same time invokes subroutine IONIC for all ionic species (including H^+) occurring in the dissociation equations (see 3.2.7).

Card 9 sets the time for invoking STEADY for the group consisting of the species e^-, OH, and H (see Table I).

Card 10 labels OH and H for processing by subroutine STEADY, Option 2, and "skips" all reactions that convert one of the species e^-, H, and OH into another without affecting other species. Because the same time is punched on cards 9 and 10, no calculation is initiated.

Card 11 adds e^- to the group to be processed by subroutine STEADY, Option 2, and invokes this subroutine. It furthermore gives the instruction MREP = 3 to repeat three times the entire calculation program up to 1.389×10^{-3} sec, i.e., up to 4.167×10^{-3} sec.

Card 12 defines the end of the calculation.

*Since the time specified on a Dose Rate Card denotes the end of the respective time interval, all instructions on a given card come into effect at the time specified on the previous card.

3.2.6 Parameter Card

No Accuracy Factor is specified; therefore the default value of 0.05 is used.

The Minimum Print Interval DTPMIN is chosen so as to cause a printout of two pages per group of six species (~110 lines).

The specified Minimum Time Increment DTMIN = 10^{-10} sec is 1/50 of the shortest relaxation time (see Table I). The default value would be 10^{-12} sec. Because the program resets DT to DTMIN six times, the latter value would cause an unnecessary increase in computing time.

The Maximum Time Increment DTMAX = 5×10^{-6} sec is 2.5 times the default value. However, the actual value used by the computer is 3.277×10^{-6} sec (double this value would exceed the given limit).

3.2.7 Equilibrium Cards

The Equilibrium Cards contain the equations for the dissociation equilibrium of H_2O, HO_2, and H_2O_2, the asterisks representing multiplication points. Note that the third equation corresponds to reactions 28 and 29. When subroutine IONIC is invoked, reactions 12, 13, 21, 22, 28, and 29 are automatically "skipped."

3.3 Additional Remarks

The example presented in Section 3.2 has been constructed somewhat artifically to demonstrate the use of as many options of the program as possible and to provide a suitable set of test data. For a practical calculation, it would not have been necessary to invoke subroutine STEADY, Option 2, for the group of species e^-, H, and OH and to split up the reaction $e^- + H_2O_2$ for this purpose, since the thereby accomplished reduction in computing time is much less than the time wasted for unsuccessful trial runs. Also, the program would have run quite satisfactorily with the default values for DTMIN, DTMAX, and even DTPMIN (i.e., with a blank parameter card). The main purpose of specifying a smaller value of DTPMIN was to obtain a better resolution of the printed plot (see Section 5.2.2), since the plotting program PROTWR20 performs a linear interpolation between the printed concentration values.

As a further simplification, the species HO_2 could have been replaced by O_2^- where applicable, omitting the reactions 21, 22, 23, 24, and 26.

As a general rule, the subroutine IONIC and STEADY should only be used if a <u>considerable</u> reduction in computing time can thereby be achieved.

RUN NUMBER 7199 FORMATION OF H2O2 IN ALKALINE, H -SAT. H2O BY SUCCESSIVE ELECTRON PULSES FROM A LINEAR ACCELERATOR.
TIME LIMIT 2 MIN

E-	+	E-	=	OH-	+	OH-	+	H2			K(1) = 5.000E 09
E-	+	OH	=	OH-							K(2) = 3.000E 10
OH	+	OH	=	H2O2							K(3) = 4.500E 09
OH	+	O2-	=	O2	+	OH-					K(4) = 1.200E 10
OH-	+	H	=	E-	+	H2O					K(5) = 2.000E 07
E-	+	H+	=	H							K(6) = 2.400E 10
E-	+	H	=	OH-	+	H2					K(7) = 2.500E 10
E-	+	H2O2	=	OH	+	H2O2					K(8) = 1.300E 10
E-	+	H2O2	=	OH-	+	E-					K(9) = 1.300E 10
E-	+	HO2-	=	OH	+	OH-	+	OH-	-	H2O	K(10) = 3.500E 09
E-	+	H2O	=	H	+	OH-					K(11) = 1.600E 01
H+	+	OH-	=	H2O							K(12) = 1.430E 11
DUMMY	+	H2O	=	OH-	+	H+					K(13) = 2.599E-05
H	+	H	=	H2							K(14) = 8.000E 09
H	+	OH	=	H2O							K(15) = 2.000E 10
OH	+	H2	=	H	+	H2O					K(16) = 4.500E 07
OH	+	H2O2	=	H2O	+	HO2					K(17) = 2.300E 07
H	+	H2O2	=	OH	+	H2O					K(18) = 9.000E 07
E-	+	O2	=	O2-							K(19) = 1.900E 10
H	+	O2	=	HO2							K(20) = 1.900E 10
DUMMY	+	HO2	=	O2-	+	H+					K(21) = 8.000E 05
H+	+	O2-	=	HO2							K(22) = 5.000E 10
HO2	+	O2-	=	O2	+	HO2-					K(23) = 7.900E 07
H	+	HO2	=	H2O2							K(24) = 2.000E 10
H	+	O2-	=	HO2-							K(25) = 2.000E 10
E-	+	HO2	=	HO2-							K(26) = 2.000E 10
E-	+	O2-	=	HO2-	-	H2O	+	OH-			K(27) = 1.000E 10
OH	+	H2O2	=	HO2-	+	H2O					K(28) = 1.000E 08
H2O	+	HO2-	=	H2O2	+	OH-					K(29) = 1.022E 04

NO	NAME	CHARGE	G	S	CI	EQCO	EXT
1	E-	-1	2.800	0.0	0.0	190.000	1.850E 04
2	H+	1	2.900	0.0	1.006E-11	349.800	0.0
3	OH-	-1	0.100	0.0	1.000E-03	197.600	0.0
4	OH	0	2.700	0.0	0.0	0.0	0.0
5	H	0	0.480	0.0	0.0	0.0	0.0
6	H2	0	0.450	0.0	7.000E-04	0.0	0.0
7	H2O2	0	0.700	0.0	0.0	0.0	0.0
8	HO2-	-1	0.0	0.0	0.0	44.500	0.0
9	HO2	0	0.020	0.0	0.0	0.0	0.0
10	O2-	-1	0.0	0.0	0.0	65.000	0.0
11	O2	0	0.0	0.0	4.900E-07	0.0	0.0
12	H2O	0	0.0	0.0	5.535E 01	0.0	0.0
13	DUMMY	0	0.0	0.0	1.000E 00	0.0	0.0
14	HA+	1	0.0	0.0	1.000E-03	50.110	0.0

INITIAL CONDUCTIVITY = 2.477E-04 MHO/CM
INITIAL ABSORBANCE = 0.0 MHO/CM

NO	TIME SEC	DOSE RATE EV/L-SEC	SPECIES SKIPPED OR LABELED		CSK1 MOLES/L	CSK2 MOLES/L	REACTIONS (UN-) SKIPPED					IST	IDN	IUN	REP
1	1.000E-08	1.000E 25	H2O	DUMMY	5.530E 01	1.000E 00	0	0	0	0	0	0	0	1	0
2	5.000E-08	1.000E 25	NA+	H2	1.000E-03	7.000E-04	0	0	0	0	0	0	0	0	0
3	2.000E-06	1.000E 25	H+		0.0	0.0	0	0	0	0	0	1	0	0	0
4	4.000E-06	1.000E 25			0.0	0.0	0	0	0	0	0	1	0	0	0
5	6.000E-06	1.000E 25			0.0	0.0	0	0	0	0	0	1	0	0	0
6	6.050E-06	0.0			0.0	0.0	0	0	0	0	0	0	0	1	0
7	2.000E-05	0.0	H+		0.0	0.0	0	0	0	0	0	1	0	0	0
8	4.000E-05	0.0			0.0	0.0	0	0	0	0	0	0	1	0	0
9	3.000E-04	0.0			0.0	0.0	0	0	0	0	0	0	1	0	0
10	3.000E-04	0.0	OH	H	0.0	0.0	5	6	8	11	16	2	1	0	0
11	1.389E-03	0.0	E-		0.0	0.0	0	0	0	0	0	2	1	0	3
12	5.000E-03	0.0			0.0	0.0	0	0	0	0	0	1	1	0	0

IRRADIATION PATTERN OF THE FIRST 1.389E-03 SEC REPEATED 3 TIMES

ACCURACY FACTOR 5.000E-02
MINIMUM PRINT INTERVAL 4.000E-05 SEC
MINIMUM TIME INCREMENT 1.000E-10 SEC
MAXIMUM TIME INCREMENT 5.000E-06 SEC

H+ * OH- = H2O * 1.818D-16
H+ * O2- = HO2 * 1.600D-05
H+ * HO2- = H2O2 * 1.780D-12

TIME SECONDS	E- MOLES/L	H+ MOLES/L	OH- MOLES/L	OH MOLES/L	H MOLES/L	H2 MOLES/L
0.0	0.0	1.006E-11	1.000E-03	0.0	0.0	7.000E-04
1.000E-08	4.649E-09	2.572E-09	1.000E-03	4.482E-09	7.975E-10	7.000E-04
5.000E-08	2.324E-08	3.375E-09	1.000E-03	2.240E-08	4.000E-09	7.000E-04
2.000E-06	8.981E-07	3.403E-09	9.991E-04	8.488E-07	1.776E-07	7.000E-04
4.000E-06	1.651E-06	3.419E-09	9.983E-04	1.543E-06	3.654E-07	7.000E-04
6.000E-06	2.198E-06	3.429E-09	9.977E-04	2.048E-06	5.321E-07	7.000E-04
6.050E-06	2.186E-06	5.775E-11	9.977E-04	2.036E-06	5.319E-07	7.000E-04
2.000E-05	8.318E-07	2.611E-11	9.990E-04	6.493E-07	4.229E-07	7.000E-04
4.000E-05	4.567E-07	1.006E-11	9.992E-04	2.372E-07	2.813E-07	7.000E-04
8.096E-05	2.558E-07	1.006E-11	9.995E-04	7.203E-08	1.279E-07	7.000E-04
1.465E-04	1.424E-07	1.006E-11	9.996E-04	3.079E-08	5.286E-08	7.000E-04
2.120E-04	9.013E-08	1.006E-11	9.996E-04	1.869E-08	3.072E-08	7.000E-04
2.776E-04	6.177E-08	1.006E-11	9.997E-04	1.253E-08	2.059E-08	7.000E-04
3.000E-04	5.497E-08	1.006E-11	9.997E-04	1.109E-08	1.825E-08	7.000E-04
3.491E-04	4.193E-08	1.006E-11	9.997E-04	7.985E-09	1.618E-08	7.000E-04
4.147E-04	3.136E-08	1.006E-11	9.997E-04	5.926E-09	1.187E-08	7.000E-04
4.802E-04	2.398E-08	1.006E-11	9.997E-04	4.492E-09	8.949E-09	7.000E-04
5.457E-04	1.863E-08	1.006E-11	9.997E-04	3.466E-09	6.878E-09	7.000E-04
6.113E-04	1.465E-08	1.006E-11	9.997E-04	2.710E-09	5.360E-09	7.000E-04
6.768E-04	1.162E-08	1.006E-11	9.998E-04	2.139E-09	4.222E-09	7.000E-04
7.423E-04	9.274E-09	1.006E-11	9.998E-04	1.702E-09	3.353E-09	7.000E-04
8.079E-04	7.430E-09	1.006E-11	9.998E-04	1.382E-09	2.673E-09	7.000E-04
8.734E-04	5.987E-09	1.006E-11	9.998E-04	1.114E-09	2.146E-09	7.000E-04
9.389E-04	4.841E-09	1.006E-11	9.998E-04	8.994E-10	1.731E-09	7.000E-04
1.004E-03	3.925E-09	1.006E-11	9.998E-04	7.282E-10	1.400E-09	7.000E-04
1.070E-03	3.189E-09	1.006E-11	9.998E-04	5.910E-10	1.136E-09	7.000E-04
1.136E-03	2.596E-09	1.006E-11	9.998E-04	4.806E-10	9.232E-10	7.000E-04
1.201E-03	2.116E-09	1.006E-11	9.998E-04	3.914E-10	7.515E-10	7.000E-04
1.267E-03	1.726E-09	1.006E-11	9.998E-04	3.191E-10	6.126E-10	7.000E-04
1.332E-03	1.410E-09	1.006E-11	9.998E-04	2.605E-10	4.999E-10	7.000E-04
1.389E-03	1.183E-09	1.006E-11	9.998E-04	2.179E-10	4.194E-10	7.000E-04
1.389E-03	1.170E-08	3.246E-09	9.998E-04	1.036E-08	2.226E-09	7.000E-04
1.389E-03	4.545E-08	3.379E-09	9.997E-04	4.286E-08	8.068E-09	7.000E-04
1.391E-03	9.320E-07	3.400E-09	9.989E-04	8.830E-07	1.862E-07	7.000E-04
1.393E-03	1.681E-06	3.406E-09	9.982E-04	1.584E-06	3.775E-07	7.000E-04
1.395E-03	2.218E-06	3.410E-09	9.976E-04	2.096E-06	5.476E-07	7.000E-04
1.395E-03	2.195E-06	3.463E-11	9.976E-04	2.074E-06	5.473E-07	7.000E-04
1.409E-03	8.122E-07	1.397E-11	9.991E-04	7.023E-07	4.576E-07	7.000E-04
1.429E-03	4.447E-07	1.006E-11	9.993E-04	2.775E-07	3.281E-07	7.000E-04
1.470E-03	2.619E-07	1.006E-11	9.995E-04	9.545E-08	1.695E-07	7.000E-04
1.535E-03	1.632E-07	1.006E-11	9.997E-04	4.513E-08	8.016E-08	7.000E-04
1.601E-03	1.160E-07	1.006E-11	9.997E-04	2.939E-08	5.059E-08	7.000E-04
1.667E-03	8.910E-08	1.006E-11	9.998E-04	2.122E-08	3.649E-08	7.000E-04
1.689E-03	8.240E-08	1.006E-11	9.998E-04	1.928E-08	3.319E-08	7.000E-04
1.738E-03	6.965E-08	1.006E-11	9.998E-04	1.532E-08	2.904E-08	7.000E-04
1.804E-03	5.822E-08	1.006E-11	9.998E-04	1.235E-08	2.332E-08	7.000E-04
1.869E-03	4.979E-08	1.006E-11	9.998E-04	1.023E-08	1.929E-08	7.000E-04
1.935E-03	4.331E-08	1.006E-11	9.998E-04	8.653E-09	1.631E-08	7.000E-04
2.000E-03	3.819E-08	1.006E-11	9.998E-04	7.444E-09	1.402E-08	7.000E-04
2.066E-03	3.401E-08	1.006E-11	9.998E-04	6.507E-09	1.221E-08	7.000E-04
2.131E-03	3.057E-08	1.006E-11	9.998E-04	5.734E-09	1.076E-08	7.000E-04
2.197E-03	2.767E-08	1.006E-11	9.999E-04	5.099E-09	9.571E-09	7.000E-04
2.262E-03	2.520E-08	1.005E-11	9.999E-04	4.568E-09	8.578E-09	7.000E-04
2.328E-03	2.307E-08	1.005E-11	9.999E-04	4.120E-09	7.740E-09	7.000E-04
2.393E-03	2.121E-08	1.005E-11	9.999E-04	3.737E-09	7.023E-09	7.000E-04

2.459E-03	1.958E-08	1.005E-11	9.999E-04	3.406E-09	6.405E-09	7.000E-04
2.525E-03	1.814E-08	1.005E-11	9.999E-04	3.118E-09	5.867E-09	7.000E-04
2.590E-03	1.686E-08	1.005E-11	9.999E-04	2.866E-09	5.395E-09	7.000E-04
2.656E-03	1.571E-08	1.005E-11	9.999E-04	2.643E-09	4.978E-09	7.000E-04
2.721E-03	1.467E-08	1.005E-11	9.999E-04	2.445E-09	4.608E-09	7.000E-04
2.776E-03	1.385E-08	1.005E-11	9.999E-04	2.289E-09	4.320E-09	7.000E-04
2.778E-03	2.437E-08	3.245E-09	9.999E-04	1.243E-08	6.126E-09	7.000E-04
2.778E-03	5.813E-08	3.379E-09	9.998E-04	4.494E-08	1.197E-08	7.000E-04
2.780E-03	9.464E-07	3.399E-09	9.990E-04	8.854E-07	1.905E-07	7.000E-04
2.782E-03	1.699E-06	3.404E-09	9.983E-04	1.586E-06	3.827E-07	7.000E-04
2.784E-03	2.242E-06	3.406E-09	9.977E-04	2.098E-06	5.541E-07	7.000E-04
2.784E-03	2.219E-06	3.141E-11	9.977E-04	2.076E-06	5.538E-07	7.000E-04
2.798E-03	8.459E-07	1.106E-11	9.991E-04	6.987E-07	4.674E-07	7.000E-04
2.818E-03	4.786E-07	1.006E-11	9.994E-04	2.731E-07	3.371E-07	7.000E-04
2.859E-03	2.949E-07	1.006E-11	9.996E-04	9.293E-08	1.749E-07	7.000E-04
2.924E-03	1.939E-07	1.006E-11	9.997E-04	4.419E-08	8.270E-08	7.000E-04
2.990E-03	1.439E-07	1.006E-11	9.998E-04	2.909E-08	5.249E-08	7.000E-04
3.056E-03	1.146E-07	1.006E-11	9.998E-04	2.122E-08	3.826E-08	7.000E-04
3.078E-03	1.072E-07	1.006E-11	9.998E-04	1.935E-08	3.494E-08	7.000E-04
3.127E-03	9.236E-08	1.006E-11	9.998E-04	1.577E-08	3.120E-08	7.000E-04
3.193E-03	7.954E-08	1.006E-11	9.998E-04	1.282E-08	2.537E-08	7.000E-04
3.258E-03	6.998E-08	1.005E-11	9.999E-04	1.071E-08	2.125E-08	7.000E-04
3.324E-03	6.256E-08	1.005E-11	9.999E-04	9.149E-09	1.819E-08	7.000E-04
3.389E-03	5.663E-08	1.005E-11	9.999E-04	7.945E-09	1.584E-08	7.000E-04
3.455E-03	5.176E-08	1.005E-11	9.999E-04	6.992E-09	1.399E-08	7.000E-04
3.520E-03	4.769E-08	1.005E-11	9.999E-04	6.231E-09	1.248E-08	7.000E-04
3.586E-03	4.423E-08	1.005E-11	9.999E-04	5.596E-09	1.125E-08	7.000E-04
3.651E-03	4.126E-08	1.005E-11	9.999E-04	5.065E-09	1.022E-08	7.000E-04
3.717E-03	3.868E-08	1.005E-11	9.999E-04	4.615E-09	9.341E-09	7.000E-04
3.782E-03	3.641E-08	1.005E-11	9.999E-04	4.230E-09	8.592E-09	7.000E-04
3.848E-03	3.440E-08	1.005E-11	9.999E-04	3.897E-09	7.943E-09	7.000E-04
3.914E-03	3.260E-08	1.005E-11	9.999E-04	3.607E-09	7.376E-09	7.000E-04
3.979E-03	3.099E-08	1.005E-11	9.999E-04	3.351E-09	6.878E-09	7.000E-04
4.045E-03	2.953E-08	1.005E-11	9.999E-04	3.126E-09	6.436E-09	7.000E-04
4.110E-03	2.821E-08	1.005E-11	9.999E-04	2.924E-09	6.042E-09	7.000E-04
4.167E-03	2.715E-08	1.005E-11	9.999E-04	2.766E-09	5.733E-09	7.000E-04
4.265E-03	2.551E-08	1.005E-11	9.999E-04	2.527E-09	5.262E-09	7.000E-04
4.331E-03	2.452E-08	1.005E-11	9.999E-04	2.386E-09	4.984E-09	7.000E-04
4.396E-03	2.361E-08	1.005E-11	9.999E-04	2.257E-09	4.731E-09	7.000E-04
4.462E-03	2.276E-08	1.005E-11	9.999E-04	2.140E-09	4.500E-09	7.000E-04
4.527E-03	2.198E-08	1.005E-11	9.999E-04	2.033E-09	4.288E-09	7.000E-04
4.593E-03	2.124E-08	1.005E-11	9.999E-04	1.935E-09	4.093E-09	7.000E-04
4.658E-03	2.055E-08	1.005E-11	9.999E-04	1.844E-09	3.913E-09	7.000E-04
4.724E-03	1.991E-08	1.005E-11	9.999E-04	1.761E-09	3.747E-09	7.000E-04
4.789E-03	1.931E-08	1.005E-11	9.999E-04	1.683E-09	3.593E-09	7.000E-04
4.855E-03	1.874E-08	1.005E-11	9.999E-04	1.611E-09	3.449E-09	7.000E-04
4.920E-03	1.820E-08	1.005E-11	9.999E-04	1.544E-09	3.316E-09	7.000E-04
4.986E-03	1.770E-08	1.005E-11	9.999E-04	1.482E-09	3.191E-09	7.000E-04
5.000E-03	1.759E-08	1.005E-11	9.999E-04	1.467E-09	3.165E-09	7.000E-04

TIME SECONDS	H2O2 MOLES/L	HO2- MOLES/L	HO2 MOLES/L	O2- MOLES/L	O2 MOLES/L	H2O MOLES/L
0.0	0.0	0.0	0.0	0.0	4.900E-07	5.535E 01
1.000E-08	1.162E-09	1.202E-17	3.311E-11	3.486E-13	4.900E-07	5.530E 01
5.000E-08	5.811E-09	1.513E-15	1.637E-10	8.698E-12	4.900E-07	5.530E 01
2.000E-06	2.329E-07	1.168E-10	4.271E-09	1.216E-08	4.801E-07	5.530E 01
4.000E-06	4.672E-07	9.837E-10	6.594E-09	4.203E-08	4.532E-07	5.530E 01
6.000E-06	7.016E-07	3.078E-09	8.151E-09	7.978E-08	4.163E-07	5.530E 01
6.050E-06	7.016E-07	3.144E-09	8.017E-09	8.074E-08	4.154E-07	5.530E 01
2.000E-05	6.717E-07	5.534E-09	2.867E-09	1.758E-07	2.796E-07	5.530E 01
4.000E-05	5.521E-07	9.768E-08	1.250E-13	1.989E-07	2.095E-07	5.530E 01
8.096E-05	5.212E-07	9.223E-08	1.255E-13	1.997E-07	1.490E-07	5.530E 01
1.465E-04	4.882E-07	8.641E-08	1.200E-13	1.909E-07	1.120E-07	5.530E 01
2.120E-04	4.678E-07	8.280E-08	1.153E-13	1.834E-07	9.572E-08	5.530E 01
2.776E-04	4.544E-07	8.044E-08	1.117E-13	1.777E-07	8.658E-08	5.530E 01
3.000E-04	4.509E-07	7.981E-08	1.107E-13	1.761E-07	8.431E-08	5.530E 01
3.491E-04	4.447E-07	7.872E-08	1.088E-13	1.731E-07	8.029E-08	5.530E 01
4.147E-04	4.386E-07	7.764E-08	1.067E-13	1.698E-07	7.645E-08	5.530E 01
4.802E-04	4.340E-07	7.682E-08	1.052E-13	1.673E-07	7.371E-08	5.530E 01
5.457E-04	4.304E-07	7.619E-08	1.040E-13	1.654E-07	7.167E-08	5.530E 01
6.113E-04	4.276E-07	7.569E-08	1.030E-13	1.639E-07	7.013E-08	5.530E 01
6.768E-04	4.254E-07	7.530E-08	1.023E-13	1.627E-07	6.894E-08	5.530E 01
7.423E-04	4.237E-07	7.499E-08	1.017E-13	1.618E-07	6.801E-08	5.530E 01
8.079E-04	4.223E-07	7.474E-08	1.012E-13	1.610E-07	6.728E-08	5.530E 01
8.734E-04	4.211E-07	7.454E-08	1.008E-13	1.604E-07	6.670E-08	5.530E 01
9.389E-04	4.202E-07	7.438E-08	1.005E-13	1.599E-07	6.623E-08	5.530E 01
1.004E-03	4.195E-07	7.425E-08	1.003E-13	1.595E-07	6.586E-08	5.530E 01
1.070E-03	4.189E-07	7.415E-08	1.001E-13	1.592E-07	6.556E-08	5.530E 01
1.136E-03	4.184E-07	7.406E-08	9.991E-14	1.590E-07	6.532E-08	5.530E 01
1.201E-03	4.180E-07	7.399E-08	9.977E-14	1.588E-07	6.512E-08	5.530E 01
1.267E-03	4.177E-07	7.393E-08	9.966E-14	1.586E-07	6.497E-08	5.530E 01
1.332E-03	4.174E-07	7.368E-08	9.957E-14	1.584E-07	6.484E-08	5.530E 01
1.389E-03	4.172E-07	7.385E-08	9.951E-14	1.583E-07	6.474E-08	5.530E 01
1.389E-03	4.208E-07	7.291E-08	7.504E-11	1.583E-07	6.474E-08	5.530E 01
1.389E-03	4.321E-07	6.998E-08	3.074E-10	1.583E-07	6.474E-08	5.530E 01
1.391E-03	7.049E-07	2.434E-08	3.500E-09	1.592E-07	6.508E-08	5.530E 01
1.393E-03	9.427E-07	1.179E-08	4.315E-09	1.580E-07	6.585E-08	5.530E 01
1.395E-03	1.164E-06	9.740E-09	4.643E-09	1.541E-07	6.668E-08	5.530E 01
1.395E-03	1.164E-06	9.735E-09	4.359E-09	1.539E-07	6.671E-08	5.530E 01
1.409E-03	1.048E-06	4.075E-09	6.989E-10	1.179E-07	6.252E-08	5.530E 01
1.429E-03	8.182E-07	1.448E-07	6.226E-14	9.902E-08	5.252E-08	5.530E 01
1.470E-03	7.263E-07	1.285E-07	5.175E-14	8.232E-08	3.921E-08	5.530E 01
1.535E-03	6.398E-07	1.132E-07	4.418E-14	7.029E-08	2.939E-08	5.530E 01
1.601E-03	5.864E-07	1.038E-07	3.994E-14	6.354E-08	2.457E-08	5.530E 01
1.667E-03	5.493E-07	9.723E-08	3.707E-14	5.898E-08	2.162E-08	5.530E 01
1.689E-03	5.389E-07	9.539E-08	3.628E-14	5.772E-08	2.085E-08	5.530E 01
1.738E-03	5.195E-07	9.196E-08	3.477E-14	5.532E-08	1.942E-08	5.530E 01
1.804E-03	4.986E-07	8.827E-08	3.313E-14	5.272E-08	1.797E-08	5.530E 01
1.869E-03	4.816E-07	8.525E-08	3.182E-14	5.063E-08	1.683E-08	5.530E 01
1.935E-03	4.672E-07	8.271E-08	3.073E-14	4.889E-08	1.592E-08	5.530E 01
2.000E-03	4.550E-07	8.055E-08	2.981E-14	4.743E-08	1.517E-08	5.530E 01
2.066E-03	4.444E-07	7.867E-08	2.902E-14	4.617E-08	1.454E-08	5.530E 01
2.131E-03	4.351E-07	7.702E-08	2.833E-14	4.508E-08	1.400E-08	5.530E 01
2.197E-03	4.269E-07	7.557E-08	2.772E-14	4.412E-08	1.353E-08	5.530E 01
2.262E-03	4.195E-07	7.427E-08	2.719E-14	4.326E-08	1.312E-08	5.530E 01
2.328E-03	4.129E-07	7.310E-08	2.671E-14	4.250E-08	1.276E-08	5.530E 01
2.393E-03	4.069E-07	7.204E-08	2.628E-14	4.181E-08	1.243E-08	5.530E 01

2.459E-03	4.015E-07	7.107E-08	2.589E-14	4.119E-08	1.214E-08	5.530E 01
2.525E-03	3.965E-07	7.019E-08	2.553E-14	4.063E-08	1.188E-08	5.530E 01
2.590E-03	3.919E-07	6.938E-08	2.521E-14	4.011E-08	1.165E-08	5.530E 01
2.656E-03	3.877E-07	6.864E-08	2.491E-14	3.964E-08	1.143E-08	5.530E 01
2.721E-03	3.839E-07	6.795E-08	2.463E-14	3.920E-08	1.123E-08	5.530E 01
2.778E-03	3.807E-07	6.740E-08	2.441E-14	3.885E-08	1.108E-08	5.530E 01
2.778E-03	3.842E-07	6.654E-08	7.463E-11	3.885E-08	1.108E-08	5.530E 01
2.778E-03	3.953E-07	6.387E-08	3.053E-10	3.886E-08	1.108E-08	5.530E 01
2.780E-03	6.638E-07	2.123E-08	3.361E-09	4.157E-08	1.128E-08	5.530E 01
2.782E-03	8.990E-07	8.066E-09	3.961E-09	4.517E-08	1.187E-08	5.530E 01
2.784E-03	1.118E-06	4.670E-09	4.077E-09	4.774E-08	1.280E-08	5.530E 01
2.784E-03	1.117E-06	4.610E-09	3.786E-09	4.782E-09	1.285E-08	5.530E 01
2.798E-03	9.768E-07	1.376E-09	1.795E-10	3.593E-09	1.447E-08	5.530E 01
2.818E-03	7.409E-07	1.311E-07	1.821E-14	2.896E-08	1.257E-08	5.530E 01
2.859E-03	6.334E-07	1.121E-07	1.456E-14	2.316E-08	9.340E-09	5.530E 01
2.924E-03	5.351E-07	9.472E-08	1.203E-14	1.913E-08	6.808E-09	5.530E 01
2.990E-03	4.748E-07	8.405E-08	1.063E-14	1.691E-08	5.535E-09	5.530E 01
3.056E-03	4.329E-07	7.663E-08	9.685E-15	1.541E-08	4.766E-09	5.530E 01
3.078E-03	4.212E-07	7.455E-08	9.424E-15	1.500E-08	4.537E-09	5.530E 01
3.127E-03	3.992E-07	7.066E-08	8.923E-15	1.420E-08	4.152E-09	5.530E 01
3.193E-03	3.753E-07	6.644E-08	8.375E-15	1.333E-08	3.755E-09	5.530E 01
3.258E-03	3.557E-07	6.297E-08	7.930E-15	1.262E-08	3.443E-09	5.530E 01
3.324E-03	3.391E-07	6.003E-08	7.559E-15	1.203E-08	3.190E-09	5.530E 01
3.389E-03	3.248E-07	5.751E-08	7.242E-15	1.152E-08	2.980E-09	5.530E 01
3.455E-03	3.124E-07	5.530E-08	6.967E-15	1.109E-08	2.801E-09	5.530E 01
3.520E-03	3.013E-07	5.335E-08	6.725E-15	1.070E-08	2.648E-09	5.530E 01
3.586E-03	2.915E-07	5.160E-08	6.510E-15	1.036E-08	2.514E-09	5.530E 01
3.651E-03	2.826E-07	5.003E-08	6.317E-15	1.005E-08	2.396E-09	5.530E 01
3.717E-03	2.745E-07	4.860E-08	6.142E-15	9.774E-09	2.291E-09	5.530E 01
3.782E-03	2.671E-07	4.729E-08	5.983E-15	9.521E-09	2.196E-09	5.530E 01
3.848E-03	2.604E-07	4.609E-08	5.837E-15	9.289E-09	2.111E-09	5.530E 01
3.914E-03	2.541E-07	4.499E-08	5.703E-15	9.075E-09	2.033E-09	5.530E 01
3.979E-03	2.483E-07	4.396E-08	5.579E-15	8.877E-09	1.963E-09	5.530E 01
4.045E-03	2.429E-07	4.300E-08	5.463E-15	8.694E-09	1.898E-09	5.530E 01
4.110E-03	2.379E-07	4.211E-08	5.355E-15	8.522E-09	1.838E-09	5.530E 01
4.167E-03	2.337E-07	4.138E-08	5.267E-15	8.382E-09	1.789E-09	5.530E 01
4.265E-03	2.271E-07	4.021E-08	5.127E-15	8.158E-09	1.712E-09	5.530E 01
4.331E-03	2.230E-07	3.948E-08	5.040E-15	8.020E-09	1.665E-09	5.530E 01
4.396E-03	2.191E-07	3.880E-08	4.957E-15	7.889E-09	1.621E-09	5.530E 01
4.462E-03	2.155E-07	3.815E-08	4.879E-15	7.765E-09	1.580E-09	5.530E 01
4.527E-03	2.120E-07	3.753E-08	4.806E-15	7.647E-09	1.542E-09	5.530E 01
4.593E-03	2.087E-07	3.694E-08	4.735E-15	7.536E-09	1.505E-09	5.530E 01
4.658E-03	2.055E-07	3.639E-08	4.669E-15	7.430E-09	1.471E-09	5.530E 01
4.724E-03	2.025E-07	3.585E-08	4.605E-15	7.328E-09	1.438E-09	5.530E 01
4.789E-03	1.996E-07	3.535E-08	4.544E-15	7.231E-09	1.408E-09	5.530E 01
4.855E-03	1.969E-07	3.486E-08	4.486E-15	7.139E-09	1.378E-09	5.530E 01
4.920E-03	1.943E-07	3.439E-08	4.430E-15	7.050E-09	1.350E-09	5.530E 01
4.986E-03	1.917E-07	3.395E-08	4.377E-15	6.965E-09	1.324E-09	5.530E 01
5.000E-03	1.912E-07	3.385E-08	4.365E-15	6.947E-09	1.318E-09	5.530E 01

TIME SECONDS	DUMMY MOLES/L	HA+ MOLES/L	CONDC MHO/CM	ABSC /CM	DT SEC	
0.0	1.000E 00	1.000E-03	2.183E-10	0.0	1.000E-10	0.0
1.000E-08	1.00CE 00	1.000E-03	1.659E-09	8.600E-05	4.000E-10	0.0
5.000E-08	1.000E 00	1.000E-03	2.095E-09	4.299E-04	4.000E-10	0.0
2.000E-06	1.00CE 00	1.000E-03	-5.966E-09	1.662E-02	5.120E-08	0.0
4.00CE-06	1.000E 00	1.000E-03	-1.554E-08	3.055E-02	5.120E-08	0.0
6.000E-06	1.000E 00	1.000E-03	-2.488E-08	4.067E-02	5.120E-08	0.0
6.050E-06	1.00CE 00	1.000E-03	-2.683E-08	4.044E-02	4.000E-10	0.0
2.000E-05	1.000E 00	1.000E-03	-2.930E-08	1.539E-02	5.120E-08	0.0
4.000E-05	1.000E 00	1.000E-03	-4.449E-08	8.448E-03	8.192E-07	0.0
8.096E-05	1.000E 00	1.000E-03	-4.229E-08	4.732E-03	8.192E-07	0.0
1.465E-04	1.000E 00	1.000E-03	-3.925E-08	2.634E-03	1.638E-06	0.0
2.120E-04	1.000E 00	1.000E-03	-3.740E-08	1.667E-03	1.638E-06	0.0
2.776E-04	1.00CE 00	1.000E-03	-3.602E-08	1.143E-03	1.638E-06	0.0
3.000E-04	1.000E 00	1.000E-03	-3.575E-08	1.017E-03	1.638E-06	0.0
3.491E-04	1.000E 00	1.000E-03	-3.494E-08	7.757E-04	1.638E-06	0.0
4.147E-04	1.000E 00	1.000E-03	-3.436E-08	5.801E-04	3.277E-06	0.0
4.802E-04	1.000E 00	1.000E-03	-3.382E-08	4.437E-04	3.277E-06	0.0
5.457E-04	1.000E 00	1.000E-03	-3.335E-08	3.447E-04	3.277E-06	0.0
6.113E-04	1.000E 00	1.000E-03	-3.325E-08	2.710E-04	3.277E-06	0.0
6.768E-04	1.000E 00	1.000E-03	-3.287E-08	2.149E-04	3.277E-06	0.0
7.423E-04	1.000E 00	1.000E-03	-3.270E-08	1.716E-04	3.277E-06	0.0
8.079E-04	1.000E 00	1.000E-03	-3.245E-08	1.375E-04	3.277E-06	0.0
8.734E-04	1.000E 00	1.000E-03	-3.249E-08	1.108E-04	3.277E-06	0.0
9.389E-04	1.000E 00	1.000E-03	-3.241E-08	8.957E-05	3.277E-06	0.0
1.004E-03	1.000E 00	1.000E-03	-3.215E-08	7.262E-05	3.277E-06	0.0
1.070E-03	1.000E 00	1.000E-03	-3.216E-08	5.901E-05	3.277E-06	0.0
1.136E-03	1.000E 00	1.000E-03	-3.200E-08	4.802E-05	3.277E-06	0.0
1.201E-03	1.00CE 00	1.000E-03	-3.212E-08	3.914E-05	3.277E-06	0.0
1.267E-03	1.000E 00	1.000E-03	-3.201E-08	3.193E-05	3.277E-06	0.0
1.332E-03	1.000E 00	1.000E-03	-3.193E-08	2.608E-05	3.277E-06	0.0
1.389E-03	1.000E 00	1.000E-03	-3.210E-08	2.189E-05	3.277E-06	0.0
1.389E-03	1.000E 00	1.000E-03	-3.014E-08	2.165E-04	4.000E-10	0.0
1.389E-03	1.000E 00	1.000E-03	-2.960E-08	8.409E-04	4.000E-10	0.0
1.391E-03	1.000E 00	1.000E-03	-2.935E-08	1.724E-02	5.120E-08	0.0
1.393E-03	1.000E 00	1.000E-03	-3.292E-08	3.110E-02	5.120E-08	0.0
1.395E-03	1.000E 00	1.000E-03	-3.590E-08	4.104E-02	5.120E-08	0.0
1.395E-03	1.00CE 00	1.000E-03	-3.786E-08	4.061E-02	4.000E-10	0.0
1.409E-03	1.000E 00	1.000E-03	-2.162E-08	1.503E-02	5.120E-08	0.0
1.429E-03	1.000E 00	1.000E-03	-3.846E-08	8.227E-03	8.192E-07	0.0
1.470E-03	1.000E 00	1.000E-03	-3.235E-08	4.845E-03	8.192E-07	0.0
1.535E-03	1.000E 00	1.000E-03	-2.752E-08	3.020E-03	1.638E-06	0.0
1.601E-03	1.000E 00	1.000E-03	-2.488E-08	2.147E-03	1.638E-06	0.0
1.667E-03	1.000E 00	1.000E-03	-2.314E-08	1.648E-03	1.638E-06	0.0
1.689E-03	1.000E 00	1.000E-03	-2.250E-08	1.524E-03	1.638E-06	0.0
1.738E-03	1.000E 00	1.000E-03	-2.160E-08	1.289E-03	1.638E-06	0.0
1.804E-03	1.000E 00	1.000E-03	-2.047E-08	1.077E-03	3.277E-06	0.0
1.869E-03	1.000E 00	1.000E-03	-1.973E-08	9.211E-04	3.277E-06	0.0
1.935E-03	1.000E 00	1.000E-03	-1.905E-08	8.013E-04	3.277E-06	0.0
2.000E-03	1.000E 00	1.000E-03	-1.844E-08	7.064E-04	3.277E-06	0.0
2.066E-03	1.000E 00	1.000E-03	-1.810E-08	6.292E-04	3.277E-06	0.0
2.131E-03	1.000E 00	1.000E-03	-1.775E-08	5.655E-04	3.277E-06	0.0
2.197E-03	1.000E 00	1.000E-03	-1.727E-08	5.118E-04	3.277E-06	0.0
2.262E-03	1.000E 00	1.000E-03	-1.689E-08	4.661E-04	3.277E-06	0.0
2.328E-03	1.000E 00	1.000E-03	-1.671E-08	4.267E-04	3.277E-06	0.0
2.393E-03	1.000E 00	1.000E-03	-1.636E-08	3.924E-04	3.277E-06	0.0

2.459E-03	1.000E 00	1.000E-03	-1.625E-08	3.623E-04	3.277E-06	0.0
2.525E-03	1.000E 00	1.000E-03	-1.604E-08	3.356E-04	3.277E-06	0.0
2.590E-03	1.000E 00	1.000E-03	-1.573E-08	3.118E-04	3.277E-06	0.0
2.656E-03	1.000E 00	1.000E-03	-1.563E-08	2.906E-04	3.277E-06	0.0
2.721E-03	1.000E 00	1.000E-03	-1.548E-08	2.714E-04	3.277E-06	0.0
2.778E-03	1.000E 00	1.000E-03	-1.518E-08	2.563E-04	3.277E-06	0.0
2.778E-03	1.000E 00	1.000E-03	-1.345E-08	4.509E-04	4.000E-10	0.0
2.778E-03	1.000E 00	1.000E-03	-1.295E-08	1.075E-03	4.000E-10	0.0
2.780E-03	1.000E 00	1.000E-03	-1.330E-08	1.751E-02	5.120E-08	0.0
2.782E-03	1.000E 00	1.000E-03	-1.756E-08	3.144E-02	5.120E-08	0.0
2.784E-03	1.000E 00	1.000E-03	-2.126E-08	4.147E-02	5.120E-08	0.0
2.784E-03	1.000E 00	1.000E-03	-2.333E-08	4.105E-02	4.000E-10	0.0
2.798E-03	1.000E 00	1.000E-03	-1.048E-08	1.565E-02	5.120E-08	0.0
2.818E-03	1.000E 00	1.000E-03	-2.727E-08	8.854E-03	8.192E-07	0.0
2.859E-03	1.000E 00	1.000E-03	-2.216E-08	5.456E-03	8.192E-07	0.0
2.924E-03	1.000E 00	1.000E-03	-1.809E-08	3.586E-03	1.638E-06	0.0
2.990E-03	1.000E 00	1.000E-03	-1.586E-08	2.661E-03	1.638E-06	0.0
3.056E-03	1.000E 00	1.000E-03	-1.430E-08	2.120E-03	1.638E-06	0.0
3.078E-03	1.000E 00	1.000E-03	-1.387E-08	1.983E-03	1.638E-06	0.0
3.127E-03	1.000E 00	1.000E-03	-1.294E-08	1.709E-03	1.638E-06	0.0
3.193E-03	1.000E 00	1.000E-03	-1.217E-08	1.472E-03	3.277E-06	0.0
3.258E-03	1.000E 00	1.000E-03	-1.126E-08	1.295E-03	3.277E-06	0.0
3.324E-03	1.000E 00	1.000E-03	-1.097E-08	1.157E-03	3.277E-06	0.0
3.389E-03	1.000E 00	1.000E-03	-1.026E-08	1.048E-03	3.277E-06	0.0
3.455E-03	1.000E 00	1.000E-03	-9.881E-09	9.575E-04	3.277E-06	0.0
3.520E-03	1.000E 00	1.000E-03	-9.677E-09	8.822E-04	3.277E-06	0.0
3.586E-03	1.000E 00	1.000E-03	-9.109E-09	8.183E-04	3.277E-06	0.0
3.651E-03	1.000E 00	1.000E-03	-8.964E-09	7.633E-04	3.277E-06	0.0
3.717E-03	1.000E 00	1.000E-03	-8.658E-09	7.155E-04	3.277E-06	0.0
3.782E-03	1.000E 00	1.000E-03	-8.484E-09	6.735E-04	3.277E-06	0.0
3.848E-03	1.000E 00	1.000E-03	-8.076E-09	6.363E-04	3.277E-06	0.0
3.914E-03	1.000E 00	1.000E-03	-8.004E-09	6.031E-04	3.277E-06	0.0
3.979E-03	1.000E 00	1.000E-03	-7.698E-09	5.733E-04	3.277E-06	0.0
4.045E-03	1.000E 00	1.000E-03	-7.509E-09	5.464E-04	3.277E-06	0.0
4.110E-03	1.000E 00	1.000E-03	-7.538E-09	5.219E-04	3.277E-06	0.0
4.167E-03	1.000E 00	1.000E-03	-7.232E-09	5.023E-04	3.277E-06	0.0
4.265E-03	1.000E 00	1.000E-03	-7.174E-09	4.720E-04	3.277E-06	0.0
4.331E-03	1.000E 00	1.000E-03	-7.087E-09	4.537E-04	3.277E-06	0.0
4.396E-03	1.000E 00	1.000E-03	-6.767E-09	4.368E-04	3.277E-06	0.0
4.462E-03	1.000E 00	1.000E-03	-6.738E-09	4.211E-04	3.277E-06	0.0
4.527E-03	1.000E 00	1.000E-03	-6.650E-09	4.065E-04	3.277E-06	0.0
4.593E-03	1.000E 00	1.000E-03	-6.446E-09	3.930E-04	3.277E-06	0.0
4.658E-03	1.000E 00	1.000E-03	-6.403E-09	3.803E-04	3.277E-06	0.0
4.724E-03	1.000E 00	1.000E-03	-6.214E-09	3.683E-04	3.277E-06	0.0
4.789E-03	1.000E 00	1.000E-03	-6.214E-09	3.572E-04	3.277E-06	0.0
4.855E-03	1.000E 00	1.000E-03	-6.024E-09	3.467E-04	3.277E-06	0.0
4.920E-03	1.000E 00	1.000E-03	-6.083E-09	3.367E-04	3.277E-06	0.0
4.986E-03	1.000E 00	1.000E-03	-5.937E-09	3.274E-04	3.277E-06	0.0
5.000E-03	1.000E 00	1.000E-03	-5.894E-09	3.254E-04	3.277E-06	0.0

TIME NEEDED FOR THIS RUN: 0.91 MIN

4. THE FORTRAN PROGRAM

4.1 Subroutines

Besides the subroutines IONIC and STEADY described in Section 2, program WR20 includes the following subroutines:

SCAN: Determines the charge of a species from the number of + or - signs in its name.

STORE: Stores time and concentrations values selected for output. Calculates once the initial conductivity $\varkappa_0$ and the optical absorbance A_0, and periodically their changes with time $\Delta\varkappa(t)$ and $\Delta A(t)$:

$$\varkappa_0 = \left(\sum_j Q_j \Lambda_j \gamma_j\right) \Big/ 1000,$$

$$A_0 = \sum_j \epsilon_j \gamma_j,$$

$$\Delta\varkappa(t) = -\varkappa_0 + \left(\sum_j Q_j \Lambda_j c_j(t)\right) \Big/ 1000,$$

$$\Delta A(t) = -A_0 + \sum_j \epsilon_j c_j(t),$$

γ_j being the initial value of c_j, Λ_j the equivalent conductance, and ϵ_j the molar absorptivity.

In addition to these subroutines, the program requires the ANL-AMD Library Function TLEFT (not included in the source deck), which gives the real time (in hundredths of a second) left for the ASP job.

This function is used to perform periodical time checks and to obtain a printout of all stored results if either the time limit of an individual run is reached, or 30 sec are left of the time specified on the Job Card.

If the function TLEFT should not be available, one can make the program operational by adding to the source deck the following dummy function subroutine:

```
FUNCTION TLEFT(X)
TLEFT = 5000.
RETURN
END
```

In this case, no periodical time checks will be performed, and exceeding the ASP job time limit will cause an abnormal termination of the job, with no results printed out.

4.2 FORTRAN Notation

Table II lists most variables and constants used in program WR20 and/or its subroutines. Arrays are included in the list, but no dimensions are given. The list does not include indices of DO loops, Statement Function names, and the names of some quantities that are only used through a few consecutive statements and whose definition is clearly evident from the source-deck listing.

TABLE II. FORTRAN Notation in WR20 and Subroutines

FORTRAN Notation	Notation in Text,[a] if Different	Explanation
A	A_{mi}	Name of species in reaction equation
A0	A_0	Coefficient of quadratic equation
A1, A2	A_1, A_2	Same[b]
AAC		Same as AC, rearranged for output
AAN		Same as AN, rearranged for output
ABSC	ΔA	Absorbance change
ABSCHG		Sum of absolute values of species charges
ABSI	A_0	Initial absorbance
AC	A_j'	Name of species in list of species
ACCFAC	q	Accuracy factor
AE	H^+, HA_i^-, etc.	Name of species in dissociation equation
AM	β_{pm}	Coefficients of Adam's extrapolation formula
AN		Headings in concentration tables (MOLES/L, etc.)
B		+ or - sign in reaction equations
BEGIN		Begin of calculation (real time) in units of 0.01 sec
BL		Four blanks
BLANK		Eight blanks
C	c_j	Concentration
CC		Concentration values stored for output
CCMAX		Maximum value of CC
CCMIN		Minimum value CC
CH		Charge of species (REAL*8)
CHARGE	Q_j	Charge of species (INTEGER)
CHGSUM		Algebraic sum of charges (initial value)
CI	γ_j	Initial concentration
COMENT		Comment on additional comment cards
CONDC	$\Delta\kappa$	Conductivity change

[a]In this report and/or in ANL-7199.
[b]Also used as name of statement function in subroutine IONIC.

TABLE II (Contd.)

FORTRAN Notation	Notation in Text,[a] if Different	Explanation
CONDI	κ_0	Initial conductivity
CP		In main program: concentrations, rearranged in groups of six In subroutine STEADY: intermediate concentration value
C0		Intermediate concentration value
CSK		Concentration of a skipped species
DCDT	$\dot{c}_j$	dc_j/dt
DFDC	$\partial f_i/\partial c_j$	See ANL-7199, p. 11
DFDCAB		Absolute value of DFDC
DR	I	Dose rate
DT		Time increment used for integrating algorithm
DTMAX	τ_{max}	Maximum Time Increment
DTMIN	τ_{min}	Minimum Time Increment
DTP		Model time elapsed since last printout of concentrations
DTPMIN	$\Delta t_{p,min}$	Minimum Print Interval
DTREQ	τ_r	Required time increment
EQ	K_i	Dissociation constant entered on data cards
EQ2	K_2	Dissociation constant for second stage of dissociation
EQCO	Λ_j	Equivalent conductance
EXT	ϵ_j	Molar absorptivity
F	$F([H^+])$	Function used for Newton's method (in subroutine IONIC)
FP		Previous value of F
G	G_j	Radiation yield
HPLUS	$[H^+]$, $[OH^-]$	Concentration of first species of dissociation equation
IDIF		Total number of steps (old time increments) in "link" routine (see ANL-7199, Fig. 1)
IFAIL		Index that becomes 1 if subroutine IONIC or STEADY fails
ILINK		Index controlling "link" routine (see ANL-7199, Fig. 1)
ION		Ionic Equilibrium Instruction
IPUNCH		Controls storage on tape of output for plotting purposes
ISHIFT		Index controlling rearrangement of dissociation equations
ISK		ISK = 1 labels reactions skipped on cards with IST ≤ 1
ISK1		ISK1 = 1 labels reactions involved in ionic dissociation or recombination
ISK2		ISK2 = 1 labels reactions skipped on cards with IST ≥ 2
ISKIP		Similar to ISHIFT
IST		Steady State Instruction
ISTEP		Index determining step size in "link" routine (see ANL-7199, Fig. 1)
IUN		Unskipping Instruction
IWARN		Becomes 1 after printout of poor-convergence warning
JEND		Number of eight-character comment words
JSK		JSK = 1 labels skipped species
JSK1		Labels species processed by STEADY and determines the option to be used

TABLE II (Contd.)

FORTRAN Notation	Notation in Text,[a] if Different	Explanation
KOEFF	α_{ji}	Coefficients of differential equations
KOEFL	$-\delta_j^{1i} - \delta_j^{2i}$	Contribution to KOEFF by left side of reaction equation
KOMENT		Comment on Run Number Card
KSK		KSK = 1 labels reactions to be skipped
LCYCL	p	Order of approximation in Adam's formula
LEQ		Identifier for species processed by IONIC
LETTER		Same as NAME, but each character one four-byte word
LIMT		Time limit for run in minutes
LT		Running number of printed line
M1	$-_{1i}$	Number of first species in reaction equation
M2	$-_{2i}$	Number of second species in reaction equation
MAXIEQ		Maximum value occuring for ION and/ or IST
MINUS		- sign (in subroutine SCAN)
MORE		Number of additional comment cards
MREP		Repetition factor
MT		Total number of time intervals (taking into account the repetition factor)
NAME		Name of species (in subroutine SCAN)
NC		Total number of species
NC1 - NC4		NC + 1, 2, 3, 4
NEQ	n_{eq}	Number of dissociation equations
NORUN		Run number
NR		Number of reactions
NREP		Same as MREP
NRS		Number of a reaction to be skipped
NT		Number of Dose Rate Cards
NT1		Number of Dose Rate Cards in first group with ION = IST = 0
NT2		Number of Dose Rate Cards up to and including the one with MREP > 1
P		Either a blank or the word PLOT
PL		The word PLOT
PLUS		+ sign (in subroutine SCAN)
PROD	$k_i c'_{1i} c'_{2i}$	This product
Q		Normalization factor
RF	g_j	Rate of formation (radiation-induced and thermal)
RK	k_i	Rate constant
RNTM		Time, in minutes, used for one run
S	s_j	Rate of spontaneous (thermal) formation
SB, SE		Headings for printed results
SG-SJ		Same
SLOPE	$\Delta c_j/\tau$	Slope of straight line connecting successive points of $c_j(t)$

TABLE II (Contd.)

FORTRAN Notation	Notation in Text,[a] if Different	Explanation
SPSK		Name of species to be skipped
SUM1		Sum of the concentrations of a group of species processed by subroutine STEADY, Option 2, after an iteration step
SUM0		Initial value of the same sum
TEST		Test values in the subroutines IONIC and STEADY
T		End of (model-) time interval specified on Dose Rate Card
TIME		Model time
TLEFT		Real time left for the ASP job, in units of 0.01 sec (This is an ANL-AMD library function.)
TLIM		Time limit for one run, in the same units
TMT		T(MT); model time at end of run
TNT2		Model time up to which calculation is repeated
TOTAL	T_{i0}	Total amount of the ith acid (or base) in dissociation equations
TT		Model times at which concentrations are printed out
XMAX		Same as CCMAX, renumbered
XMIN		Same as CCMIN, renumbered
ZEIT		Real time encountered at periodic time checks, in units of 0.01 sec

4.3 Source-deck Listing

The complete FORTRAN IV source deck of program WR20 and its subroutines (except TLEFT) is listed below:

```
C     PROGRAM WR20 FOR REACTION KINETICS. VERSION OF 3-12-70.          WR20   1
C     FOR IBM-360/75 SYSTEM. K. SCHMIDT.                               WR20   2
      REAL*8 C,PROD,DCDT,SLOPE,KOMENT,COMENT,EQ,EQ2                    WR20   3
      REAL*8 AC,AAC,A,AN,AAN,SPSK,AE,AM(4,5)/                          WR20   4
     1  +1.5000000000,+1.9166666667,+2.2916666667,+2.6402777778,       WR20   5
     2  -0.5000000000,-1.3333333333,-2.4583333333,-3.8527777778,       WR20   6
     3  +0.0000000000,+0.4166666666,+1.5416666666,+3.6333333333,       WR20   7
     4  -0.0000000000,-0.0000000000,-0.3750000000,-1.7694444444,       WR20   8
     5  +0.0000000000,+0.0000000000,+0.0000000000,+0.3486111111/       WR20   9
      REAL*8 BLANK/'          '/,SB/'MOLES/L'/,SE/'CONDC'/,            WR20  10
     1  SF/'ABSC'/,SG/'DT'/,SH/' MHO/CM'/,SI/'  /CM'/,SJ/'  SEC'/      WR20  11
      INTEGER CHARGE,P,BL/'     '/,PL/'PLOT'/                          WR20  12
      REAL*4 MINUS/'-'/                                                WR20  13
      COMMON/BLOCK1/AC(30),C(30),CHARGE(28),NC,NR,IFAIL,IWARN          WR20  14
      COMMON/BLOCK2/AE(3,21),EQ(21),EQ2(21),LEQ(4,21),NEQ              WR20  15
      COMMON/BLOCK3/A(51,6),ISK1(50)                                   WR20  16
      COMMON/BLOCK4/TIME,TT(500),CC(30,500),CONDI,DT,ABSI,EQCO(28),    WR20  17
     1   EXT(28),LT,DTP,NC1,NC2,NC3                                    WR20  18
      COMMON/BLOCK5/RF(27),RK(51),M1(50),M2(50),KOEFL(27,50),          WR20  19
     1   KOEFF(27,50),JSK(30),JSK1(30),ISK(50)                         WR20  20
      DIMENSION PROD(50),DR(51), G(28), S(28), CI(30), T(51),          WR20  21
     1   B(51,6),DCDT(30,20),IST(51),NRS(5,51),CCMAX(30),CCMIN(30),CP(6)WR20  22
     2   ,AAC(6),XMAX(6),XMIN(6),AN(30),AAN(6),SPSK(2,51),             WR20  23
     3   CSK(2,51),KOMENT(7),COMENT(90),IUN(51),ION(51),KSK(50),ISK2(50)WR20  24
      PRINT 999                                                        WR20  25
    1 READ(5,200,END=600,ERR=600)NORUN,LIMT,IPUNCH,KOMENT,MORE         WR20  26
    8 BEGIN=-TLEFT(0.)                                                 WR20  27
    4 IF(LIMT.LE.0)LIMT=2                                              WR20  28
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      TLIM=LIMT*6000-500                                                WR20  29
    2 P=BL                                                              WR20  30
      IF(IPUNCH.GT.0)P=PL                                               WR20  31
      PRINT 300,NORUN,KOMENT,NORUN,P                                    WR20  32
      IF(MORE)3,3,1003                                                  WR20  33
 1003 JEND=MORE*10                                                      WR20  34
      READ(5,211)(COMENT(J),J=1,JEND)                                   WR20  35
      PRINT 211,(COMENT(J),J=1,JEND)                                    WR20  36
    3 PRINT 317,LIMT                                                    WR20  37
C     READ, COUNT AND PRINT CHEMICAL REACTIONS                          WR20  38
      DO 5 I=1,51                                                       WR20  39
      READ(5,201)(A(I,K),K=1,3),(B(I,K),A(I,K),K=4,6),RK(I)             WR20  40
      IF(I.EQ.1)PRINT 308                                               WR20  41
      IF (RK(I)) 5,6,5                                                  WR20  42
    5 PRINT 301,(A(I,K),K=1,3),(B(I,K),A(I,K),K=4,6),I,RK(I)            WR20  43
    6 NR=I-1                                                            WR20  44
C     READ, COUNT AND PRINT SPECIES ETC.                                WR20  45
      PRINT 302                                                         WR20  46
      DO 10 J=1,28                                                      WR20  47
      READ(5,203)AC(J),CHARGE(J),G(J),S(J),CI(J),EQCO(J),EXT(J)         WR20  48
      IF(CHARGE(J).EQ.0)CALL SCAN(CHARGE(J),AC(J))                      WR20  49
    9 IF (AC(J)-BLANK) 10,11,10                                         WR20  50
   10 PRINT 303,J,AC(J),CHARGE(J),G(J),S(J),CI(J),EQCO(J),EXT(J)        WR20  51
   11 NC=J-1                                                            WR20  52
C     DEFINE SOME VALUES                                                WR20  53
      NC1=NC+1                                                          WR20  54
      NC2=NC+2                                                          WR20  55
      NC3=NC+3                                                          WR20  56
      DO 12 J=NC1,30                                                    WR20  57
   12 CI(J)=0.                                                          WR20  58
C     COMPUTE AND PRINT INITIAL CONDUCTIVITY AND OPTICAL DENSITY        WR20  59
C     AND CHECK BALANCE OF CHARGE                                       WR20  60
      CONDI=0.                                                          WR20  61
      ABSI=0.                                                           WR20  62
      CHGSUM=0.                                                         WR20  63
      ABSCHG=0.                                                         WR20  64
      DO 100 M=1,NC                                                     WR20  65
      CONDI=CONDI+CI(M)*EQCO(M)*ABS(FLOAT(CHARGE(M)))*0.001             WR20  66
      CHGSUM=CHGSUM+CI(M)*FLOAT(CHARGE(M))                              WR20  67
      ABSCHG=ABSCHG+CI(M)*ABS(FLOAT(CHARGE(M)))                         WR20  68
  100 ABSI=ABSI+CI(M)*EXT(M)                                            WR20  69
      PRINT 400,CONDI,NORUN,ABSI                                        WR20  70
      IF(ABSCHG.EQ.0.)GO TO 13                                          WR20  71
      IF(ABS(CHGSUM)/ABSCHG.GT.0.0005)PRINT 401,CHGSUM                  WR20  72
C     READ, COUNT AND PRINT DOSE RATE VALUES                            WR20  73
   13 PRINT 304                                                         WR20  74
      MAXIEQ=0                                                          WR20  75
      NREP=0                                                            WR20  76
      NT1=1                                                             WR20  77
      NT2=1                                                             WR20  78
      DO 15 K=1,51                                                      WR20  79
      READ(5,205)T(K),DR(K),SPSK(1,K),SPSK(2,K),CSK(1,K),CSK(2,K)       WR20  80
     1   ,(NRS(M,K),M=1,5),IST(K),ION(K),IUN(K),MREP                    WR20  81
      IF(T(K))14,19,14                                                  WR20  82
   14 MAXIEQ=MAX0(MAXIEQ,IST(K),ION(K))                                 WR20  83
      IF(MAXIEQ.EQ.0)NT1=K                                              WR20  84
      NREP=MAX0(MREP,NREP,1)                                            WR20  85
      IF(NREP.LE.1)NT2=K+1                                              WR20  86
   15 PRINT 305,K,T(K),DR(K),SPSK(1,K),SPSK(2,K),CSK(1,K),CSK(2,K)      WR20  87
     1   ,(NRS(M,K),M=1,5),IST(K),ION(K),IUN(K),MREP                    WR20  88
   19 NT=K-1                                                            WR20  89
      IF(NREP.LE.1)GO TO 21                                             WR20  90
      PRINT 318,T(NT2),NREP                                             WR20  91
      TNT2=T(NT2)                                                       WR20  92
C     READ OR DEFINE, AND PRINT, SOME PARAMETERS FOR COMPUTATION        WR20  93
   21 READ(5,206)ACCFAC,DTPMIN,DTMIN,DTMAX                              WR20  94
      IF (ACCFAC.LE.0..AND.MAXIEQ.EQ.0)ACCFAC=0.1                       WR20  95
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                                                                        WR20  96
      IF (ACCFAC.LE.0..AND.MAXIEQ.NE.0)ACCFAC=0.05                      WR20  97
      MT=(NREP-1)*NT2+NT                                                WR20  98
      TMT=T(NT)                                                         WR20  99
      IF(NREP.GT.1.AND.NT2.EQ.NT)TMT=FLOAT(NREP)*T(NT)                  WR20 100
      IF(DTPMIN.LE.0.)DTPMIN=TMT/FLOAT(54-MT)                           WR20 101
      IF(DTPMIN.LT. TMT /FLOAT(500-MT))DTPMIN= TMT /FLOAT(500-MT)       WR20 102
      IF (DTMIN.LE.0.)DTMIN=T(NT1)/50000.                               WR20 103
      IF(DTMAX.EQ.0.AND.MAXIEQ.EQ.0)DTMAX=TMT/2000.                     WR20 104
      IF(DTMAX.EQ.0.AND.MAXIEQ.NE.0)DTMAX=TMT/5000.                     WR20 105
      PRINT 306,ACCFAC,DTPMIN,DTMIN,DTMAX                               WR20 106
C     READ AND PRINT EQUATIONS FOR IONIC EQUILIBRIUM                    WR20 107
      IFAIL=0                                                           WR20 108
      CALL EQUIL1                                                       WR20 109
      IF(IFAIL.NE.0)GO TO 535                                           WR20 110
      PRINT 999                                                         WR20 111
C     INITIALIZE, CALCULATE COEFFICIENTS OF DIFFERENTIAL EQUATIONS      WR20 112
      DO 31 I=1,NR                                                      WR20 113
      ISK(I)=0                                                          WR20 114
      ISK2(I)=0                                                         WR20 115
      M1(I)=0                                                           WR20 116
      M2(I)=0                                                           WR20 117
      DO 30 J=1,NC                                                      WR20 118
      KOEFF(J,I)=0                                                      WR20 119
      KOEFL(J,I)=0                                                      WR20 120
      IF (AC(J)-A(I,1)) 23,22,23                                        WR20 121
   22 KOEFF(J,I)=KOEFF(J,I)-1                                           WR20 122
      M1(I)=J                                                           WR20 123
   23 IF (AC(J)-A(I,2)) 25,24,25                                        WR20 124
   24 KOEFF(J,I)=KOEFF(J,I)-1                                           WR20 125
      M2(I)=J                                                           WR20 126
   25 KOEFL(J,I)=KOEFF(J,I)                                             WR20 127
      DO 30 K=3,6                                                       WR20 128
      IF (AC(J)-A(I,K)) 30,26,30                                        WR20 129
   26 KOEFF(J,I)=KOEFF(J,I)+1                                           WR20 130
      IF (B(I,K)-MINUS) 30,27,30                                        WR20 131
   27 KOEFF(J,I)=KOEFF(J,I)-2                                           WR20 132
   30 CONTINUE                                                          WR20 133
      IF(M1(I).EQ.0.OR.M2(I).EQ.0)GO TO 592                             WR20 134
   31 CONTINUE                                                          WR20 135
C     INITIALIZE                                                        WR20 136
      DO 50 J=1,30                                                      WR20 137
      C(J)=DBLE(CI(J))                                                  WR20 138
      JSK(J)=0                                                          WR20 139
      JSK1(J)=0                                                         WR20 140
   50 CC(J,1)=CI(J)                                                     WR20 141
      TIME=0.                                                           WR20 142
      DT=DTMIN                                                          WR20 143
      LT=0                                                              WR20 144
      IWARN=0                                                           WR20 145
      CALL STORE                                                        WR20 146
      DO 120 IREP=1,NREP                                                WR20 147
      NEND=NT                                                           WR20 148
      IF(IREP.LT.NREP)NEND=NT2                                          WR20 149
C     START SOLVING DIFFERENTIAL EQUATIONS                              WR20 150
      DO 120 IT=1,NEND                                                  WR20 151
      IF(IUN(IT).NE.0)DT=DTMIN                                          WR20 152
      IF(IREP.GE.2.AND.IT.LE.NT2)T(IT)=T(IT)+TNT2                       WR20 153
C     SKIPPING AND LABELING OF SPECIES                                  WR20 154
      DO 450 M=1,2                                                      WR20 155
      IF (SPSK(M,IT)-BLANK) 431,450,431                                 WR20 156
  431 DO 435 J=1,NC                                                     WR20 157
      IF (SPSK(M,IT)-AC(J)) 435,432,435                                 WR20 158
  432 JSK(J)=1                                                          WR20 159
      IF(IUN(IT).LT.0.OR.IST(IT).GE.2)JSK(J)=0                          WR20 160
      JSK1(J)=IST(IT)                                                   WR20 161
      IF (IST(IT).EQ.0.AND.IUN(IT).GE.0)C(J)=CSK(M,IT)                  WR20 162
      GO TO 450
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  435 CONTINUE                                                          WR20 163
  450 CONTINUE                                                          WR20 164
C     SKIPPING AND UNSKIPPING OF REACTIONS                              WR20 165
      DO 470 M=1,5                                                      WR20 166
      IF (NRS(M,IT)) 470,470,455                                        WR20 167
  455 I=NRS(M,IT)                                                       WR20 168
      IF(IST(IT).LE.1)ISK(I)=1                                          WR20 169
      IF(IST(IT).GE.2)ISK2(I)=1                                         WR20 170
      IF(IUN(IT).LT.0)ISK(I)=0                                          WR20 171
  470 CONTINUE                                                          WR20 172
      DO 460 I=1,NR                                                     WR20 173
      KSK(I)=0                                                          WR20 174
      IF(IST(IT).EQ.0)ISK2(I)=0                                         WR20 175
      IF(ISK(I).EQ.1.OR.ISK1(I)*ION(IT).GE.1.OR.ISK2(I).EQ.1)KSK(I)=1   WR20 176
  460 CONTINUE                                                          WR20 177
C     AUTOMATIC UNSKIPPING OR UNLABELING                                WR20 178
      DO 475 J=1,NC                                                     WR20 179
      IF(IST(IT).EQ.0.AND.JSK1(J).GT.0)JSK(J)=0                         WR20 180
      IF(IUN(IT).LE.-2)JSK(J)=0                                         WR20 181
      IF(IST(IT).EQ.0)JSK1(J)=0                                         WR20 182
  475 CONTINUE                                                          WR20 183
      DO 485 I=1,NR                                                     WR20 184
      IF(IUN(IT).LE.-2)ISK(I)=0                                         WR20 185
  485 CONTINUE                                                          WR20 186
C     END OF SKIPPING ROUTINE                                           WR20 187
  490 IF (TIME-T(IT)) 34,120,120                                        WR20 188
   34 DO 35 L=1,NC                                                      WR20 189
   35 RF(L)=S(L)+(DR(IT)*G(L))/6.0231E+25                               WR20 190
      LCYCL=0                                                           WR20 191
      ILINK=0                                                           WR20 192
      IF (DT.GE.(2.*DTMIN))DT=DT*0.5                                    WR20 193
   36 DO 65 NCYCL=1,20                                                  WR20 194
      LCYCL=MIN0(LCYCL+1,5)                                             WR20 195
C     START CYCLE OF COMPUTATION                                        WR20 196
      TIME=TIME+DT                                                      WR20 197
      DO 51 I=1,NR                                                      WR20 198
      IF (KSK(I)) 52,52,51                                              WR20 199
   52 N1=M1(I)                                                          WR20 200
      N2=M2(I)                                                          WR20 201
      PROD(I)=C(N1)*C(N2)*DBLE(RK(I))                                   WR20 202
   51 CONTINUE                                                          WR20 203
      DO 60 L=1,NC                                                      WR20 204
      IF (JSK(L)) 43,43,60                                              WR20 205
   43 DCDT(L,NCYCL)=DBLE(RF(L))                                         WR20 206
      DO 42 I=1,NR                                                      WR20 207
      IF (KSK(I)) 44,44,42                                              WR20 208
   44 IF(KOEFF(L,I))41,42,41                                            WR20 209
   41 DCDT(L,NCYCL)=DCDT(L,NCYCL)+PROD(I)*DFLOAT(KOEFF(L,I))            WR20 210
   42 CONTINUE                                                          WR20 211
      SLOPE=0.                                                          WR20 212
      IF (ILINK) 54,54,58                                               WR20 213
C     STANDARD ROUTINE FOR COMPUTING SLOPE                              WR20 214
   54 IF (LCYCL-1) 55,55,56                                             WR20 215
   55 SLOPE=DCDT(L,NCYCL)                                               WR20 216
      GO TO 59                                                          WR20 217
   56 DO 57 K=1,LCYCL                                                   WR20 218
      INDK=NCYCL+21-K-20*((NCYCL+20-K)/20)                              WR20 219
   57 SLOPE=SLOPE+AM(LCYCL-1,K)*DCDT(L,INDK)                            WR20 220
      GO TO 59                                                          WR20 221
C     'LINK' ROUTINE FOR COMPUTING SLOPE                                WR20 222
   58 IDIF=-1                                                           WR20 223
      DO 158 K=1,5                                                      WR20 224
      ISTEP=1                                                           WR20 225
      IF ((K+ILINK).GT.6)ISTEP=2                                        WR20 226
      IDIF=IDIF+ISTEP                                                   WR20 227
      INDK=NCYCL+20-IDIF-20*((NCYCL+19-IDIF)/20)                        WR20 228
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  158 SLOPE=SLOPE+AM(4,K)*DCDT(L,INDK)                                  WR20 229
C     CALCULATE AND STORE NEW CONCENTRATIONS                            WR20 230
   59 IF (TIME.LT.T(IT)) GO TO 159                                      WR20 231
      C(L)=C(L)+SLOPE*DBLE(DT+T(IT)-TIME)                               WR20 232
      GO TO 60                                                          WR20 233
  159 C(L)=C(L)+SLOPE*DBLE(DT)                                          WR20 234
   60 CONTINUE                                                          WR20 235
      IF(TIME.LT.T(IT))GO TO 160                                        WR20 236
      TIME=T(IT)                                                        WR20 237
      LCYCL=0                                                           WR20 238
      GO TO 73                                                          WR20 239
  160 ILINK=MAX0(0,ILINK-1)                                             WR20 240
      DTP=DTP+DT                                                        WR20 241
      IF(DTP.LT.DTPMIN.OR.IST(IT).GT.0.OR.ION(IT).GT.0)GO TO 65         WR20 242
      CALL STORE                                                        WR20 243
   65 CONTINUE                                                          WR20 244
C     CHECK TIME LIMIT                                                  WR20 245
      ZEIT=-TLEFT(0.)                                                   WR20 246
      IF(ZEIT-BEGIN.GT.TLIM.OR.ZEIT+3000..GT.0.)GO TO 130               WR20 247
C     BRANCH TO EQUILIBRIUM ROUTINES                                    WR20 248
   73 IF(IST(IT).EQ.0.AND.ION(IT).EQ.0)GO TO 273                        WR20 249
      IFAIL=0                                                           WR20 250
      IF(ION(IT).GE.1)CALL EQUIL2                                       WR20 251
      IF (IST(IT).GE.1)CALL STEADY                                      WR20 252
      IF (IFAIL) 174,174,575                                            WR20 253
  575 PRINT 666                                                         WR20 254
      GO TO 130                                                         WR20 255
  174 LCYCL=0                                                           WR20 256
  273 IF(DTP.GE.DTPMIN.OR.TIME.EQ.T(IT))CALL STORE                      WR20 257
      IF (TIME.EQ.T(IT)) GO TO 120                                      WR20 258
C     REDETERMINE TIME INCREMENTS                                       WR20 259
  175 DFDCMA=0.                                                         WR20 260
      DO 360 L=1,NC                                                     WR20 261
      IF (JSK(L).GE.1)GO TO 360                                         WR20 262
      DFDC=0.                                                           WR20 263
      DO 350 I=1,NR                                                     WR20 264
      IF (KSK(I).GE.1) GO TO 350                                        WR20 265
      M1I=M1(I)                                                         WR20 266
      M2I=M2(I)                                                         WR20 267
      IF (M1I.EQ.L)DFDC=DFDC+FLOAT (KOEFF(L,I))*RK(I)*SNGL(C(M2I))      WR20 268
      IF (M2I.EQ.L)DFDC=DFDC+FLOAT (KOEFF(L,I))*RK(I)*SNGL(C(M1I))      WR20 269
  350 CONTINUE                                                          WR20 270
      DFDCAB=ABS (DFDC)                                                 WR20 271
      IF (DFDCAB.GT.DFDCMA)DFDCMA=DFDCAB                                WR20 272
  360 CONTINUE                                                          WR20 273
      DTREQ=ACCFAC/DFDCMA                                               WR20 274
      IF (DT.LE.(1.4*DTREQ).OR. DT.LT.(2.*DTMIN))GO TO 370              WR20 275
      DT=DT*0.5                                                         WR20 276
      LCYCL=0                                                           WR20 277
      GO TO 36                                                          WR20 278
  370 IF (DT.GE.(0.7*DTREQ).OR. DT.GT.(0.5*DTMAX))GO TO 36              WR20 279
      DT=2.*DT                                                          WR20 280
      ILINK=4                                                           WR20 281
      GO TO 36                                                          WR20 282
  120 CONTINUE                                                          WR20 283
C     DIFFERENTIAL EQUATIONS SOLVED                                     WR20 284
C     DETERMINE MINIMA AND MAXIMA OF FUNCTIONS (FOR PLOTTING)           WR20 285
  130 DO 121 M=1,30                                                     WR20 286
      CCMAX(M)=0.                                                       WR20 287
  121 CCMIN(M)=0.                                                       WR20 288
      DO 125 M=1,NC3                                                    WR20 289
      DO 125 LL=1,LT                                                    WR20 290
      IF (CC(M,LL).GT.CCMAX(M))CCMAX(M)=CC(M,LL)                        WR20 291
      IF (CC(M,LL).LT.CCMIN(M))CCMIN(M)=CC(M,LL)                        WR20 292
  125 CONTINUE                                                          WR20 293
C     DEFINE COLUMN HEADINGS                                            WR20 294
      DO 220 J=1,NC                                                     WR20 295
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  220 AN(J)=SB                                                          WR20 296
      DO 225 J=NC3,30                                                   WR20 297
      AC(J)=BLANK                                                       WR20 298
  225 AN(J)=BLANK                                                       WR20 299
      AC(NC1)=SE                                                        WR20 300
      AC(NC2)=SF                                                        WR20 301
      AC(NC3)=SG                                                        WR20 302
      AN(NC1)=SH                                                        WR20 303
      AN(NC2)=SI                                                        WR20 304
      AN(NC3)=SJ                                                        WR20 305
C     ARRANGE RESULTS FOR OUTPUT.                                       WR20 306
      IGROUP=(NC3+5)/6                                                  WR20 307
      DO 150 IG=1,IGROUP                                                WR20 308
      IF (IPUNCH.GT.0)WRITE(7,315)NORUN,IG,LT,T(NT),KOMENT,MORE         WR20 309
      IF(IPUNCH.GT.0.AND.MORE.GT.0)WRITE(7,411)(COMENT(J),J=1,JEND)     WR20 310
      WRITE(7,411)BLANK                                                 WR20 311
      DO 140 L=1,6                                                      WR20 312
      IGL=(IG-1)*6+L                                                    WR20 313
      AAC(L)=AC(IGL)                                                    WR20 314
      AAN(L)=AN(IGL)                                                    WR20 315
      XMAX(L)=CCMAX(IGL)                                                WR20 316
  140 XMIN(L)=CCMIN(IGL)                                                WR20 317
      PRINT 316,(AAC(L),L=1,6),NORUN,(AAN(L),L=1,6)                     WR20 318
      IF (IPUNCH) 142,142,141                                           WR20 319
  141 WRITE(7,310)(AAC(L),L=1,6),(AAN(L),L=1,6)                         WR20 320
      WRITE(7,311)(XMAX(L),L=1,6)                                       WR20 321
      WRITE(7,312)(XMIN(L),L=1,6)                                       WR20 322
  142 DO 144 LL=1,LT                                                    WR20 323
      DO 145 L=1,6                                                      WR20 324
      IGL=(IG-1)*6+L                                                    WR20 325
  145 CP(L)=CC(IGL,LL)                                                  WR20 326
C     PUNCH AND/OR PRINT RESULTS                                        WR20 327
      IF (IPUNCH.GT.0)WRITE(7,313)TT(LL),(CP(L), L=1,6)                 WR20 328
      IF(MOD(LL,59).EQ.56.AND.LT.GT.57)PRINT 999                        WR20 329
  144 PRINT 313,TT(LL),(CP(L),L=1,6)                                    WR20 330
      IF(IG.NE.IGROUP)PRINT 999                                         WR20 331
      IF (IPUNCH.GT.0)WRITE(7,998)                                      WR20 332
  150 CONTINUE                                                          WR20 333
      IF (ZEIT-BEGIN.GT.TLIM)GO TO 595                                  WR20 334
      IF(ZEIT+3000..GT.0.)GO TO 599                                     WR20 335
      RNTM=(-TLEFT(0.)-BEGIN)/6000.                                     WR20 336
      PRINT 700,RNTM                                                    WR20 337
      PRINT 999                                                         WR20 338
      GO TO 1                                                           WR20 339
  592 PRINT 319,A(I,1),A(I,2)                                           WR20 340
  535 PRINT 666                                                         WR20 341
      PRINT 999                                                         WR20 342
      GO TO 1                                                           WR20 343
  595 PRINT 667,NORUN                                                   WR20 344
      GO TO 535                                                         WR20 345
  599 PRINT 669                                                         WR20 346
  600 STOP                                                              WR20 347
  200 FORMAT(1X,I4,I3,I2,6A8,A7,I1)                                     WR20 348
  201 FORMAT(2(A5,1X),A5,3(A1,A5),E10.3)                                WR20 349
  203 FORMAT(A5,I5,5E10.3)                                              WR20 350
  205 FORMAT(2E10.3,2A5,2E10.3,5I3,I2,I1,I2,I5)                         WR20 351
  206 FORMAT(4E10.3)                                                    WR20 352
  211 FORMAT(1X,A7,9A8)                                                 WR20 353
  300 FORMAT (1X,10HRUN NUMBER,I5,4X,6A8,A7,45X,I5,2X,A4)               WR20 354
  301 FORMAT(6X,A5,5H +    ,A5,5H=     ,A5,3(1X,A4,A5),2X,2HK(,         WR20 355
     1  I2,3H) =,1PE10.3)                                               WR20 356
  302 FORMAT(//6X,'NO',3X,'NAME',3X,'CHARGE',4X,'G',9X,'S',11X,'CI',    WR20 357
     1   10X,'EQCO',7X,'EXT'/)                                          WR20 358
  303 FORMAT(I8,3X,A5,I6,F9.3,1P2(2X,E10.3,1X),0PF10.3,2X,1PE10.3)      WR20 359
  304 FORMAT(6X,2HNO,4X,4HTIME,4X,9HDOSE RATE,3X,7HSPECIES,6X,4HCSK1,7X,WR20 360
     1 4HCSK2,7X,9HREACTIONS,5X,'I I I     R'/32X,'SKIPPED',30X,'(UN-)', WR20 361
     2 7X,'S O U     E'/12X,3HSEC,5X,8HEV/L-SEC,2X,10HOR LABELED,4X,    WR20 362
     3   7HMOLES/L,4X,7HMOLES/L,6X,7HSKIPPED,6X,'T N N     P'/)         WR20 363
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  305 FORMAT(I8,1P2(E10.3,1X), A5, 1X,A5,2(1X,E10.3),3P5I3,I4,2I2,I5)   WR20 364
  306 FORMAT(////6X,15HACCURACY FACTOR,8X,1PE10.3/                      WR20 365
     2   6X,23HMINIMUM PRINT INTERVAL ,1PE10.3,4H SEC/                  WR20 366
     3   6X,23HMINIMUM TIME INCREMENT ,E10.3,4H SEC/                    WR20 367
     4   6X,23HMAXIMUM TIME INCREMENT ,E10.3,4H SEC//)                  WR20 368
  308 FORMAT(//)                                                        WR20 369
  310 FORMAT (6X,4HTIME,3X,6(5X,A5,1X)//                                WR20 370
     15X,7HSECONDS,6(4X,A7)/)                                           WR20 371
  311 FORMAT(6X,5H*MAX*,2X,1P6(1X,E10.3))                               WR20 372
  312 FORMAT(6X,5H*MIN*,2X,1P6(1X,E10.3)/)                              WR20 373
  313 FORMAT(2X,1P7(1X,E10.3))                                          WR20 374
  315 FORMAT(I4,1H*,I1,1H*,I3,1PE10.3,1X,6A8,A7,I3)                     WR20 375
  316 FORMAT(6X,'TIME',3X,6(5X,A5,1X),46X,I5//                          WR20 376
     1  5X,'SECONDS',6(4X,A7)/)                                         WR20 377
  317 FORMAT(1X,'TIME LIMIT',I3,' MIN')                                 WR20 378
  318 FORMAT(/6X,'IRRADIATION PATTERN OF THE FIRST',1PE10.3,' SEC ',    WR20 379
     1   'REPEATED',I5,' TIMES')                                        WR20 380
  319 FORMAT(/1X,'SPECIES ',A6,'AND/OR ',A6,' NOT LISTED')              WR20 381
  400 FORMAT(1H1/6X,'INITIAL CONDUCTIVITY =',1X,1PE10.3,1X,'MHO/CM',78X,WR20 382
     1       I5/6X,'INITIAL ABSORBANCE   =',1X,1PE10.3,1X,'MHO/CM'/)   WR20 383
  401 FORMAT(6X,'WARNING, NO BALANCE OF CHARGE. NET CHARGE =',1PE10.3,  WR20 384
     1  ' EQUIVALENTS'/6X,'SUBROUTINE  IONIC  WILL NOT WORK PROPERLY'/) WR20 385
  411 FORMAT(A7,9A8,1X)                                                 WR20 386
  666 FORMAT (1X,'RUN ABANDONED')                                       WR20 387
  667 FORMAT(1X,'TIME LIMIT FOR RUN  ',I5,' REACHED ')                  WR20 388
  669 FORMAT(1X,'TIME FOR JOB IS RUNNING OUT, JOB TERMINATED')          WR20 389
  700 FORMAT(4X,'TIME NEEDED FOR THIS RUN ',F6.2,' MIN')                WR20 390
  998 FORMAT (79X,1H-)                                                  WR20 391
  999 FORMAT (1H1)                                                      WR20 392
      END                                                               WR20 393
      SUBROUTINE STORE                                                  WR20 394
C     CALCULATE CONDUCTIVITY AND ABSORBANCE. STORE SET OF OUTPUT VALUES WR20 395
      REAL*8 C,AC                                                       WR20 396
      INTEGER CHARGE                                                    WR20 397
      COMMON/BLOCK1/AC(30),C(30),CHARGE(28),NC,NR,IFAIL,IWARN           WR20 398
      COMMON/BLOCK4/TIME,TT(500),CC(30,500),CONDI,DT,ABSI,EQCO(28),     WR20 399
     1   EXT(28),LT,DTP,NC1,NC2,NC3                                     WR20 400
      CONDC=-CONDI                                                      WR20 401
      ABSC=-ABSI                                                        WR20 402
      LT=LT+1                                                           WR20 403
      DO 20 L=1,NC                                                      WR20 404
      IF(C(L).GT.1.D25)C(L)=1.D25                                       WR20 405
      IF(C(L).LT.1.D-50)C(L)=0.D0                                       WR20 406
      CC(L,LT)=SNGL(C(L))                                               WR20 407
      TT(LT)=TIME                                                       WR20 408
      CONDC=CONDC+SNGL(C(L)) *EQCO(L)*ABS(FLOAT(CHARGE(L)))*0.001       WR20 409
   20 ABSC=ABSC+SNGL(C(L))*EXT(L)                                       WR20 410
      CC(NC1,LT)=CONDC                                                  WR20 411
      CC(NC2,LT)=ABSC                                                   WR20 412
      CC(NC3,LT)=DT                                                     WR20 413
      IF (NC3-30) 25,40,40                                              WR20 414
   25 NC4=NC3+1                                                         WR20 415
      DO 30 L=NC4,30                                                    WR20 416
   30 CC(L,LT)=0.                                                       WR20 417
   40 DTP=0.                                                            WR20 418
      RETURN                                                            WR20 419
      END                                                               WR20 420
      SUBROUTINE SCAN(CHARGE,NAME)                                      WR20 421
      REAL*8 NAME                                                       WR20 422
      REAL*4 PLUS/'+'/,MINUS/'-'/,LETTER(8)                             WR20 423
      INTEGER CHARGE                                                    WR20 424
      WRITE(8,101)NAME                                                  WR20 425
  101 FORMAT(A8)                                                        WR20 426
      REWIND 8                                                          WR20 427
      READ(8,102)LETTER                                                 WR20 428
  102 FORMAT(8A1)                                                       WR20 429
      REWIND 8                                                          WR20 430
```

```
      CHARGE=0                                                          WR20 431
      DO 50 I=1,5                                                       WR20 432
      IF(LETTER(I).EQ.PLUS)CHARGE=CHARGE+1                              WR20 433
      IF(LETTER(I).EQ.MINUS)CHARGE=CHARGE-1                             WR20 434
   50 CONTINUE                                                          WR20 435
      RETURN                                                            WR20 436
      END                                                               WR20 437
      SUBROUTINE IONIC                                                  WR20 438
C     READ AND PRINT EQUILIBRIUM EQUATIONS                              WR20 439
      REAL*8 AC,AE,BLANK/'        '/,C,HPLUS,TOTAL,K1,K2,H,DEN,A1,A2,   WR20 440
     1 DA12,T,CC,F,FP,CH,DCH,A,EQ,EQ2                                   WR20 441
      INTEGER CHARGE                                                    WR20 442
      COMMON/BLOCK1/AC(30),C(30),CHARGE(28),NC,NR,IFAIL,IWARN           WR20 443
      COMMON/BLOCK2/AE(3,21),EQ(21),EQ2(21),LEQ(4,21),NEQ               WR20 444
      COMMON/BLOCK3/A(51,6),ISK1(50)                                    WR20 445
      DIMENSION ISHIFT(20),ISKIP(20),TOTAL(20)                          WR20 446
C     DEFINE SOME FUNCTIONS                                             WR20 447
      DEN(H,K1,K2)=H**2+K1*H+K1*K2                                      WR20 448
      A1(H,K1,K2,T)=K1*T*H/DEN(H,K1,K2)                                 WR20 449
      A2(H,K1,K2,T)=K1*K2*T/DEN(H,K1,K2)                                WR20 450
      DA1(H,K1,K2,T)=K1*T*(K1*K2-H**2)/DEN(H,K1,K2)**2                  WR20 451
      DA2(H,K1,K2,T)=-K1*K2*T*(2.D0*H+K1)/DEN(H,K1,K2)**2               WR20 452
      LEQQ(I,K)=LEQ(I,K)                                                WR20 453
      DCH(J)=DBLE(FLOAT(CHARGE(J)))                                     WR20 454
      CC(I,K)=C(LEQQ(I,K))                                              WR20 455
      ENTRY EQUIL1                                                      WR20 456
      DO 510 K=1,21                                                     WR20 457
      READ(5,211)(AE(M,K),M=1,3),EQ(K)                                  WR20 458
      IF (AE(1,K)-BLANK) 510,511,510                                    WR20 459
  510 PRINT 311,(AE(M,K),M=1,3),EQ(K)                                   WR20 460
  511 NEQ=K-1                                                           WR20 461
      IF(NEQ.LE.0)RETURN                                                WR20 462
C     IDENTIFY SPECIES INVOLVED IN IONIC EQUILIBRIUM                    WR20 463
      DO 520 K=1,NEQ                                                    WR20 464
      DO 520 M=1,3                                                      WR20 465
      DO 515 L=1,NC                                                     WR20 466
      IF (AC(L)-AE(M,K))  515,512,515                                   WR20 467
  512 LEQ(M,K)=L                                                        WR20 468
      GO TO 520                                                         WR20 469
  515 CONTINUE                                                          WR20 470
      IF (L-NC) 520,520,526                                             WR20 471
  520 CONTINUE                                                          WR20 472
C     ERROR CHECK                                                       WR20 473
      DO 525 K=1,NEQ                                                    WR20 474
      IF (AE(1,K)-AE(1,1)) 526,525,526                                  WR20 475
  525 CONTINUE                                                          WR20 476
C     LABEL REACTIONS INVOLVED IN IONIC EQUILIBRIUM                     WR20 477
      DO 450 I=1,NR                                                     WR20 478
      ISK1(I)=0                                                         WR20 479
      DO 450 N=1,NEQ                                                    WR20 480
      IF((AE(2,N).EQ.A(I,2).AND.AE(3,N).EQ.A(I,3)).OR.                  WR20 481
     1 (AE(2,N).EQ.A(I,3).AND.AE(3,N).EQ.A(I,2)))ISK1(I)=1              WR20 482
  450 CONTINUE                                                          WR20 483
C     CHECK FOR 2ND DISSOCIATION STAGE, RENUMBER                        WR20 484
      ISKIP(1)=0                                                        WR20 485
      ISHIFT(1)=0                                                       WR20 486
      DO 630 K=1,NEQ                                                    WR20 487
      ISKIP(K+1)=0                                                      WR20 488
      ISHIFT(K+1)=ISHIFT(K)                                             WR20 489
      LEQ(4,K)=NC+1                                                     WR20 490
      EQ2(K)=0.                                                         WR20 491
      IF (ISKIP(K)) 630,605,630                                         WR20 492
  605 IF (LEQ(3,K)-LEQ(2,K+1)) 610,526,610                              WR20 493
  610 IF (LEQ(2,K)-LEQ(3,K+1)) 630,615,630                              WR20 494
  615 EQ2(K)=EQ(K+1)                                                    WR20 495
      LEQ(4,K)=LEQ(2,K+1)                                               WR20 496
      ISHIFT(K+1)=ISHIFT(K)+1                                           WR20 497
```

```
      ISKIP(K+1)=1                                                      WR20 498
  630 CONTINUE                                                          WR20 499
      DO 650 K=1,NEQ                                                    WR20 500
      IF (ISKIP(K)) 650,635,650                                         WR20 501
  635 EQ(K-ISHIFT(K))=EQ(K)                                             WR20 502
      EQ2(K-ISHIFT(K))=EQ2(K)                                           WR20 503
      DO 640 M=1,4                                                      WR20 504
  640 LEQ(M,K-ISHIFT(K))=LEQ(M,K)                                       WR20 505
  650 CONTINUE                                                          WR20 506
      NEQ=NEQ-ISHIFT(NEQ)                                               WR20 507
      GO TO 530                                                         WR20 508
  526 PRINT 777                                                         WR20 509
      IFAIL=1                                                           WR20 510
  530 RETURN                                                            WR20 511
  211 FORMAT (3(A5,1X),2X,E10.3)                                        WR20 512
  311 FORMAT (6X,A5,5H *    ,A5,5H =    ,A5,4H *  ,1PE10.3)             WR20 513
  777 FORMAT (1X,'ERROR IN EQUILIBRIUM EQUATIONS')                      WR20 514
      ENTRY EQUIL2                                                      WR20 515
C     COMPUTE EQUILIBRIUM OF IONIC SPECIES                              WR20 516
      CH=DCH(LEQQ(1,1))                                                 WR20 517
      DO 10 K=1,NEQ                                                     WR20 518
   10 TOTAL(K)=CC(2,K)+CC(3,K)+CC(4,K)                                  WR20 519
      DO 100 NSTEP=1,100                                                WR20 520
      FP=CH                                                             WR20 521
      DO 20 N=1,NEQ                                                     WR20 522
      C(LEQQ(2,N))=A1(CC(1,1),EQ(N),EQ2(N),TOTAL(N))                    WR20 523
      C(LEQQ(4,N))=A2(CC(1,1),EQ(N),EQ2(N),TOTAL(N))                    WR20 524
   20 FP=FP+CH*(DA1(CC(1,1),EQ(N),EQ2(N),TOTAL(N))*DCH(LEQQ(2,N))       WR20 525
     1   +DA2(CC(1,1),EQ(N),EQ2(N),TOTAL(N))*DCH(LEQQ(4,N)))            WR20 526
      F=0.D0                                                            WR20 527
      DO 30 J=1,NC                                                      WR20 528
   30 F=F+C(J)*DCH(J)                                                   WR20 529
      HPLUS=CC(1,1)-F/FP                                                WR20 530
      IF(HPLUS.LE.0)HPLUS=0.2D0*CC(1,1)                                 WR20 531
      DO 40 N=1,NEQ                                                     WR20 532
      C (LEQQ(2,N))=A1(HPLUS,EQ(N),EQ2(N),TOTAL(N))                     WR20 533
      C (LEQQ(4,N))=A2(HPLUS,EQ(N),EQ2(N),TOTAL(N))                     WR20 534
   40 C (LEQQ(3,N))=TOTAL(N)-CC(2,N)-CC(4,N)                            WR20 535
      TEST=SNGL(DABS(HPLUS-CC(1,1))/(HPLUS+CC(1,1)))                    WR20 536
      C(LEQQ(1,1))=HPLUS                                                WR20 537
      IF(TEST.LT.1.E-6)GO TO 120                                        WR20 538
  100 CONTINUE                                                          WR20 539
  110 IFAIL=1                                                           WR20 540
      PRINT 888                                                         WR20 541
  120 RETURN                                                            WR20 542
  888 FORMAT(1X,'NO CONVERGENCE IN  IONIC . CHECK DATA.')               WR20 543
      END                                                               WR20 544
      SUBROUTINE STEADY                                                 WR20 545
C     CALCULATES STEADY STATE CONCENTRATIONS OF FAST REACTING SPECIES   WR20 546
      REAL*8 NN,C,A0,A1,A2,CC(27,3),DENOM,C0(27),SUM0(5),SUM1,Q,CP(27)  WR20 547
      COMMON/BLOCK1/NN(30),C(30),NNN(28),NC,NR,IFAIL,IWARN              WR20 548
      COMMON/BLOCK5/RF(27),RK(51),M1(50),M2(50),KOEFL(27,50),           WR20 549
     1   KOEFF(27,50),JSK(30),JSK1(30),ISK(50)                          WR20 550
      SABS(A0)=ABS(SNGL(A0))                                            WR20 551
      DO 2 L=2,5                                                        WR20 552
      SUM0(L)=0.D0                                                      WR20 553
      DO 2 J=1,NC                                                       WR20 554
      IF(JSK1(J).NE.L)GO TO 2                                           WR20 555
      CP(J)=C(J)                                                        WR20 556
      SUM0(L)=SUM0(L)+C(J)                                              WR20 557
    2 CONTINUE                                                          WR20 558
      DO 150 N=1,50                                                     WR20 559
      DO 10 J=1,NC                                                      WR20 560
      IF(JSK1(J).GT.0)CC(J,1)=C(J)                                      WR20 561
   10 C0(J)=C(J)                                                        WR20 562
      TEST=0.                                                           WR20 563
      DO 100 K=1,2                                                      WR20 564
```

```
      DO 80 JJ=1,NC                                                     WR20 565
      J=JJ                                                              WR20 566
      IF(MOD(N,2).EQ.1)J=NC+1-JJ                                        WR20 567
      IF (JSK1(J).EQ.0) GO TO 80                                        WR20 568
      A0=DBLE(RF(J))                                                    WR20 569
      A1=0.D0                                                           WR20 570
      A2=0.D0                                                           WR20 571
      DO 50 I=1,NR                                                      WR20 572
      IF (ISK(I).NE.0)GO TO 50                                          WR20 573
    7 M1I=M1(I)                                                         WR20 574
      M2I =M2(I)                                                        WR20 575
      IF (KOEFL(J,I).EQ.-2)A2=A2+DBLE(RK(I)*FLOAT(KOEFF(J,I)))          WR20 576
      IF (KOEFL(J,I).NE.-1) GO TO 30                                    WR20 577
      IF (M1I.NE.J) GO TO 20                                            WR20 578
      A1=A1+DBLE(RK(I)*FLOAT(KOEFF(J,I)))*C(M2I)                        WR20 579
   20 IF (M2I.NE.J) GO TO 30                                            WR20 580
      A1=A1+DBLE(RK(I)*FLOAT(KOEFF(J,I)))*C(M1I)                        WR20 581
   30 IF (KOEFL(J,I).EQ.0.AND.KOEFF(J,I).NE.0) A0=A0+DBLE(RK(I)*        WR20 582
     1   FLOAT(KOEFF(J,I)))*C(M1I)*C(M2I)                               WR20 583
   50 CONTINUE                                                          WR20 584
      IF (A2.EQ.0.D0)C(J)=-A0/A1                                        WR20 585
      IF (A2.NE.0.D0) C(J)    = (-A1-DSQRT(A1*A1-4.D0*A0*A2))/(2.D0*A2) WR20 586
   80 CONTINUE                                                          WR20 587
      DO 95 L=2,5                                                       WR20 588
      SUM1=0.D0                                                         WR20 589
      DO 85 J=1,NC                                                      WR20 590
      IF(JSK1(J).EQ.L)SUM1=SUM1+C(J)                                    WR20 591
   85 CONTINUE                                                          WR20 592
      IF(SUM1.EQ.0.D0)GO TO 95                                          WR20 593
      Q=SUM0(L)/SUM1                                                    WR20 594
      DO 90 J=1,NC                                                      WR20 595
      IF(JSK1(J).EQ.L)C(J)=C(J)*Q                                       WR20 596
   90 CONTINUE                                                          WR20 597
   95 CONTINUE                                                          WR20 598
      DO 100 J=1,NC                                                     WR20 599
      IF(JSK1(J).GT.0)CC(J,K+1)=C(J)                                    WR20 600
  100 CONTINUE                                                          WR20 601
      DO 120 J=1,NC                                                     WR20 602
      IF(JSK1(J) .EQ.0)GO TO 120                                        WR20 603
      IF(JSK1(J).GT.1)GO TO 110                                         WR20 604
      DENOM=CC(J,1)-2.D0*CC(J,2)+CC(J,3)                                WR20 605
      IF(DENOM.EQ.0.D0) GO TO 111                                       WR20 606
  105 C(J)=(CC(J,1)*CC(J,3)-CC(J,2)*CC(J,2))/DENOM                      WR20 607
      C(J)=0.1D0*C0(J)+0.9D0*C(J)                                       WR20 608
      GO TO 115                                                         WR20 609
  110 C(J)=(CC(J,3)+CP(J))*0.5D0                                        WR20 610
      CP(J)=CC(J,3)                                                     WR20 611
      GO TO 115                                                         WR20 612
  111 C(J)=(CC(J,2)+CC(J,3))*0.5D0                                      WR20 613
  115 DEN=SABS(C(J))+SABS(C0(J))                                        WR20 614
      IF(DEN.GT.0)TEST=TEST+SABS(C(J)-C0(J))/DEN                        WR20 615
  120 CONTINUE                                                          WR20 616
      IF (TEST.LE.2.E-6.AND.N.GT.2)GO TO 160                            WR20 617
  150 CONTINUE                                                          WR20 618
      IF (TEST.LE.1.E-4)GO TO 159                                       WR20 619
      IFAIL=1                                                           WR20 620
      PRINT 666                                                         WR20 621
      GO TO 160                                                         WR20 622
  159 IF(IWARN.EQ.0)PRINT 667                                           WR20 623
      IWARN=1                                                           WR20 624
  160 RETURN                                                            WR20 625
  666 FORMAT (1X, 'INSUFFICIENT CONVERGENCE IN SUBROUTINE  STEADY ')    WR20 626
  667 FORMAT(1X,  'WARNING  POOR CONVERGENCE IN SUBROUTINE  STEADY ')   WR20 627
      END                                                               WR20 628
```

5. PLOTTING PROGRAMS

Two programs have been written for plotting the results calculated by program WR20. To be able to use these programs, one has to store the results of WR20 on a temporary storage device, normally a disk. This is simply accomplished by punching the digit 1 (IPUNCH) in Col. 10 of the Run Number Card (see 3.1.1). The necessary Job Control Language is described in Section 5.3.

5.1 PLOTWR20, a Program for Plotting WR20 Results on a 780 Calcomp Plotter

This program allows one to plot any or all output columns (concentrations of species, CONDC or ABSC) of one or several runs of WR20 in the same ASP job. Columns printed out on the same page are plotted in the same frame. The size of each frame can be chosen individually. All scaling operations are performed automatically.

The column ABSC can also be plotted on an Optical Transmission Scale. If this is done, no other columns on the same page can be plotted. By appropriately choosing the frame size, one can directly compare theoretical plots with the oscilloscope picture of an absorption signal produced in a pulse radiolysis or flash photolysis experiment.

5.1.1 Data Cards

One data card is required for each species (including CONDC and/or ABSC) of a particular run. It contains the following data:

NRUN, the Run Number

Col. 2-5, FORMAT: I5

SPEC, the Name of the Species

Col. 6-10, FORMAT: A5

LGTH, the Length of the Frame (time axis) in inches. Maximum value 10.0, default value 10.0.

Col. 11-15, FORMAT: F5.2

HGT, the Height of the Frame in inches. Default value 5.0.

Col. 16-20, FORMAT: F5.2

AMPL, the Amplification Factor. Leave blank unless an Optical Transmission Plot is desired. The plot will be scaled so that the specified frame height HGT corresponds to 100/AMPL % transmission.

Col. 21-30, FORMAT: E10.3

PTH, the Optical Path Length, in cm, of absorption cell (only for transmission plot). Default value 1.0.

Col. 31-40, FORMAT: E10.3

Up to 50 such data cards may be stacked. Cards with a run number not used in the job are ignored. No blank card is required at the end of the plotting data.

5.1.2 Example of Plot

Figure 2 shows a plot of the species O_2 and H_2O_2 as calculated in run 7199, using the data cards

b7199O2bbbb5.00

b7199H2O2bb5.00

b indicating a blank space.

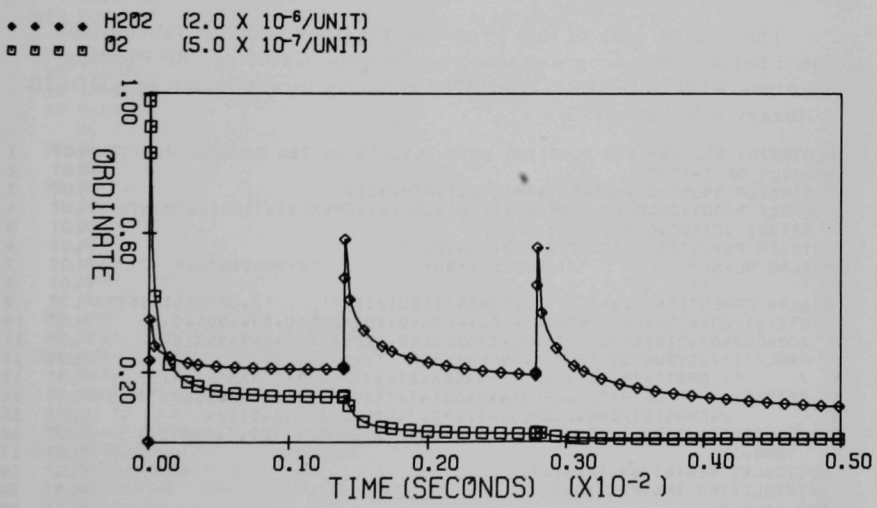

Fig. 2. CALCOMP Plot of $[O_2]$ and $[H_2O_2]$ from Run 7199, Created by Program PLOTWR20

Together with this plot, the following printout appears:

```
PLOTTING INSTRUCTIONS
7199   H2O2    5.00 * 5.00 INCHES  AMPL.=  0.0  PATH= 1.00E 00 CM
7199   O2      5.00 * 5.00 INCHES  AMPL.=  0.0  PATH= 1.00E 00 CM
H2O2 OF RUN #7199 FOUND ON DISK
O2   OF RUN #7199 FOUND ON DISK
END OF PLOT
```

Other possible, self-explanatory messages are

(1) NO DATA CARDS WITH PLOTTING INSTRUCTIONS

(2) DATA REFERRED TO IN PLOTTING INSTRUCTION NOT ON DISK

(3) ERROR IN WR20 OUTPUT

(4) NO PLOT FROM THIS JOB

5.1.3 Source Deck of Program PLOTWR20

The source deck of this program, together with its subroutines, is listed below. The program also requires the Calcomp 780 Plotting subroutines PLOTS (PRD24-2, at ANL recently incorporated in AMDLIB as a library subroutine).

```
C     PLOTWR20, PROGRAM FOR PLOTTING WR20 RESULTS ON 780 CALCOMP PLOTTERPLOT   1
C     VERSION OF 3-13-70                                              PLOT   2
      DIMENSION NRUN(50),HGT(50),AMPL(50),PTH(50),                    PLOT   3
     1 SPACE( 5000),CSUP(6),CINF(6),II(6),SCF(6),CMAX(6),T(502),CMIN(6),PLOT   4
     2  XX(502),C(500,6),VORD(4)                                      PLOT   5
      INTEGER PSY(6)/Z05,Z00,Z0A,Z0B,Z04,Z03/                         PLOT   6
      REAL*8 BLANK/'        '/,SPEC(50)/50*'        '/,WORD(6)/6*     PLOT   7
     1  '        '/                                                   PLOT   8
      REAL*4 COMENT(14)/14*'    '/,KOMENT(180)/180*'    '/,CR/Z15151515/PLOT   9
     1,PSY1(6)/Z05400540,Z00400040, Z0A400A40,Z0B400B40,Z04400440,    PLOT  10
     2  Z03400340/,DIV(4)/Z40674071,Z702E6040,Z2F616455,Z49635D15/,    PLOT  11
     3  PARL/'('/,SYRUN(3)/'RUN ','NUMB','ER  '/,ARRAY1(4)            PLOT  12
     4  /'    ','ORDI','NATE','    '/,ARRAY2(4)/'    ','TRAN','SMIS',  PLOT  13
     5  'SION'/,     LGTH(50),LENGTH,VABS(4)/'TIME','(SEC','ONDS',')  'PLOT  14
     6          /,CMNS(6)/6*0./,CPLU(6)/6*0./,NIHIL/Z40114011/,       PLOT  15
     7   FINISH(8)/'END ','OF P','LOT.','-K. ','SCHM','IDT.','-F11',  PLOT  16
     8   '638.'/                                                      PLOT  17
      LOGICAL*1 YES(6)/6*.FALSE./                                     PLOT  18
C     INITIALIZING INSTRUCTIONS                                       PLOT  19
      END FILE 7                                                      PLOT  20
      REWIND 7                                                        PLOT  21
      NERR=0                                                          PLOT  22
      CALL PLOTS(SPACE, 5000)                                         PLOT  23
      CALL PLOT(8.5,0.,23)                                            PLOT  24
      CALL SYMBOL(-0.2,0.,0.2,FINISH(5),90.,16)                       PLOT  25
C     READ PLOTTING INSTRUCTIONS FROM CARDS                           PLOT  26
      DO 20 I=1,50                                                    PLOT  27
      READ(5,501,END=21,ERR=20)NRUN(I),SPEC(I),LGTH(I),HGT(I),AMPL(I), PLOT  28
     1   PTH(I)                                                       PLOT  29
```

```
  501 FORMAT(I5,A5,2F5.2,3E10.3)                                        PLOT  30
      IMAX=I                                                            PLOT  31
      IF(HGT(I).LE.0.)HGT(I)=5.                                         PLOT  32
      IF(LGTH(I).LE.0.)LGTH(I)=10.                                      PLOT  33
      IF(PTH(I).LE.0.)PTH(I)=1.                                         PLOT  34
   20 CONTINUE                                                          PLOT  35
C     START MAIN CYCLE                                                  PLOT  36
   21 IF(IMAX.EQ.0)GO TO 801                                            PLOT  37
      PRINT 650                                                         PLOT  38
  650 FORMAT(1H1/1X,'PLOTTING INSTRUCTIONS'/)                           PLOT  39
      DO 10 I=1,IMAX                                                    PLOT  40
   10 PRINT 651,NRUN(I),SPEC(I),LGTH(I),HGT(I),AMPL(I),PTH(I)           PLOT  41
  651 FORMAT(I 8,3X,A5,F08.2,' *',F6.2,' INCHES',3X,'AMPL.=',F7.2,2X,   PLOT  42
     1   'PATH=',1PE10.3,' CM')                                         PLOT  43
   25 DO 200 KDUMMY=1,50                                                PLOT  44
      READ(7,702,END=800,ERR=802)NORUN,LT,TMAX,COMENT,MORE              PLOT  45
  702 FORMAT(I4,3X,I3,E10.3,1X,14A4,I2,1X)                              PLOT  46
      JEND=20*MORE                                                      PLOT  47
      IF(JEND.GT.0)READ(7,703)(KOMENT(J),J=1,JEND)                      PLOT  48
  703 FORMAT(20A4)                                                      PLOT  49
      READ(7,704)(WORD(J),J=1,6)                                        PLOT  50
  704 FORMAT(/12X,6(6X,A5),2X///)                                       PLOT  51
      NSKIP=0                                                           PLOT  52
      DO 30 I=1,IMAX                                                    PLOT  53
      IF(NORUN.NE.NRUN(I))GO TO 30                                      PLOT  54
      DO 29 J=1,6                                                       PLOT  55
      IF(SPEC(I).NE.WORD(J))GO TO 29                                    PLOT  56
      YES(J)=.TRUE.                                                     PLOT  57
      NSKIP=NSKIP+1                                                     PLOT  58
      II(J)=I                                                           PLOT  59
      PRINT 652,WORD(J),NRUN(I)                                         PLOT  60
  652 FORMAT(/1X,A5,' OF RUN  ',I5,' FOUND ON DISK')                    PLOT  61
      NERR=1                                                            PLOT  62
   29 CONTINUE                                                          PLOT  63
   30 CONTINUE                                                          PLOT  64
   33 IF(NSKIP)35,35,31                                                 PLOT  65
   35 MSKIP=LT+4                                                        PLOT  66
      DO 37 M=1,MSKIP                                                   PLOT  67
   37 READ(7,703)DUMMY                                                  PLOT  68
      GO TO 200                                                         PLOT  69
   31 DO 32 J=1,6                                                       PLOT  70
      IF(.NOT.YES(J))GO TO 32                                           PLOT  71
      I=II(J)                                                           PLOT  72
      HEIGHT=HGT(I)                                                     PLOT  73
      LENGTH=LGTH(I)                                                    PLOT  74
      AMPLIF=AMPL(I)                                                    PLOT  75
      GO TO 40                                                          PLOT  76
   32 CONTINUE                                                          PLOT  77
   40 READ(7,705)(CMAX(J),J=1,6)                                        PLOT  78
  705 FORMAT(13X,6(1X,E10.3),1X)                                        PLOT  79
      READ(7,705)(CMIN(J),J=1,6)                                        PLOT  80
      READ(7,703)DUMMY                                                  PLOT  81
      DO 50 L=1,LT                                                      PLOT  82
   50 READ(7,706,ERR=803)T(L),(C(L,J),J=1,6)                            PLOT  83
  706 FORMAT(2X,7(1X,E10.3),1X)                                         PLOT  84
      READ(7,703)DUMMY                                                  PLOT  85
C     DETERMINE FRAME SIZE AND SCALE FACTORS                            PLOT  86
      DO 60 J=1,6                                                       PLOT  87
      CPLU(J)=0.                                                        PLOT  88
      CMNS(J)=0.                                                        PLOT  89
      IF(.NOT.YES(J))GO TO 60                                           PLOT  90
      CALL KSRND(CSUP(J),DUMMY,CMAX(J),2.,2.5,5.,10.,10.,10.,10.,10.,N) PLOT  91
      CALL KSRND(DUMMY,CINF(J),CMIN(J),2.,2.5,5.,10.,10.,10.,10.,10.,N) PLOT  92
      IF(AMPLIF.NE.0.)GO TO 60                                          PLOT  93
      IF(CSUP(J).GT.0..AND.CINF(J).GT.0.)CINF(J)=0.                     PLOT  94
      IF(CSUP(J).LT.0..AND.CINF(J).LT.0.)CSUP(J)=0.                     PLOT  95
      IF(CSUP(J)+CINF(J))52,54,54                                       PLOT  96
```

```
 52 CMNS(J)=-HEIGHT                                                     PLOT  97
    SCF(J)=-1./CINF(J)                                                  PLOT  98
    CPLU(J)=AMAX1(HEIGHT/4.,CSUP(J)*SCF(J)*HEIGHT)                      PLOT  99
    GO TO 60                                                            PLOT 100
 54 CPLU(J)=HEIGHT                                                      PLOT 101
    SCF(J)=1./CSUP(J)                                                   PLOT 102
    CMNS(J)=CINF(J)*SCF(J)*HEIGHT                                       PLOT 103
    IF(-CMNS(J).LT.0.004)CMNS(J)=0.                                     PLOT 104
    IF(-CMNS(J).GE.0.004.AND.-CMNS(J).LT.HEIGHT/4.)CMNS(J)=-HEIGHT/4.   PLOT 105
 60 CONTINUE                                                            PLOT 106
    HOLD=HEIGHT                                                         PLOT 107
    IF(AMPLIF.NE.0.)GO TO 62                                            PLOT 108
    HSUP =AMAX1(CPLU(1),CPLU(2),CPLU(3),CPLU(4),CPLU(5),CPLU(6))        PLOT 109
    HINF=-AMIN1(CMNS(1),CMNS(2),CMNS(3),CMNS(4),CMNS(5),CMNS(6))        PLOT 110
    HEIGHT=HSUP+HINF                                                    PLOT 111
    CCSUP=HSUP/HOLD                                                     PLOT 112
    CCINF=-HINF/HOLD                                                    PLOT 113
 62 IF(AMPLIF.EQ.0.)GO TO 70                                            PLOT 114
    CCSUP=100.                                                          PLOT 115
    CCINF=100.-(100./AMPLIF)                                            PLOT 116
    HSUP=HOLD                                                           PLOT 117
 70 DO 80 L=1,LT                                                        PLOT 118
    DO 80 J=1,6                                                         PLOT 119
    IF(.NOT.YES(J))GO TO 80                                             PLOT 120
    IF(AMPLIF)74,74,72                                                  PLOT 121
 72 I=II(J)                                                             PLOT 122
    C(L,J)=100.*10.**(-C(L,J)*PTH(I))                                   PLOT 123
    IF(C(L,J).LT.2.*CCINF-CCSUP)C(L,J)=2.*CCINF-CCSUP                   PLOT 124
    GO TO 77                                                            PLOT 125
 74 C(L,J)=C(L,J)*SCF(J)                                                PLOT 126
    IF(C(L,J).LT.CCINF)C(L,J)=CCINF                                     PLOT 127
 77 IF(C(L,J).GT.CCSUP)C(L,J)=CCSUP                                     PLOT 128
 80 CONTINUE                                                            PLOT 129
    CALL KSRND(TSUP,DUMMY,TMAX,2.,5.,10.,10.,10.,10.,10.,10.,N)         PLOT 130
    T(LT+1)=0.                                                          PLOT 131
    T(LT+2)=TSUP/LENGTH                                                 PLOT 132
    CALL PLOT(0.,-0.2,3)                                                PLOT 133
    CALL PLOT(0.,0.,2)                                                  PLOT 134
    CALL PLOT(0.,10.2,3)                                                PLOT 135
    CALL PLOT(0.,10.,2)                                                 PLOT 136
    CALL SYMBOL(0.9,1.5,0.1,SYRUN(1),90.,11)                            PLOT 137
    FPN=NORUN                                                           PLOT 138
    CALL NUMBER(-0.0,-0.0,-0.0,FPN,90.,-1)                              PLOT 139
    CALL SYMBOL(-0.0,-0.0,-0.0,BLANK,90.,1)                             PLOT 140
    CALL SYMBOL(-0.0,-0.0,-0.0,COMENT(1),90.,55)                        PLOT 141
    DO 95 M=1,MORE                                                      PLOT 142
    IF(MORE.EQ.0)GO TO 95                                               PLOT 143
    J1=(M-1)*20+1                                                       PLOT 144
    CALL SYMBOL(-0.0,-0.0,-0.0,CR,90.,1)                                PLOT 145
    CALL SYMBOL(-0.0,-0.0,-0.0,KOMENT(J1),90.,80)                       PLOT 146
 95 CONTINUE                                                            PLOT 147
    DO 96 IDUMMY=1,2                                                    PLOT 148
 96 CALL SYMBOL(-0.0,-0.0,-0.0,CR,90.,1)                                PLOT 149
    N4=0                                                                PLOT 150
    DO 100 J=1,6                                                        PLOT 151
    IF(.NOT.YES(J))GO TO 100                                            PLOT 152
    N4=N4+1                                                             PLOT 153
    DO 98 NDUMMY=1,2                                                    PLOT 154
 98 CALL SYMBOL(-0.0,-0.0,-0.0,PSY1(N4),90.,4)                          PLOT 155
    CALL SYMBOL(-0.0,-0.0,-0.0,WORD(J),90.,6)                           PLOT 156
    IF(AMPLIF.NE.0.)PRINT 656,WORD(J)                                   PLOT 157
656 FORMAT(1X,A5,' (    TRANSMISSION )')                                PLOT 158
    IF(AMPLIF.NE.0.)GO TO 99                                            PLOT 159
    SCFRC=1./SCF(J)                                                     PLOT 160
    NEXP=0                                                              PLOT 161
    SCFREC=SCFRC                                                        PLOT 162
    DO 396 K=1,100                                                      PLOT 163
```

```
      IF(SCFREC.GE..9)GO TO 397
      SCFREC=10.*SCFREC
  396 NEXP=NEXP-1
  397 FEXP=-NEXP
      CALL SYMBOL(-0.0,-0.0,-0.0,PARL,90.,1)
      CALL NUMBER(-0.0,-0.0,-0.0,SCFREC,90.,1)
      CALL SYMBOL(-0.0,-0.0,-0.0,DIV(1),90.,7)
      CALL NUMBER(-0.0,-0.0,-0.0,FEXP,90.,-1)
      CALL SYMBOL(-0.0,-0.0,-0.0,DIV(3),90.,8)
   99 IF(N4.EQ.3)CALL WHERE(X2,Y2,DUMMY)
      IF(N4.EQ.1)CALL WHERE(X1,Y1,DUMMY)
      IF(N4.EQ.3)CALL SYMBOL(X1,Y1+1.1,0.1,NIHIL,90.,2)
  100 CONTINUE
C     DRAW FRAME AND AXIS
      IF(N4.LT.3)CALL WHERE(X2,Y2,DUMMY)
      CALL PLOT(X2+0.3,(10.-LENGTH)/2.,3)
      CALL WHERE(ULX,ULY,DUMMY)
      CALL PLOT(ULX,ULY+LENGTH,2)
      CALL PLOT(ULX+HEIGHT,ULY+LENGTH,2)
      IF(CCINF.LT.0.)CALL PLOT(ULX+HEIGHT,ULY,2)
      CALL PLOT(ULX+HSUP,ULY,23)
      DO 105 K=1,4
      VORD(K)=ARRAY1(K)
      IF(AMPLIF.NE.0.)VORD(K)=ARRAY2(K)
  105 CONTINUE
      CALL KSRND(RL,DUMMY,LENGTH*0.999,2.,2.5,4.,5.,10.,10.,10.,10.,N)
      DVA=10.*RL/LENGTH
      H=HOLD
      IF(AMPLIF.NE.0.)H=H*100./(100.-CCINF)
      CALL KSRND(RH,DUMMY,H*0.999,2.,2.5,4.,5.,10.,10.,10.,10.,N)
      DVO=10.*RH/H
      CALL AXIS(0.,0.,VABS,-14,1.001*LENGTH,90.,T(LT+1),T(LT+2),DVA)
      DELTAC=(CCSUP -CCINF )/HEIGHT
      XX(LT+1)=0.
      XX(LT+2)=1./HOLD
      CALL AXIS(-HSUP,0.,VORD,-16,1.001*HEIGHT,0.,CCSUP ,-DELTAC,DVO)
C     DRAW CURVES
      NP=0
      DO 150 J=1,6
      IF(.NOT.YES(J))GO TO 150
      NP=NP+1
      IF(AMPLIF.NE.0.)GO TO 115
      DO 110 L=1,LT
  110 XX(L)=-C(L,J)
      GO TO 120
  115 DO 117 L=1,LT
  117 XX(L)=2.*CCINF-C(L,J)
      XX(LT+1)=CCINF
      XX(LT+2)=(100.-CCINF)/HOLD
  120 CALL LINE(XX,T,LT,1,2,PSY(NP))
      YES(J)=.FALSE.
  150 CONTINUE
C     MOVE TO NEXT PLOT
      XNEXT=8.5-ULX-HSUP
      IF(ULX+HEIGHT.GT.8.)XNEXT=HEIGHT-HSUP+1.
      CALL PLOT(XNEXT,-ULY,23)
  200 CONTINUE
  800 IF(NERR.NE.0)GO TO 820
  815 IF(NERR.EQ.0)PRINT 600
  600 FORMAT(1H1/' DATA REFERRED TO IN PLOTTING INSTRUCTIONS NOT ON DISK
     1')
      GO TO 810
  801 PRINT 601
  601 FORMAT(1H1/' NO DATA CARDS WITH PLOTTING INSTRUCTIONS')
      GO TO 810
  802 PRINT 602
  602 FORMAT(1H1/' ERROR IN WR20 OUTPUT')
      GO TO 820
```

```
803 PRINT 602                                                          PLOT 232
    MSKIP=LT+1-L                                                       PLOT 233
    DO 205 M=1,MSKIP                                                   PLOT 234
205 READ(7,703)DUMMY                                                   PLOT 235
    GO TO 25                                                           PLOT 236
810 PRINT 610                                                          PLOT 237
610 FORMAT(/' NO PLOT FROM THIS JOB')                                  PLOT 238
820 CALL PLOT(0.,-0.2,3)                                               PLOT 239
    CALL PLOT(0.,0.,2)                                                 PLOT 240
    CALL PLOT(0.,10.2,3)                                               PLOT 241
    CALL PLOT(0.,10.,2)                                                PLOT 242
830 CALL SYMBOL(0.3,0.,0.2,FINISH(1),90.,32)                           PLOT 243
    CALL PLOT(10.,0.,23)                                               PLOT 244
    CALL PLOT(0.,0.,999)                                               PLOT 245
    PRINT 615                                                          PLOT 246
615 FORMAT(/ ' END OF PLOT')                                           PLOT 247
    STOP                                                               PLOT 248
    END                                                                PLOT 249
    SUBROUTINE KSRND(XSUP,XINF,X,A1,A2,A3,A4,A5,A6,A7,A8,N)            PLOT 250
    DIMENSION A(10)                                                    PLOT 251
    Y=X                                                                PLOT 252
    IF(X)411,406,407                                                   PLOT 253
411 X=-X                                                               PLOT 254
    GO TO 407                                                          PLOT 255
406 XINF=0.                                                            PLOT 256
    XSUP=0.                                                            PLOT 257
    N=0                                                                PLOT 258
    GO TO 413                                                          PLOT 259
407 DLG = ALOG10(X)                                                    PLOT 260
    IF(DLG)401,402,402                                                 PLOT 261
401 DLG = DLG-1.                                                       PLOT 262
402 LG=DLG                                                             PLOT 263
    XMANT=X/10.**LG                                                    PLOT 264
    A(1)=1.                                                            PLOT 265
    A(2)=A1                                                            PLOT 266
    A(3)=A2                                                            PLOT 267
    A(4)=A3                                                            PLOT 268
    A(5)=A4                                                            PLOT 269
    A(6)=A5                                                            PLOT 270
    A(7)=A6                                                            PLOT 271
    A(8)=A7                                                            PLOT 272
    A(9)=A8                                                            PLOT 273
    A(10)=10.                                                          PLOT 274
    DO 404 K=1,10                                                      PLOT 275
    IF(XMANT-A(K))410,403,404                                          PLOT 276
410 XINF=A(K-1)*10.**LG                                                PLOT 277
    XSUP=A(K)*10.**LG                                                  PLOT 278
    N=K                                                                PLOT 279
    GO TO 405                                                          PLOT 280
403 XINF=A(K)*10.**LG                                                  PLOT 281
    XSUP=XINF                                                          PLOT 282
    N=K                                                                PLOT 283
    GO TO 405                                                          PLOT 284
404 CONTINUE                                                           PLOT 285
405 IF(Y)412,413,413                                                   PLOT 286
412 XINFR=XINF                                                         PLOT 287
    XINF=-XSUP                                                         PLOT 288
    XSUP=-XINFR                                                        PLOT 289
    X=-X                                                               PLOT 290
413 RETURN                                                             PLOT 291
    END                                                                PLOT 292
```

5.2 PROTWR20, a Program for Plotting WR20 Results on the Printer

Program PROTWR20 performs a function similar to PLOTWR20, except that the plot is produced by the printer. Each plot is on a separate frame. An Optical Transmission Plot is not possible.

5.2.1 Data Cards

As for PLOTWR20, one data card is required for each species of any run. It contains the following data:

NRUN, the Run Number

Col. 2-5, FORMAT: I5

SPEC, the Name of the Species (including CONDC and/or ABSC).

Col. 6-10, FORMAT: A5

NLINE, the Length of the Plot, given as the number of printed lines. The computer uses the nearest value of (10n + 1). Recommended values are 51 (one page) and 121 (two pages). The default value is 51.

Col. 11-15, FORMAT: I5

NY1, the Width of the Plot, given as number of printed characters. Permitted values: 51 or 101. Default values if NY1 is ≤50 is entered: 51, otherwise 101.

Col. 16-20, FORMAT: I5

Up to 50 data cards are allowed.

5.2.2 Example of Plot

Figure 3 shows a plot of H_2O_2 as calculated in run 7199. The data card used was, with b indicating blanks,

b7199H2O2bbb121

In the program PROTWR20, the ordinate resolution is doubled by using as points either the character O, marking a point on the line, or the characters (), marking a point halfway between two lines.

5.2.3 Source-deck Listing

The following source-deck listing includes the program PROTWR20 and all necessary subroutines.

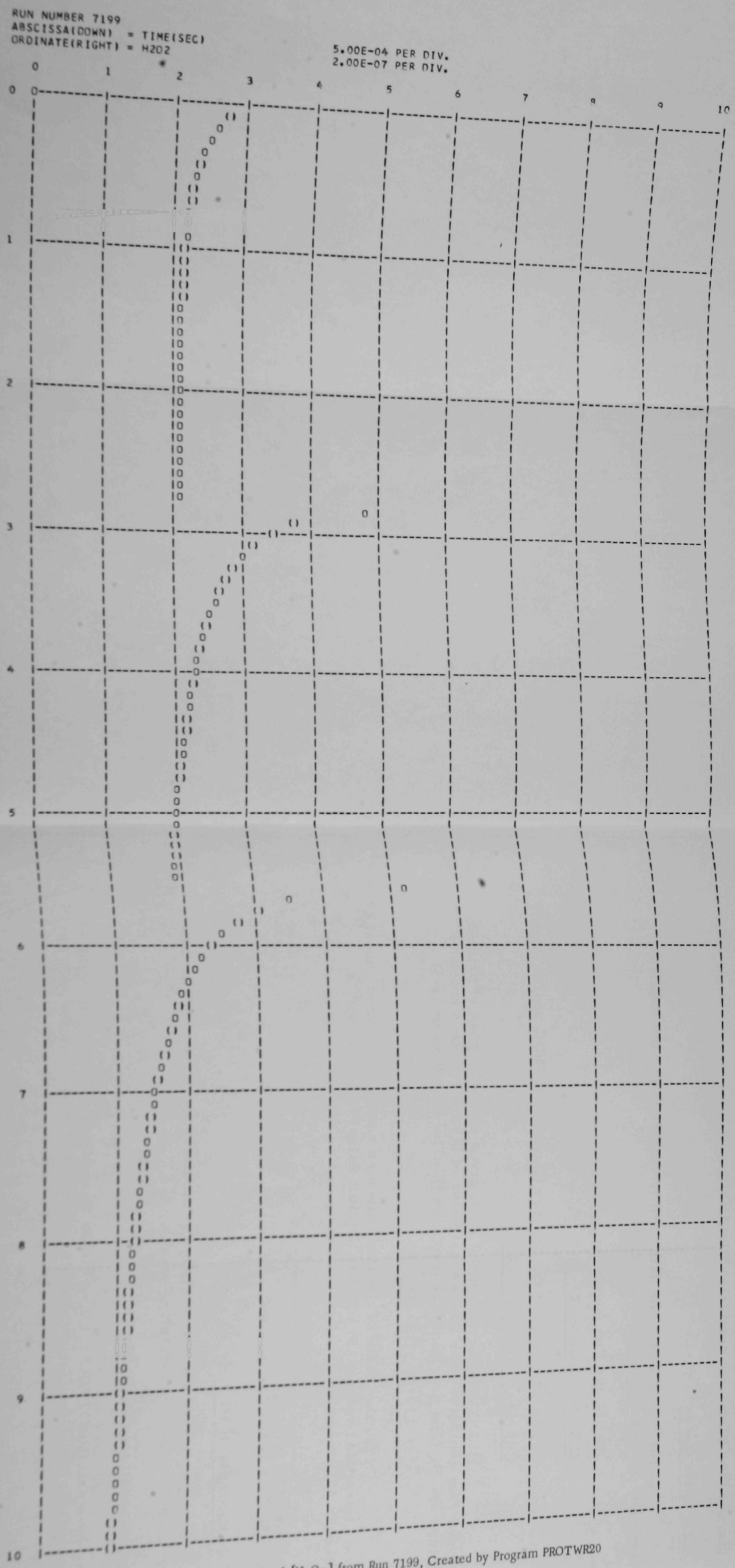

Fig. 3. Printed Plot of $[H_2O_2]$ from Run 7199, Created by Program PROTWR20

```
C     PROTWR20, PROGRAM FOR PLOTTING WR20 RESULTS ON PRINTER.
      REAL*8 SPEC(50)/50*'          '/,WORD(6)/6*'        '/
      REAL*8 ORD(3)/3*'          '/,ABSC(3)/'TIME(SEC',')        ',
     1   '          '/
      REAL*4 COMENT(14),CMAX(6),CMIN(6),T(502),C(500,6),XX(502),YY(501),
     1   TIME(501),AROUND(8)/2.,2.5,6*5./
      LOGICAL*1 YES(6)/6*.FALSE./
      INTEGER NRUN(50),NLINE(50),NY1(50),NY(6),NL(6)
      ENDFILE7
      REWIND7
      NERR=0
      DO20I=1,50
      READ(5,501, END=21,ERR=20)NRUN(I),SPEC(I),NLINE(I),NY1(I)
  501 FORMAT(I5,A5,2I5)
      IF(NLINE(I).EQ.0)NLINE(I)=51
      IMAX=I
   20 CONTINUE
   21 IF(IMAX.EQ.0)GO TO 801
   25 DO200KDUMMY=1,50
      READ(7,702,END=800,ERR=802)NORUN,LT,TMAX,MORE
  702 FORMAT(I4,3X,I3,E10.3,57X,I2)
      DO28J=1,MORE
      IF(MORE.EQ.0)GOTO28
      READ(7,703)DUMMY
  703 FORMAT(A1)
   28 CONTINUE
      READ(7,704)(WORD(J),J=1,6)
  704 FORMAT(/12X,6(6X,A5)///)
      NSKIP=0
      DO30I=1,IMAX
      IF(NORUN.NE.NRUN(I))GOTO30
      DO30J=1,6
      IF(SPEC(I).NE.WORD(J))GOTO30
      YES(J)=.TRUE.
      NSKIP=NSKIP+1
      NL(J)=((NLINE(I)+5)/10)*10+1
      NY(J)=NY1(I)
      IF(NY(J).EQ.0)NY(J)=101
      NERR=1
   30 CONTINUE
   33 IF(NSKIP)35,35,40
   35 MSKIP=LT+4
      DO37M=1,MSKIP
   37 READ(7,703)DUMMY
      GOTO200
   40 READ(7,705)(CMAX(J),J=1,6)
  705 FORMAT(13X,6(1X,E10.3))
      READ(7,705)(CMIN(J),J=1,6)
      READ(7,703)DUMMY
      DO50L=1,LT
   50 READ(7,706,ERR=803)T(L),(C(L,J),J=1,6)
  706 FORMAT(2X,7(1X,E10.3))
      READ(7,703)DUMMY
      CALL ROUNDX(TMAX,TSUP,AROUND)
      DO150J=1,6
      IF(.NOT.YES(J))GOTO150
      ORD(1)=WORD(J)
      DO110L=1,LT
  110 XX(L)=C(L,J)
      NLJ=NL(J)
      DO 120 N=1,NLJ
      TIME(N)=FLOAT(N-1)*TSUP/FLOAT(NLJ-1)
      IF(TIME(N).LE.TMAX)GO TO 115
  105 YY(N)=100.*(CMAX(J)-CMIN(J))
      GO TO 120
  115 CALL INTER(LT,T,XX,TIME(N),YY(N))
  120 CONTINUE
```

```
      PRINT710,NORUN                                                    PROT  68
  710 FORMAT('1',13X,'RUN NUMBER',I5)                                   PROT  69
      CALL PROT(YY,NLJ,NY(J),TSUP,CMIN(J),CMAX(J),ABSC,ORD)             PROT  70
      YES(J)=.FALSE.                                                    PROT  71
  150 CONTINUE                                                          PROT  72
  200 CONTINUE                                                          PROT  73
      PRINT712                                                          PROT  74
  712 FORMAT('1')                                                       PROT  75
  800 IF(NERR.NE.0)GOTO820                                              PROT  76
  815 IF(NERR.EQ.0)PRINT600                                             PROT  77
  600 FORMAT('1',' DATA TO BE PLOTTED NOT ON DISK')                     PROT  78
      GOTO810                                                           PROT  79
  801 PRINT601                                                          PROT  80
  601 FORMAT('1',' NO PLOTTING INSTRUCTIONS')                           PROT  81
      GOTO810                                                           PROT  82
  802 PRINT602                                                          PROT  83
  602 FORMAT('1',' ERROR IN WR18 OUTPUT')                               PROT  84
      GOTO820                                                           PROT  85
  803 PRINT603,L                                                        PROT  86
  603 FORMAT(//' ERROR IN ROW  ',I4,' OF TABLE, REST OF TABLE FLUSHED') PROT  87
      MSKIP=LT+1-L                                                      PROT  88
      DO205M=1,MSKIP                                                    PROT  89
  205 READ(7,703)DUMMY                                                  PROT  90
      GOTO25                                                            PROT  91
  810 PRINT610                                                          PROT  92
  610 FORMAT(/'  NO PLOT FROM THIS JOB')                                PROT  93
  820 STOP                                                              PROT  94
      END                                                               PROT  95
      SUBROUTINE PROT(Y,NLINE,NY1,XMAX,Y1,Y2,ABSC,ORD)                  PROT  96
      INTEGER SCX/0/,SCY(11)                                            PROT  97
      REAL*8 ABSC(3),ORD(3)                                             PROT  98
      REAL A(101),Y(NLINE),BLANK/' '/,I/' '/,                           PROT  99
     1   DASH/'-'/,CIRCLE/'O'/,LPAR/'('/,RPAR/')'/                      PROT 100
      REAL AROUND(8)/2.,2.5,6*5./                                       PROT 101
      NX10=(NLINE+5)/10                                                 PROT 102
      NLINE=10*NX10+1                                                   PROT 103
      IF(NY1.GT.51)NY1=101                                              PROT 104
      IF(NY1.LE.50)NY1=51                                               PROT 105
      NY10=NY1/10                                                       PROT 106
      IF(Y1.GT.0.)Y1=0.                                                 PROT 107
      IF(Y2.LT.0.)Y2=0.                                                 PROT 108
      IF(Y1.EQ.0.)NEG=0                                                 PROT 109
      IF(Y2.EQ.0.)NEG=10                                                PROT 110
      IF(Y1.EQ.0..OR.Y2.EQ.0.)GO TO 5                                   PROT 111
      NEG=-Y1/(Y2-Y1)*10.+1                                             PROT 112
      IF(NEG.GT.5)NEG=NEG-1                                             PROT 113
    5 Y21=Y2-Y1                                                         PROT 114
   10 CALL ROUNDX (Y21,DY,AROUND)                                       PROT 115
      YMAX=FLOAT(10-NEG)/10.*DY                                         PROT 116
      YMIN=-FLOAT(NEG)/10.*DY                                           PROT 117
      IF(Y2.GT.YMAX.OR.Y1.LT.YMIN)GOTO15                                PROT 118
      GOTO20                                                            PROT 119
   15 Y21=(YMAX-YMIN)*1.25                                              PROT 120
      GOTO10                                                            PROT 121
   20 Y2=YMAX                                                           PROT 122
      Y1=YMIN                                                           PROT 123
      DO25J=1,11                                                        PROT 124
   25 SCY(J)=-NEG-1+J                                                   PROT 125
      DELTAX=XMAX/10.                                                   PROT 126
      DELTAY=(Y2-Y1)/10.                                                PROT 127
      PRINT501,ABSC,DELTAX,ORD,DELTAY                                   PROT 128
  501 FORMAT(14X,'ABSCISSA(DOWN)  = ',3A8, 2X,1PE9.2,' PER DIV.'/       PROT 129
     1       14X,'ORDINATE(RIGHT) = ',3A8, 2X,1PE9.2,' PER DIV.')       PROT 130
      IF(NY1.EQ.51)GOTO30                                               PROT 131
      IF(NY1.EQ.101)GOTO40                                              PROT 132
   30 PRINT 502,SCY                                                     PROT 133
      GOTO50                                                            PROT 134
```

```
 40 PRINT503,SCY                                                    PROT 135
502 FORMAT(/15X,11(I3,2X)/)                                         PROT 136
503 FORMAT(/15X,11(I3,7X)/)                                         PROT 137
 50 DO100N=1,NLINE                                                  PROT 138
    Z    =(Y(N)-Y1)/(Y2-Y1)*FLOAT(NY1-1)+1.                         PROT 139
    DO60M=1,NY1                                                     PROT 140
    A(M)=BLANK                                                      PROT 141
    IF(FLOAT((N-1)/NX10).EQ.FLOAT(N-1)/FLOAT(NX10))A(M)=DASH        PROT 142
 60 CONTINUE                                                        PROT 143
    DO 70 M=1,NY1,NY10                                              PROT 144
 70 A(M)=I                                                          PROT 145
    IZ=Z                                                            PROT 146
    FZ=IZ                                                           PROT 147
    IF(IZ.LT.1.OR.IZ.GE.NY1)GOTO 92                                 PROT 148
    IF(Z    .LE.(FZ+0.25))GOTO80                                    PROT 149
    IF(Z    .GT.(FZ+0.25).AND.Z    .LT.(FZ+0.75))GO TO 90           PROT 150
    A(IZ+1)=CIRCLE                                                  PROT 151
    GO TO 92                                                        PROT 152
 80 A(IZ)=CIRCLE                                                    PROT 153
    GO TO 92                                                        PROT 154
 90 A(IZ)=LPAR                                                      PROT 155
    A(IZ+1)=RPAR                                                    PROT 156
 92 IF(FLOAT((N-1)/NX10).EQ.FLOAT(N-1)/FLOAT(NX10))GO TO 97         PROT 157
 95 PRINT 510,(A(M),M=1,NY1)                                        PROT 158
    GO TO 100                                                       PROT 159
 97 SCX=N/NX10                                                      PROT 160
    PRINT505,SCX,(A(M),M=1,NY1)                                     PROT 161
505 FORMAT(12X,I3,2X,101A1)                                         PROT 162
510 FORMAT(17X,101A1)                                               PROT 163
100 CONTINUE                                                        PROT 164
    RETURN                                                          PROT 165
    END                                                             PROT 166
    SUBROUTINE ROUNDX(X,R,A)                                        PROT 167
    DIMENSION A(8),B(10)                                            PROT 168
    B(1)=1.                                                         PROT 169
    B(10)=10.                                                       PROT 170
    IF(X)10,5,15                                                    PROT 171
  5 R=0.                                                            PROT 172
    GO TO 100                                                       PROT 173
 10 Y=-X                                                            PROT 174
    GO TO 20                                                        PROT 175
 15 Y=X                                                             PROT 176
 20 LY100=ALOG10(Y)+100.                                            PROT 177
    LY=LY100-100                                                    PROT 178
    YMANT=Y*10.**(-LY)                                              PROT 179
    YLIM=1.                                                         PROT 180
    DO 22 I=2,9                                                     PROT 181
 22 B(I)=A(I-1)                                                     PROT 182
    DO 50 I=1,9                                                     PROT 183
    IF(YMANT-B(I))50,50,25                                          PROT 184
 25 YLIM=B(I+1)                                                     PROT 185
 50 CONTINUE                                                        PROT 186
    R=Y/X*YLIM*10.**LY                                              PROT 187
100 RETURN                                                          PROT 188
    END                                                             PROT 189
    SUBROUTINE INTER(LT,AX,AY,X,Y)                                  PROT 190
    DIMENSION AX(1),AY(1)                                           PROT 191
    IF(X-AX(1))10,5,10                                              PROT 192
  5 Y=AY(1)                                                         PROT 193
    GO TO 100                                                       PROT 194
 10 DO 20 L=2,LT                                                    PROT 195
    IF(X.LT.AX(L))GO TO 25                                          PROT 196
 20 CONTINUE                                                        PROT 197
    IF(X.LE.AX(LT))GO TO 25                                         PROT 198
    Y=AY(LT)                                                        PROT 199
    GO TO 100                                                       PROT 200
 25 Y=AY(L-1)+(X-AX(L-1))*(AY(L)-AY(L-1))/(AX(L)-AX(L-1))           PROT 201
100 RETURN                                                          PROT 202
    END                                                             PROT 203
```

5.3 Structure of Input Deck Containing WR20 and Plotting Program

Figure 4 shows the structure of the input deck used on the IBM 360/75 system of the Applied Mathematics Division, Argonne National Laboratory.

The cards /*SETUP... and //GO·PLOTTAPE.... are omitted for PROTWR20.

```
//WR20PLOT JOB (F11638,05,00,03),'K.SCHMIDT',MSGLEVEL=1,
//       REGION=140K,CLASS=C
//*COMMENT.-THE ACCOUNTING CARD IS INSERTED HERE.**********************
/*SETUP  DDNAME=PLOTTAPE,DEVICE=2400-7,ID=(CALCMP,RING,SAVE,NL)
//PART1 EXEC FTHLG
//EDT.SYSIN DD *
//*COMMENT.-THE WR20 OBJECT DECK IS INSERTED HERE.**********************
/*
//GO.FT07F001 DD UNIT=2314,SPACE=(80,(500,250)),
//       DISP=(NEW,PASS),DSNAME=+TABLES,
//       DCB=(RECFM=FB,LRECL=80,BLKSIZE=800)
//GO.FT08F001 DD UNIT=2314,SPACE=(80,(1,1)),
//       DISP=(NEW,DELETE),DSNAME=+CHARGE,
//       DCB=(RECFM=F,BLKSIZE=8)
//GO.SYSIN DD *
//*COMMENT.-THE DATA FOR WR20 ARE INSERTED HERE.***********************
/*
//PART2 EXEC FTHLG
//EDT.SYSIN DD *
//*COMMENT.-THE PLOTWR20 OR PROTWR20 OBJECT DECK IS INSERTED HERE.******
 NAME G(R)
/*
//GO.FT07F001 DD DSNAME=*.PART1.GO.FT07F001,DISP=(MOD,DELETE)
//GO.PLOTTAPE DD UNIT=TAPE7TRK,LABEL=(,BLP),DISP=(,PASS)
//GO.SYSIN DD *
//*COMMENT.-THE PLOTTING DATA ARE INSERTED HERE.***********************
/*
```

Fig. 4. Structure of the Input Deck for Running the Program WR20 and PLOTWR20 (or PROTWR20) on the IBM 360/75 System at ANL. If PROTWR20 is to be used, the cards /*SETUP... and //GO·PLOTTAPE must be removed.

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