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COMPOSITION(U) MATERIALS RESEARCH LABS ASCOT VALE
(AUSTRALIA) G J JENKS ET AL. MAY 83 MRL-R-882

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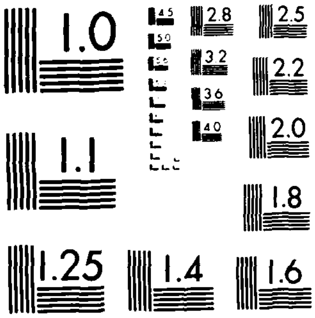

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AR-003-292

(12)

DEPARTMENT OF DEFENCE

DEFENCE SCIENCE AND TECHNOLOGY ORGANISATION

MATERIALS RESEARCH LABORATORIES

MELBOURNE, VICTORIA

REPORT

MRL-R-882

DETONATION PARAMETERS FOR AUSTRALIAN HIGH-EXPLOSIVES COMPOSITION

G.J. Jenks, [illegible] [illegible]inskas and D.A. Price*

Approved for Public Release

* Vacation Student at MRL (1981-82) now at
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DOCUMENT CONTROL DATA SHEET

REPORT NO.	AR NO.	REPORT SECURITY CLASSIFICATION
MRL-R-882	AR-003-292	UNCLASSIFIED

TITLE

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REPORT DATE	TASK NO.	SPONSOR
MAY, 1983	DST 82/200	DSTO

CLASSIFICATION/LIMITATION REVIEW DATE

CLASSIFICATION/RELEASE AUTHORITY
Superintendent, MRL
Physical Chemistry Division

SECONDARY DISTRIBUTION

Approved for Public Release

ANNOUNCEMENT

Announcement of this report is unlimited

KEYWORDS
HIGH EXPLOSIVE AMMUNITION
EXPLOSIVES
DETONATION
PARAMETERS
COMPUTER PROGRAMS

COSATI GROUPS 19010

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CONTENTS

DETONATION PARAMETERS FOR AUSTRALIAN HIGH-EXPLOSIVES COMPOSITION

1. INTRODUCTION

High explosives are a fundamental ingredient in most weapons and devices used by the Australian Defence Force. Some explosives are manufactured in Australia while others are imported. High explosives may be a single chemical compound (such as TNT) or a mixture (such as Composition B). Even for Composition B, the explosive components are mixed in different proportions in Australia from those used overseas.

The choice of explosive depends on its sensitivity during manufacture, storage and transport, its performance and of course its cost. Different environments (such as underwater in the warhead of a torpedo or in an air-burst artillery shell) dictate different explosive compositions.

Systems analysts require data on explosive parameters so that weapon performance can be predicted. If necessary, the weapon design can be modified to optimise the terminal effectiveness.

The explosive parameters of interest in such an analysis are detonation velocity, pressure, temperature and energy output. Their experimental measurement is usually slow and potentially hazardous. Moreover, the accuracy to which these measurements are made could result in erroneous conclusions particularly when similar compositions are being compared.

Theoretical estimates of detonation parameters are based on suitable high-pressure equations-of-state for the gaseous detonation products. The three most commonly used are BKW [1], JWL [2] and JCZ [3].

Of these, BKW has been employed extensively both within Australia and overseas for the last fifteen years. Not only has it generated detonation parameters so that explosive performance can be assessed, but has provided input data for large hydrodynamic codes used in weapon studies. Two codes in operation in Australia are the one- and two-dimensional Lagrangian programs, SIN, [5,6] and 2DL [7].

The first BKW program [4] available in Australia was written for a batch-oriented process on a CDC 3600 computer although the earlier versions were compiled in a machine language for an IBM 7030 machine. Following its modification to permit running on the Cyber 76 computer in the CSIRO computing network (CSIRONET), an interactive program USERBKW was developed. By this approach, the input data deck is compiled directly from a series of questions and from data already available. Results can then be obtained reliably and at minimum cost.

This Report describes USERBKW and presents a table of detonation parameters of high explosive compositions of current interest in Australia.

2. THE BKW PROGRAM

The BKW Code [4] employs the Becker-Kistiakowsy-Wilson (BKW) equation of state [8] to calculate the detonation properties of explosives. It is also possible from these calculations to obtain the Hugoniot, the isentrope through the C-J point and the coefficients to fits of pressure, energy and temperature along the isentrope. The fits of these results are used in reactive hydrodynamic codes to calculate the appropriate equations of state.

The BKW equation of state is normally used in the empirical form:

$$\frac{PV}{RT} = 1 + \gamma \, e^{\beta\gamma}$$

where $\gamma = K\left[V(T + \theta)^{\alpha}\right]^{-1}$

$K = \kappa \sum_i x_i k_i$

$k_i = 10.46 \, v_i$

P being the pressure
V the molar gas volume
R the gas constant
T the absolute temperature
x_i the mole fraction of component i
k_i is the covolume
v_i is the effective volume (in A^{03}) occupied by a rotating molecule.

The constants α, β, κ and θ are determined experimentally, and are discussed more fully elsewhere [8].

Steady-state time-independent behaviour is assumed in the use of this code. Detonation products are considered to be in instantaneous chemical equilibrium. In practice, however, the detonation process is a complex time-dependent one and appropriate caution in the use of the results is naturally required.

The code itself contains a number of subroutines that operate under the control of the main program. This main routine handles only the input and output of data besides the control of the code. All computations are performed in the subroutines. The program requires the calculation to proceed iteratively by minimising the free energy.

3. SOURCES OF DATA

For the explosive, the necessary input data are elemental composition, heat of formation, density and formula weight. For an explosive mixture, the fraction by weight, the elemental composition and heat of formation of each component are required.

The heats of formation for some substances are listed in various publications [8,9,10,11,12].

For other compounds, reliable estimates may be obtained by assuming that the heat of formation is independent of the path by which the reaction proceeds. Under this approach, the elements in their standard states are assumed to pass through the monatomic gaseous elements to the product compound. Bond energies are reasonably well-known, and BKW is not very sensitive to the heat of formation used to describe the explosive.

The parameters α, β, κ and θ have been carefully calibrated. In general, the set of parameters which best fits RDX ($\alpha = 0.5$, $\beta = 0.16$, $\kappa = 10.91$, $\theta = 400$) are used [8]. If the explosive composition is deficient in oxygen and produces significant concentrations of solid carbon, the TNT parameters are more appropriate ($\alpha = 0.5$, $\beta = 0.09585$, $\kappa = 12.685$ and $\theta = 400$).

The covolume for each species is given by 10.46 v_i where v_i is in $A^{\circ 3}$. It represents the spherical volume of the rotating molecule where its radius is the maximum dimension of the molecule as measured from the centre of mass. Covolumes for the usual product species are listed [4], [8] or may be calculated from the Van der Waals radii, values of which are tabulated for some elements.

The BKW code requires the entropy of the product species to be expressed as a polynomial function of temperature. While these data are available for most common species [8], information for other products is available through tables [11], [12] or through the TDF program [13].

As BKW uses basically iterative techniques, some parameters have to be selected initially so that convergence during the program takes place. For example, initial estimates of pressure and temperature must be of the right order. BKW is written to ensure realistic initial values are selected for CHNO-type (RDX, TNT) explosives. If an appreciably different explosive is used, new values of these parameters must be selected. Typical values of these modified parameters are given elsewhere [14].

For example, if there is an error in the gas volume VBOS(1) (at parameter 2) should be changed. If the Hugoniot temperature is incorrect, HUGBOS (at parameter 5) should be amended. APGCJ (parameters 11) or BPGCJ (parameter 12) should be altered if there are too many iterations in calculating the detonation pressure.

It may be noted that aluminium containing explosives tend to give a much higher temperature than non-aluminised explosives

4. THE USER INTERFACE

The original BKW program [4] required as input a deck of punched cards in a complicated format specifying the density, the components of the explosive mixture, the detonation products and a large number of physical and numerical constants related to them. So complicated is the input that is requires a knowledge of the BKW program, the editor program, the FORTRAN language and the reference books for obtaining the numerical constants. Data preparation is both tedious and error prone, since the input is a precise sequence of spaces and numbers. There is thus a clear need for a user interface package, such as USERBKW, to allow users with a minimum of technical knowledge to prepare data for BKW in a flexible, reliable and efficient manner.

USERBKW is written as a FORTRAN program for the CSIRONET Cyber 7600, although it can be readily modified for other computers. It runs under the CIO interactive sub-system, ie it asks questions of, and reads answers from, the user sitting at a remote terminal. USERBKW also maintains three database files, namely BKWCMP, BKWGAS and BKWSOL. BKWCMP contains information on standard components of explosives, while BKWGAS and BKWSOL contain information on gaseous and solid detonation products. These files can be updated from USERBKW, and their internal formats are given in Appendix I. Appendix II provides the listing.

The questions asked by USERBKW are straightforward to answer. Questions requiring a "yes or no" type answer have the characters (Y/N) at the end of the question. The default answer (that is, the effective answer if nothing but a line-feed is typed) is "N". When asked to specify a component or a product, the answer required is a name of up to six characters. For example, TNT is a component, H2 is a gaseous product and SOLC is a solid product. Typing a question mark in answer to such a question evokes a list of standard components or products on file. The program will automatically look up the appropriate formula and physical constants if on file; otherwise the user is required to supply all such data.

In answer to the question "what is the formula of ....", a chemical formula must be given. The formula must be a sequence of element symbols, each of which is followed by a number or spaces or both. Brackets may be used. For example, the formula for hydrous copper sulphate is CU S 04 (H20)5. Element symbols must not be run together as in CO which is cobalt not carbon dioxide. Formulae should not be confused with names. For example, the gaseous product carbon dioxide has formula C 02 but has name CO2. If common element symbols are used in the formula, the program will automatically work out the formula weight.

Some questions, (such as asking for the percentage composition) require a numerical answer. Others may represent a number of alternatives and require the user to type a single letter (and line feed) to indicate his choice. Examples of the latter are the menus which allow the user to inspect and edit data at will. There are three such menus, the main menu, the component menu and the product menu.

The first question that USERBKW asks is whether the user wants to read back in a previously generated deck. The answer to this, under normal circumstances, is "no". The next question asks the user to type a title of up to 62 characters. This title, together with the date, will appear on each page of the BKW output. The next question will ask the user for the loading density of the explosive (e.g. 2 g/cm^3).

After this the user is requested to specify a component of the explosive. If the specified component is not on file, the user will be required to type in its formula and heat of formation. In any case, the user will have to give the percentage of explosive by mass. If, when all components have been specified, the sum of the composition does not equal 100%, the program will go to the component menu for the user to edit the components until it does.

After the components have been considered, the detonation products must be specified and then their amounts estimated. Usually, if the explosive is a C-H-N-O explosive, this is done automatically; otherwise the detonation products will be explicitly requested, and then estimates will be asked for. There are three methods of making estimates, explicitly, by which the user gives his estimates, hierarchically, by which the user gives priorities with first priority being given to the product most likely to be formed (e.g. priority 1 = H2O, priority 2 = CO2); and by default estimates. If an attempt at estimation is indequate, the user is told. He can either try again, or temporarily ignore the error until more products can be added later through the product menu.

The next item to be considered is the set of parameters for the Becker-Kistiakowsky-Wilson equation of state. After this, if all data are present and correct, the user may have the program generate an "object deck", which is the main output of the package. The object deck contains a complete job for running under the ED subsystem. This job "chains" to the BKW program and submits all appropriate data. If the user answers "yes", to the question "do you want to generate a deck at this stage?" the object deck is generated as a file after the user gives a file name and a user identification for it. Otherwise the user may inspect and edit the data by menu operations, and generate an object deck later.

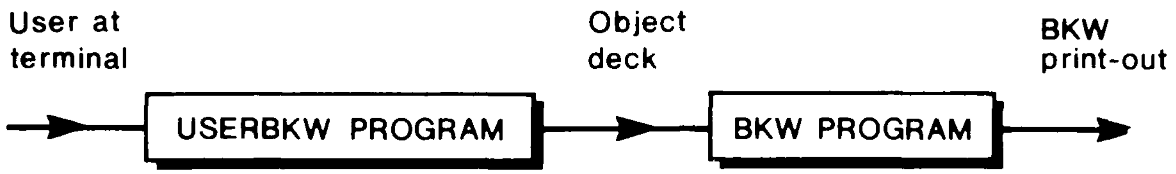

Figure 1. USERBKW is the "frontend" of a program "chain".

A maximum of 12 components may comprise an explosive mixture, which cannot have more than 10 elements. There can be up to 20 gaseous and 5 solid detonation products, none of which may contain an element not present in the mixture. If editing data in the component or product menus, changes such as changing the composition, or adding another detonation product, will necessitate re-estimation of the product quantities. Similarly, removal of a component will require reconsideration of the detonation products.

The USERBKW user interface, while working closely with the BKW program, was deliberately written as a separate program. This is desirable. The software is easier to manage for the logically distinct tasks of data preparation and numerical processing, and it is more convenient to run as different programs. USERBKW takes fractions of a central processor second to execute, and uses a high priority, whereas BKW, like most "number crunching" programs, consumes relatively large amounts of CPU time, and should therefore be run at the cheaper non-prime priority.

The user will find that the package is simple to grasp, fast to operate, and that it achieves the goal of facilitating reliable calculations through the BKW code.

5. RESULTS

The input data for a BKW run on Australian Composition B (RDX 55%, TNT 45%) at a density of 1.65 is shown in Appendix III. The corresponding output showing detonation parameters, isentrope and Hugoniot and curve-fitting coefficients are given in Appendix IV.

Detonation parameters for other explosive compositions of interest in Australia are listed in Table I.

TABLE 1

DETONATION PARAMETERS

Composition	Density g/cm^3	Gamma	Det. Temp. K	Det. Vel. m/s	Det. Pressure GPa
TNT	1.56	2.81	2980	6680	18.3
TNT	1.64	2.84	2920	6920	20.4
RDX/wax 92/8	1.43	2.84	2970	7320	20.2
RDX/wax 92/8	1.57	2.90	2790	7810	24.5
RDX/wax 92/8	1.67	2.94	2630	8190	28.4
Composition B	1.65	2.92	2860	7760	25.3
H6 (Note 1)	1.80	3.16	5300	7370	23.5
Ammonium Picrate	1.42	2.92	2590	6780	16.6
Ammonium Picrate	1.50	2.96	2500	7070	18.9
Ammonium Nitrate	0.67	2.01	5810	5880	7.7
Ammonium Nitrate	0.80	2.11	5750	6340	10.4
Ammonium Nitrate	1.00	2.26	5600	7000	15.2
Ammonium Nitrate	1.70	2.76	4360	9660	42.1
RDX/wax 91/9	1.60	2.92	2680	7920	25.6
RDX/wax 91/9	1.55	2.90	2760	7730	23.7
PBX W 106	1.65	2.87	3030	8200	28.6
PBX W 106	1.68	2.89	2980	8310	29.8
PBX W 106	1.715	2.90	2920	8440	31.3
RDX/TNT 60/40	1.715	2.94	2760	8050	28.2
Amatol 50/50 (Note 2)	1.00	2.43	3950	6430	12.1
Amatol 50/50	1.20	2.74	2530	6230	12.5
NQ/TNT 50/50 (TNT)	1.594	2.68	3830	7860	26.8
NQ/TNT 60/40 (TNT)	1.60	2.67	4000	8080	28.5
NQ/TNT 60/40 (RDX)	1.60	2.77	3860	8280	29.1
NQ/TNT 50/50 (RDX)	1.594	2.80	3700	8070	27.3
NQ/TNT 40/60 (RDX)	1.586	2.82	3540	7840	25.6
NQ/TNT 40/60 (TNT)	1.586	2.72	3670	7640	24.9
Nitroguanidine	1.65	2.88	2890	8690	32.1
Nitroguanidine	1.715	2.92	2760	8950	35.0
Amatol 50/50 (TNT)	1.59	2.84	2250	7280	22.0
Amatol 50/50 (RDX)	1.59	3.02	2060	7700	23.5
Amatol 80/20	1.46	3.02	1740	7490	20.4
Torpex	1.72	2.90	5271	7150	22.5
Hexal 17	1.74	3.01	4950	7710	25.8
Nitroguanidine	1.62	2.87	2960	8570	30.7
Astrolite	1.30	2.99	1660	7780	19.7
Astrolite	1.41	3.04	1500	8300	24.0
RDX/TNT/AN 62/10/28	1.625	2.96	2390	8100	27.0
RDX/AN 48.1/51.9	1.68	3.10	1878	8550	30.0
PETN/AN 66.5/33.5	1.60	2.94	2440	8000	25.9

TABLE 1

(Continued)

RDX/TNT/AN 48.5/10/40.5	1.670	3.03	2120	8360	29.0
RDX/TNT/AN 25/10/65	1.678	3.09	1730	8530	29.8
Tetryl	1.50	2.83	3170	6970	19.0
Metabel (Note 3)	1.608	2.75	3010	7330	23.0

Note 1 H6: RDX 43%, TNT 30%, Al 22%, NC 0.6%, Wax 4.4%.
Note 2 Amatol: ammonium nitrate, TNT.
Note 3 Metabel: PETN 70%, TNT 4%, DNT 20%, NC 3% Wax 3%.

General Note: (RDX) or (TNT) denotes that the calculations were carried out with RDX or TNT parameters.

6. CONCLUSION

BKW has proved a most successful tool in predicting detonation parameters. It is fast, efficient, reliable and cheap to use. USERBKW has simplified the operation of the BKW code.

7. ACKNOWLEDGEMENTS

The authors wish to record their thanks to Dr C.L. Mader for invaluable comments and assistance, and to Dr L.J. Johnston and Mr G.K. Manzie who obtained some of the results over many years.

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APPENDIX I - MAINTENANCE OF USERBKW

The FORTRAN EXTENDED source listing for USERBKW, as giv
Appendix II, is well documented with comments, and the maintenanc
should be familiar with these before making any changes. The pro
under the CSIRONET/SCOPE 2.1 operating system. As with most I-O
programs, it relies on its environment. Subroutines PAGE and PSS
instance, depend on the terminals in use, while other parts of th
make calls to the operating system for file cataloguing operation

USERBKW does a lot of error checking for the benefit of
and may often issue messages in the form of "**ERROR**...". Such
for the information of the user. Very rarely, though, a diagnost
the form "=DIAG=..." may be issued. Such an occurrence may indic
presence of a bug, and should be drawn to the attention of the ma
programmer.

The three database files BKWCMP (for components), BKWGA
products) and BKWSOL (solid products) should be maintained by the
within the program (e.g. by using the file option in the componen
menus). Entries in these files may be created, deleted or update
entries may be protected against accidental deletion by the use o
from within USERBKW. All users are encouraged to create entries
temporarily, where this will circumvent tedious retyping of the m

BKWCMP is logical file TAPE1, and contains the followin
about components: name, comment, formula, protection, heat of fo
formula weight. Each entry is a single line in the format (1H0,
2G12.6).

BKWGAS is logical file TAPE2 and contains the following
on gaseous products: name, comment, formula, protection, heat of
entropy constants A, B, C, D, E and IC, and the covolume. Each e
the format (1H0, A6, 4A10, 6A10, A1, G12.6/1X, 7G14.8), which tak
lines.

BKWSOL is TAPE3 with information on solid products as f
name, comment, formula, protection, heat of formation, formula we
constants A, B, C, D, E and IC, covolume, specific volume and the
Fickett solid equation of state parameters A_S, B_S, C_S, D_S, E_S, A_1
C_3. Each entry is in the format 1H0, A6, 4A10, 6A10, A1, 2G12.6/
9G14.8/1X, 9G14.8) and uses three consecutive lines.

For each of these three files a file entry is deemed tc
there is the character zero (0) in the first column of the line.
function SEEK). A file usually ends with an end-of-partition mar
by a comment on the last change made to it. (See subroutine SEAI
information such as the internal formats of the files is irreleva
user, and is only provided here for the benefit of the maintenanc

APPENDIX II

1 Sheet Microfiche

APPENDIX III

```
 [illegible]
[illegible] Version 10/01/84
  [illegible]
Entering 7000 mode...wait
          WELCOME TO  USERBKW , THE USER INTERFACE FOR THE BKW PROGRAM.


 DO YOU WANT TO READ IN A PREVIOUSLY GENERATED DECK ?  [Y/N]     [DEFAULT='NO']
 n


 TYPE A TITLE FOR THIS RUN (E.G. NAME OF EXPLOSIVE) :
:[illegible] composition b


 WHAT DENSITY IS TO BE USED FOR THE EXPLOSIVE ?  [G/CC]
:1.65
 DO YOU ALSO WANT CALCULATION TO BE PERFORMED FOR ANOTHER DENSITY ?  [Y/N]
:n


 SPECIFY A COMPONENT OF THE UNREACTED EXPLOSIVE :
   [A SHORT NAME OF UP TO 6 CHARACTERS IS REQUIRED.   E.G. TNT]
   [FOR A LIST OF STANDARD COMPONENTS, TYPE A QUESTION MARK '?'.]
:rdx

 WHAT PERCENTAGE OF THE UNREACTED EXPLOSIVE WILL BE RDX     ?
:55


 ARE THERE ANY OTHER EXPLOSIVE COMPONENTS ?  [Y/N]
:y


 SPECIFY A COMPONENT OF THE UNREACTED EXPLOSIVE :
:tnt

 WHAT PERCENTAGE OF THE UNREACTED EXPLOSIVE WILL BE TNT     ?
:45


 ARE THERE ANY OTHER EXPLOSIVE COMPONENTS ?  [Y/N]
:n

                      COMPONENT EXPLOSIVE            COMPOSITION
                      -------------------            -----------

                            RDX                          55.00 %
                            TNT                          45.00 %

                            ------                       --------
                            TOTAL                       100.00 %


 THE ELEMENTAL COMPOSITION OF 100.000      GRAM OF EXPLOSIVE IS :-
        2.129695      MOLE OF   C
        2.474301      MOLE OF   H
        2.080060      MOLE OF   N
        2.674422      MOLE OF   O

 THE ESTIMATES OF THE   11 GASEOUS PRODUCTS ARE :-
        1.238151      MOLE OF   H2O
       0.             MOLE OF   H2
       0.             MOLE OF   O2
        .718136       MOLE OF   CO2
       0.             MOLE OF   CO
       0.             MOLE OF   NH3
       0.             MOLE OF   H
       0.             MOLE OF   NO
        1.040030      MOLE OF   N2
       0.             MOLE OF   OH
       0.             MOLE OF   CH4

 THE ESTIMATES OF THE    1 SOLID PRODUCT(S) ARE :-
        1.411559      MOLE OF   SOLC


 CONSIDER THE BKW EQUATION OF STATE PARAMETERS : ALPHA,BETA,THETA & KAPPA

 DO YOU WANT PARAMETERS TO FIT  RDX [R] , TNT [T]  OR OTHER [O] ?  [DEFAULT R]
:r


 DO YOU WANT TO GENERATE A DECK AT THIS STAGE ?  [Y/N]
:y
 WHICH FILE DO YOU WANT GENERATED AS AN OBJECT DECK ?
  compb
 WHAT IS THE USER ID FOR THIS FILE ?
 dfc[illegible]

 DECK GENERATION SUCCESSFUL
```

```
 DO YOU WANT TO QUIT YET ?  [Y/N]
:y
7000 Job exiting
CIO active mode
:o,ed
ED version 10/01/84
WORKFILE RECOVERY INITIATED.
1** 7000 SCOPE 2.1.5-590 MOD 11/01/84  13.02.17.** 19/01/84      84019
:*/attach(comrb,sn=dfc4522,id=dfcjjm)/
BKWDECK(T20) 19/01/84 AUSTRALIAN COMPOSITION B
:0,
BKWDECK(T20) 19/01/84 AUSTRALIAN COMPOSITION B
GETSET(DFC4522)
ATTACH(BKWBIN,BKWBIN,SN=DFC4522,ID=DFCJJM)
BKWBIN.
*EOS
    0    1    1    1              0    2    0    0   USERBKW
 AUSTRALIAN COMPOSITION B                                       19/01/84
    4   11   12
 .500000000000      .160000000000      400.000000000      10.9097784436
C      H      N      O
       303.1500            .1000000E-05
H2O    H2     O2     CO2    CO     NH3    H      NO     N2     OH     CH4
SOLC
       100.0000
       222.1180            33970.00            .5500000            1.650000    RDX
       3.000000            6.000000            6.000000            6.000000
       227.1340           -1440.000            .4500000            1.650000    TNT
       7.000000            5.000000            3.000000            6.000000
 1.65000000000
 1.23815072844     0.                  0.                  .718135830729
0.                 0.                  0.                 0.
 1.04002979542     0.                  0.                  1.41155909629
 42.5884200000      .148080500000E-01-.263918100000E-05 .192045300000E-09
0.                  1342.82840000      -57107.0000000      250.000000000
 39.7034700000      .114382900000E-01-.220122200000E-05 .167776100000E-09
0.                  1175.89620000      0.                  80.0000000000
 47.0309000000      .128714700000E-01-.250021700000E-05 .190157000000E-09
0.                  1035.37650000      0.                  350.000000000
 47.4811200000      .195446300000E-01-.372129600000E-05 .277030000000E-09
0.                  746.280970000      -93968.0000000      600.000000000
 45.3408200000      .123816100000E-01-.241640300000E-05 .182818100000E-09
0.                  1121.58830000      -27201.0000000      390.000000000
 42.0181600000      .191166200000E-01-.316433000000E-05 .219780100000E-09
0.                  1206.96120000      -9368.00000000      476.000000000
 26.3911000000      .812137200000E-02-.169074000000E-05 .131682300000E-09
0.                  794.631620000       51619.0000000      40.0000000000
 38.4149800000      .126938600000E-01-.249460000000E-05 .189321300000E-09
0.                  1209.24970000       21477.0000000      386.000000000
 43.9234000000      .122250100000E-01-.237900500000E-05 .179832200000E-09
0.                  1139.16130000      0.                  380.000000000
 42.4179200000      .115684700000E-01-.222665900000E-05 .168915500000E-09
0.                  1183.51750000       3560.00000000      413.000000000
 38.7568600000      .236401300000E-01-.370795700000E-05 .247071400000E-09
0.                  1042.42790000      -16000.0000000      528.000000000
 .246151900000      .717985500000E-02-.129755000000E-05 .934999500000E-10
0.                 -258.204390000      0.                 0.
SOLF
 .444444440000      .830935840000      -1.39381810000      .672569720000
 .113537260000      .649155880000E-02-.226705350000      .120516570000
 .831600000000E-01-.175590000000      .155310000000      12.0111500000
      0.                2.000000           0.                  1.000000
      0.                2.000000           0.                  0.
      0.               0.                  0.                  2.000000
       1.000000        0.                  0.                  2.000000
       1.000000        0.                  0.                  1.000000
      0.                3.000000            1.000000           0.
      0.                1.000000           0.                  0.
      0.               0.                   1.000000            1.000000
      0.               0.                   2.000000           0.
      0.                1.000000           0.                  1.000000
       1.000000         4.000000           0.                  0.
       1.000000        0.                  0.                  0.
 !
*EOF
:E [illegible]
1** 7000 SCOPE 2.1.5 590 MOD 11/01/84  13.02.17.** 19/01/84      84019
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APPENDIX IV

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 * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
          [illegible] BEGIN
                           [illegible] 4
                           REWIND [illegible]
                             [illegible] ANTMATRIX [illegible] MOUNT [illegible]
                             [illegible] PARAMETER [illegible]
                           ATTACH(BEWLIN,BEWLIN[illegible])
                           REWIND
                             [illegible] REQUIRED
                             [illegible] EXECUTION [illegible]
                               END [illegible]
                               [illegible] SECOND EXECUTION TIME

[illegible]

       COEFFICIENT [illegible] INTEGRATION CONSTANT [illegible]
[illegible]   .4[illegible]E+02   .14[illegible]E-01   .26[illegible]E-[illegible]
              .1[illegible]E+04   [illegible]          [illegible]
              .4[illegible]E+0[illegible]   [illegible]   .41[illegible]
              .11[illegible]E+04   [illegible]   [illegible]
              .49[illegible]E+0[illegible]   [illegible]   [illegible]
              .11[illegible]E+01   [illegible]   [illegible]
              .118[illegible]E+03   [illegible]   [illegible]
              .164[illegible]E+04   [illegible]   [illegible]
[illegible]   .2461[illegible]E+0[illegible]   [illegible]   [illegible]
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  [illegible] BKW CALCULATION FOR THE EXPLOSIVE
  [illegible] COMPOSITION B                                           19/01/84

  THE COMPUTED C-J PRESSURE IS         .2543040774E+00    MEGABARS

  THE COMPUTED DETONATION VELOCITY IS        .7764271863E+00    CM/MICROSECOND

  THE COMPUTED C-J TEMPERATURE IS        .2863259488E+04    DEGREES KELVIN

  THE COMPUTED C-J VOLUME       .4[illegible]E+00  CC/GM OF EXPLOSIVE

  THE COMPUTED GAMMA IS      .[illegible]E+01

  THE VOLUME OF THE GAS IS       .[illegible]E+02  CC/MOLE OF GAS AND THERE ARE       .3024047062E+01   MOLES OF GAS

  [illegible]
  [illegible]

  THE COMPOSITION OF THE DETONATION MIXTURE

  SPECIES    NO. OF MOLES
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
  [illegible] BKW HUGONIOT FOR THE DETONATION PRODUCTS OF
  [illegible] COMPOSITION B                                           19/01/84

  PRESSURE       [illegible]E+00 VOLUME      .[illegible]E+00 TEMPERATURE      .3700359089E+04
  SHOCK VELOCITY       [illegible]E+00 PARTICLE VELOCITY     .3505580342E+00 UNITS ARE MBARS,CC/GM, DEG K, AND CM/MICROSECOND

  SPECIES    NO. OF MOLES
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]

  PRESSURE       [illegible] VOLUME      .[illegible]E+00 TEMPERATURE      .347866[illegible]E+04
  SHOCK VELOCITY       [illegible]E+00 PARTICLE VELOCITY     .[illegible]E+00 UNITS ARE MBARS,CC/GM, DEG K, AND CM/MICROSECOND

  SPECIES    NO. OF MOLES
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]

  PRESSURE       .3[illegible]E+00 VOLUME      .38[illegible]E+00 TEMPERATURE      .3282261128E+04
  SHOCK VELOCITY       .[illegible]14E+00 PARTICLE VELOCITY     .2951474751E+00 UNITS ARE MBARS,CC/GM, DEG K, AND CM/MICROSECOND

  SPECIES    NO. OF MOLES
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             [illegible]
             [illegible]
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             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]
             [illegible]

  PRESSURE       [illegible] VOLUME      .[illegible] TEMPERATURE      .[illegible]E+04
  SHOCK VELOCITY       [illegible] PARTICLE VELOCITY     [illegible] UNITS ARE MBARS,[illegible]

  SPECIES    NO. OF MOLES
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             [illegible]
             [illegible]
             [illegible]
             [illegible]
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[illegible]      .[illegible]E+00 VOLUME      .4265215973E+00 TEMPERATURE =    .2969110179E+04
[illegible]      .[illegible]74274153E+00 PARTICLE VELOCITY =  .2320809546E+00 UNITS ARE MBARS,CC/GM, DEG K, AND CM/MICROSECON

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H                .[illegible]4465096[illegible]E-02
[illegible]      .5[illegible]48040[illegible]69E-05
[illegible]      .6[illegible]81[illegible]4[illegible]42E+00
[illegible]      .4245609510E-01
[illegible]      .1[illegible]1430420[illegible]E-03
H                .8036014333E-0[illegible]
[illegible]      .1[illegible]286[illegible]390[illegible]E-0[illegible]
N2               .10399176491E+0[illegible]
[illegible]      .20[illegible]45[illegible]45[illegible]48E-06
[illegible]      .45496[illegible]E-05
[illegible]      .1389[illegible]9908E+01

[illegible]      .2[illegible]E+00 VOLUME =    .4537658986E+00 TEMPERATURE =    .2854565073E+04

  [illegible]   NO OF MOLES
[illegible]      .1234163204E+01
[illegible]      .3[illegible]284392[illegible]E-02
[illegible]      .[illegible]44091[illegible]E-05
[illegible]      .6934[illegible]161106E+00
[illegible]      .[illegible]
[illegible]      .1[illegible]
                 .1[illegible]829112[illegible]E-0[illegible]
[illegible]      .[illegible]
[illegible]      .1[illegible]
[illegible]      .[illegible]
[illegible]      .[illegible]
[illegible]      .1[illegible]

[illegible]      .[illegible]E+00 VOLUME      [illegible]4429202E+00 TEMPERATURE =    .2770263051E+04

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[illegible]      .[illegible]
[illegible]      .[illegible]E+00
[illegible]      .[illegible]E-01
[illegible]      .[illegible]
[illegible]      .[illegible]44744[illegible]
[illegible]      .[illegible]
[illegible]      .[illegible]
[illegible]      .[illegible]
[illegible]      .[illegible]
[illegible]      .[illegible]

[illegible]      .[illegible]E+00 VOLUME      .[illegible]4544451[illegible]3E+00 TEMPERATURE =    .27[illegible]1687253[illegible]E+04

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[illegible]      .[illegible]
[illegible]      .[illegible]

[illegible]      .[illegible] VOLUME      .[illegible]E+00 TEMPERATURE      .[illegible]E+04

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[illegible]      .[illegible]
[illegible]      .[illegible]
[illegible]      .[illegible]
[illegible]      .[illegible]
[illegible]      .[illegible]
[illegible] NEW [illegible] ENTROPY [illegible] NEW [illegible]
[illegible] TAN [illegible]                                   1[illegible] 01 84
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 [illegible]   [illegible]E+01   [illegible]E+00ENV   [illegible]E+01ENV#2   .2619226551E+01ENV#3   .1144[illegible]   [illegible]V#4

 N [illegible]   .2749504804E+01   .4640643398E+00ENV   [illegible]E+01ENV#2   .1957 4[illegible]6E 01ENV#3   [illegible]4330E   [illegible]#4

 [illegible]   .2544[illegible]E+01   .5199[illegible]2834E+00ENE   .7962391447E+01ENE#2   .4213[illegible]51E+01ENE#3   .2097[illegible]6131E+01ENE#4

THE CONSTANT ADDED TO ENERGIES WAS   .1000000000E+01

  PRESSURE (MBARS)   VOLUME (CC/GM)    TEMPERATURE (DEG K)   ENERGY(MB-CC/GM)   GAMMA            PARTICLE VELOCITY
  .2514040[illegible]E+00   .4511141133E+00   .2363259434E+04   .1197021298E+00   .2826210698E+01   [illegible]
  .1942280588E+00   .4981135514E+00   .2718250095E+04   .1094197[illegible]E+00   .2293345858E+01   .2512087842E+0[illegible]
  .1134456444E+00   .5505087528E+00   .2572881485E+04   .1002455[illegible]E+00   .2762658208E+01   .7206892446E+0[illegible]
  .1[illegible]2545[illegible]E+00   .6094216428E+00   .2432642618E+04   .9342836298E-01   .2724998006E+01   .3459366495E+[illegible]
  .[illegible]4[illegible]E-01   .6760735138E+00   .2298598888E+04   .8721736298E-01   .2633762992E+01   [illegible]
  [illegible]E-01   .7518998718E+00   .2171531458E+04   .9191619678E-01   .2637456098E+01   .426[illegible]4931[illegible]
  [illegible]E-01   .8385499358E+00   .2051985491E+04   [illegible]4998E-01   .2557539911E+01   .4630[illegible]
  [illegible]E-01   .9380445588E+00   .1940292648E+04   .[illegible]3452655E-01   .2534531706E+01   .4969[illegible]
  [illegible]E-01   .1052782278E+01   .1874[illegible]E+04   .7268334911E-01   .2475[illegible]E+01   .5284[illegible]
  [illegible]E-01   .1185663898E+01   .1740800338E+04   .6711800628E-01   .2417592076E+01   .5579[illegible]
  .113[illegible]45E-01   .1340263998E+01   .1652273513E+04   .6454113408E-01   .2341[illegible]E+01   .5954[illegible]
  [illegible]E-01   .1520[illegible]24[illegible]E+01   .1574273614E+04   .6235[illegible]522E-01   .2270339302E+01   .6117051[illegible]
  [illegible]5425488E-02   .1735050[illegible]E+01   .1500676[illegible]E+04   .6067[illegible]99E-01   .2205989[illegible]E+01   .6354[illegible]
  [illegible]E-02   .1986420[illegible]E+01   .1433744564E+04   .5862890485E-01   .2130675427E+01   .6581070[illegible]
  [illegible]E-02   .2284051151E+01   .1371970821E+04   .5796365951E-01   .2053245511E+01   .6797[illegible]
  [illegible]E-02   .2641105498E+01   .1315628898E+04   .5567282998E-01   .1974[illegible]7953E+01   .6994[illegible]
  [illegible]E-02   .3069375839E+01   .1265380813E+04   .5441530718E-01   .1994688298E+01   .7184[illegible]
  [illegible]E-02   .3594111448E+01   .1215998874E+04   .5320795592E-01   .1815506474E+01   .7364[illegible]
  [illegible]E-02   .4212294128E+01   .1171[illegible]E+04   .5214217701E-01   .1773[illegible]E+01   .7574[illegible]
  [illegible]E-[illegible]   .4979[illegible]E+01   .1129425[illegible]E+04   .5119242918E-01   .1663799941E+01   [illegible]
  [illegible]E-03   .5920[illegible]432E+01   .1[illegible]E+04   .5041[illegible]E-01   .1595245[illegible]E+01   .7954410[illegible]
  [illegible]E-03   .7094648818E+01   .1052[illegible]E+04   .4960522068E-01   .1534142E+01   .8605[illegible]
  [illegible]E-03   .8531[illegible]E+01   .1018[illegible]E+04   .4884877998E-01   .1494343[illegible]E+01   .9150[illegible]E+00
  [illegible]E-03   .1034825[illegible]E+02   .9810[illegible]E+03   .4814050518E-01   .1446272828E+01   .929[illegible]E+00
  [illegible]E-03   .1259928[illegible]E+02   .9477742458E+03   .4747485148E-01   .1426201[illegible]4E+01   .9431[illegible]E+00
  [illegible]E-03   .1544[illegible]E+02   .9142574748E+03   .4694[illegible]148E-01   .1427[illegible]60E+01   .95[illegible]
  [illegible]E-03   .190[illegible]E+02   .8811274848E+03   .4627443368E-01   .1457069138E+01   .9701283908E+00
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  [illegible]E+00   .3905[illegible]E+00   .3094[illegible]E+04   .1387956048E+00   .2862124[illegible]E+01   0.
  [illegible]E+00   .3720295[illegible]E+00   .3157214218E+04   .1464498142E+00   .2877105098E+01   0.
  [illegible]E+00   .3540227018E+00   .3[illegible]9408[illegible]E+04   .1550099952E+00   .2882604478E+01   0.
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  [illegible]E+00   .3[illegible]41[illegible]4E+00   .3386[illegible]E+04   .1766804128E+00   .2899469548E+01   0.
  [illegible]E+00   .293402[illegible]E+00   .3485[illegible]47E+04   .1905011408E+00   .2906556318E+01   0.
  [illegible]E+00   .2947[illegible]E+00   .3539[illegible]E+04   .2020[illegible]568E+00   .2910681048E+01   0.
 [illegible] STATE VARIABLES AS COMPUTED FROM THE LEAST SQUARES FIT

  [illegible]   FIT [illegible]   RAW TEMPERATURE   FIT TEMPERATURE   RAW ENERGY + C   FIT ENERGY
  [illegible]   [illegible]E+00   .2363259434E+04   .2[illegible]6254[illegible]E+04   .1197021298E+00   .1129[illegible]
  [illegible]   [illegible]E+00   .2718250095E+04   .2693854[illegible]1E+04   .1094197378E+00   .1092[illegible]E+0[illegible]
  [illegible]   [illegible]E+00   .2572881485E+04   .255[illegible]E+04   .1002455238E+00   .10[illegible]E+00
  [illegible]   [illegible]E+00   .2432642618E+04   .2415335998E+04   .9342836298E-01   .9414[illegible]
  [illegible]   [illegible]   .2298598888E+04   .2299[illegible]E+04   .8721736298E-01   .8694[illegible]
  [illegible]   [illegible]   .2171531458E+04   .2179906[illegible]E+04   .9191619678E-01   .8195[illegible]
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  [illegible]   [illegible]   .1940292648E+04   .1957[illegible]E+04   .7734526555E-01   .7735[illegible]
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  [illegible]   [illegible]   .1740800338E+04   .1759[illegible]E+04   .6711800628E-01   .671[illegible]
  [illegible]   [illegible]   .1652273513E+04   .1667[illegible]E+04   .6454113408E-01   .6454[illegible]
  [illegible]   [illegible]   .1574273614E+04   .1584595408E+04   .6235[illegible]522E-01   .6241[illegible]
  [illegible]   [illegible]   .1500676[illegible]E+04   .1509[illegible]E+04   .6067[illegible]99E-01   .6045[illegible]
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  [illegible]   [illegible]   .9810[illegible]E+03   .989[illegible]E+03   .4814050518E-01   .49[illegible]
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  [illegible]   [illegible]   .3[illegible]9408[illegible]E+04   .32[illegible]E+04   .1550099952E+00   .155[illegible]
  [illegible]   [illegible]   .339[illegible]55818E+04   .330[illegible]E+04   .1648454628E+00   .16[illegible]
  [illegible]   [illegible]   .3386[illegible]E+04   .3464408[illegible]E+04   .1766804128E+00   .17[illegible]
  [illegible]   [illegible]E+00   .3485[illegible]47E+04   .351[illegible]E+04   .1905011408E+00   .19[illegible]
  [illegible]   [illegible]E+00   .3539[illegible]E+04   .35[illegible]E+04   .2020[illegible]568E+00   .20[illegible]
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[illegible] PRESSURE AND COMPOSITION OF DETONATION PRODUCTS
[illegible]          NH3      H        N2       NO       OH       H4       [illegible]
[illegible]      .[illegible]14E+01   [illegible]      [illegible]      [illegible]34E+[illegible]   [illegible]
[illegible]      .1055[illegible]E-0[illegible]   [illegible]E-04   .1[illegible]E+01   [illegible]   [illegible]
[illegible]
[illegible]      .12[illegible]E+01   [illegible]E-0[illegible]   [illegible]E-04   [illegible]E+[illegible]   [illegible]
[illegible]      [illegible]   .3[illegible]E-04   .1039[illegible]E+01   .15[illegible]   [illegible]
[illegible]
[illegible]      .12[illegible]E+01   [illegible]E-01   [illegible]   [illegible]   [illegible]
[illegible]      [illegible]   [illegible]   .1079[illegible]E+01   .195[illegible]   [illegible]
[illegible]
[illegible]      .121[illegible]E+01   [illegible]E-01   .431[illegible]E-0[illegible]   [illegible]E+[illegible]   [illegible]
[illegible]      [illegible]   .431[illegible]   .1035[illegible]E+01   .212[illegible]   [illegible]
[illegible]
[illegible]      [illegible]E+01   [illegible]E-01   .1[illegible]   [illegible]   [illegible]
[illegible]      [illegible]   .3015[illegible]   .1079[illegible]E+01   .9756153[illegible]   .43[illegible]
[illegible]
[illegible]      .1195994[illegible]E+[illegible]   [illegible]E-01   .1000[illegible]E-[illegible]   .54[illegible]4E+[illegible]   [illegible]
[illegible]      [illegible]   .305324[illegible]   .1037112[illegible]1E+01   [illegible]   [illegible]
[illegible]
[illegible]      [illegible]E+01   [illegible]E-01   [illegible]   [illegible]   [illegible]
[illegible]      [illegible]   .151[illegible]E-04   .10368154[illegible]E+01   .1[illegible]   [illegible]
[illegible]
[illegible]      [illegible]   [illegible]E-01   [illegible]   [illegible]E+[illegible]   [illegible]
[illegible]      [illegible]   [illegible]   .1038[illegible]E+01   .16[illegible]   .31[illegible]
[illegible]
[illegible]      [illegible]   [illegible]   [illegible]   [illegible]E+[illegible]   [illegible]
[illegible]      [illegible]   .4[illegible]   .1[illegible]E+01   .139550572E-0[illegible]   .544[illegible]
[illegible]
[illegible]      [illegible]   [illegible]   [illegible]   .4[illegible]E+0[illegible]   [illegible]
[illegible]      [illegible]   .1[illegible]   .103[illegible]E+01   .1104[illegible]   .9[illegible]
[illegible]
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[illegible]
[illegible]      [illegible]   [illegible]   [illegible]   .[illegible]49182[illegible]E+00   [illegible]
[illegible]      [illegible]   [illegible]   .1[illegible]E+01   .5[illegible]E-0[illegible]   .1[illegible]E-01
[illegible]
[illegible]      [illegible]   [illegible]   [illegible]E-0[illegible]   .[illegible]9105[illegible]325E+[illegible]   [illegible]
[illegible]      [illegible]   [illegible]   .103[illegible]E+[illegible]   .[illegible]698[illegible]E-0[illegible]   [illegible]
[illegible]
[illegible]      [illegible]   [illegible]   [illegible]   [illegible]E+00   [illegible]
[illegible]      [illegible]   [illegible]   .10[illegible]   [illegible]141E-0[illegible]   [illegible]
[illegible]
[illegible]      [illegible]   [illegible]E+0[illegible]   [illegible]   [illegible]E+0[illegible]   [illegible]
[illegible]      [illegible]   [illegible]   .10[illegible]E+01   [illegible]   [illegible]
[illegible]
[illegible]      [illegible]   [illegible]   [illegible]   [illegible]E+00   [illegible]
[illegible]      [illegible]   [illegible]   .10[illegible]E+01   .1000000000E-0[illegible]   [illegible]
[illegible]
[illegible]      [illegible]   [illegible]   [illegible]   [illegible]E+00   [illegible]
[illegible]      [illegible]   [illegible]   .10[illegible]E+01   .1000000000E-0[illegible]   .5[illegible]41[illegible]
[illegible]
[illegible]      [illegible]   [illegible]   [illegible]   .7[illegible]E+[illegible]   [illegible]
[illegible]      [illegible]   [illegible]   .10[illegible]E+[illegible]   .1000[illegible]E-0[illegible]   [illegible]
[illegible]
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[illegible]      [illegible]   [illegible]   [illegible]   [illegible]   [illegible]
[illegible]
[illegible]      .1238A[illegible]E+01   [illegible]E-0[illegible]   .1[illegible]E-04   .1055[illegible]E+00   [illegible]
[illegible]      .40[illegible]   .2070[illegible]   .103990[illegible]E+01   .1239444[illegible]   [illegible]
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