Determination of detonation velocity and Plate Dent properties of DPX-9 and DPX-10

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Emneord

DPX-9

DPX-10

Detonasjonshastighet

Detonasjonstrykk

RDX

Godkjent av

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English summary

Two press and formable new plastic explosive compositions developed by Chemring Nobel containing RDX as main filler have been studied. Pellets pressed by Chemring Nobel AS were glued together at FFI to test charges of approximately 300 mm length and used to measure detonation velocity and detonation pressure.

For two shots of DPX-9 sats 527/09 made up of pellets with an average density of 1.657±0.015 g/cm^3 we obtained a detonation velocity of 8186±130 m/s. The detonation pressure calculated from the dent depth and charge diameter was on average 224±18 kbar for three test charges.

Accordingly for DPX-10 sats 540/09 made up of pellets with an average density of 1.631±0.019 g/cm^3, three shots gave an average detonation velocity of 8219±75 m/s. Corresponding detonation pressure calculated from the dent depth and charge diameter gave an average detonation pressure of 233±11 kbar.

Sammendrag

To pressbare og formbare nye plastiske sprengstoffkomposisjoner utviklet av Chemring Nobel AS med RDX som hovedfyllstoff har vært studert. Etter at Chemring Nobel AS hadde fremstilt pelletter ved pressing ble disse limt sammen til testladninger med en totallengde på omlag 300 mm og benyttet til bestemmelse av detonasjonshastighet og trykk ved FFI.

For DPX-9 sats 527/09 ble det for to skudd sammensatt av pelletter med en gjennomsnittlig tetthet på 1.657±0.015 g/cm^3 oppnådde en gjennomsnittlig detonasjonshastighet på 8186±130 m/s. Detonasjonstrykk beregnet ut fra eksperimentell Plate dent dybder og ladningsdiameter ble bestemt til gjennomsnittlig 224±18 kbar for tre test ladninger..

For 3 skudd med DPX-10 sats 540/09 sammensatt av pelletter med en gjennomsnittlig tetthet på 1.631±0.019 g/cm^3 ble detonasjonshastighet bestemt til 8219±75 m/s. Detonasjonstrykk beregnet ut fra dent dybder og ladningsdiameter for de samme 3 skuddene ga et gjennomsnittlig trykk på 233±11kbar.

Contents

1 Introduction

Two new compositions developed by Chemring Nobel AS have been tested with regard to detonation velocity and pressure. To experimentally determine the detonation velocity we used a cylindrical charge that contains a start and stop probe consisting of twisted copper wires, and registered the time the detonation front used from the start to the stop. The detonation pressure was measured by using of the Plate Dent test.

The tested compositions are plastic explosive containing RDX as the main filler. A nominal filler content of 87-90 wt% has been indicated from the producer. In addition to RDX the compositions contain binder/ plasticizer as DOS (dioctyl sebacate). In addition to the experimental determination of detonation velocity and pressure some Cheetah calculations (1) of a generic composition of 88.5 wt.% RDX and 11.5% DOS have been carried out. The content of plasticizer DOS is lower than 11.5 wt% but the other ingredients in the compositions have approximately the same chemical content and therefore give more or less the same product.

2 Experimentally

2.1 Detonation Velocity

The tested DPX-9 and DPX-10 charges consist of single pellets glued together to a length that reduces the uncertainty in the measurement to an acceptable level. For both compositions the used pellets were pressed by Chemring Nobel AS. Dimensions, weight and density of single pellets are given in Appendix A. The material DPX-9 used was from sats 527/09, and for DPX-10 from sats 540/09. 30 pellets of each composition were received and used to produce three test items of each composition. All three test items contained 10 pellets, pellet 1-10 in item No 1, pellet 11-20 in item No 2 and pellets 21-30 in item No 3. As sensors or measuring probes we used twisted copper wires (2).The Copper wire had a diameter of 0.15 mm with a 0.005 mm thick layer of lacquer. Two wires were twisted together and at the ends the lacquer was removed to obtain contact. We used two measuring probes, one placed between the second and third pellet and one between pellet 9 and 10. The position of the start measuring probe was selected to get a stable detonation front/velocity before starting the measurements and the position of the stop probe was selected not to influence the Dent.

To initiate the charges we use a 16 g RDX/wax (HWC) booster and a detonator No 8. Pictures of the test items are given in Figure 3.2 and 3.6.

To measure the velocity we used the set up shown in Figure 2.1 in addition to two power supplies and a scope of type: HEWLETT PACKARD 54510A. Digitizing Oscilloscope, 250 MHz 1G Sa/s. When the detonation front passes the start sensor there will go a current through the circuit and a signal is observed on the oscilloscope. The same will happen when the detonation front

reaches the stop probe. The time between these two signals is used to calculate the detonation velocity since we know the distance between the two sensors.

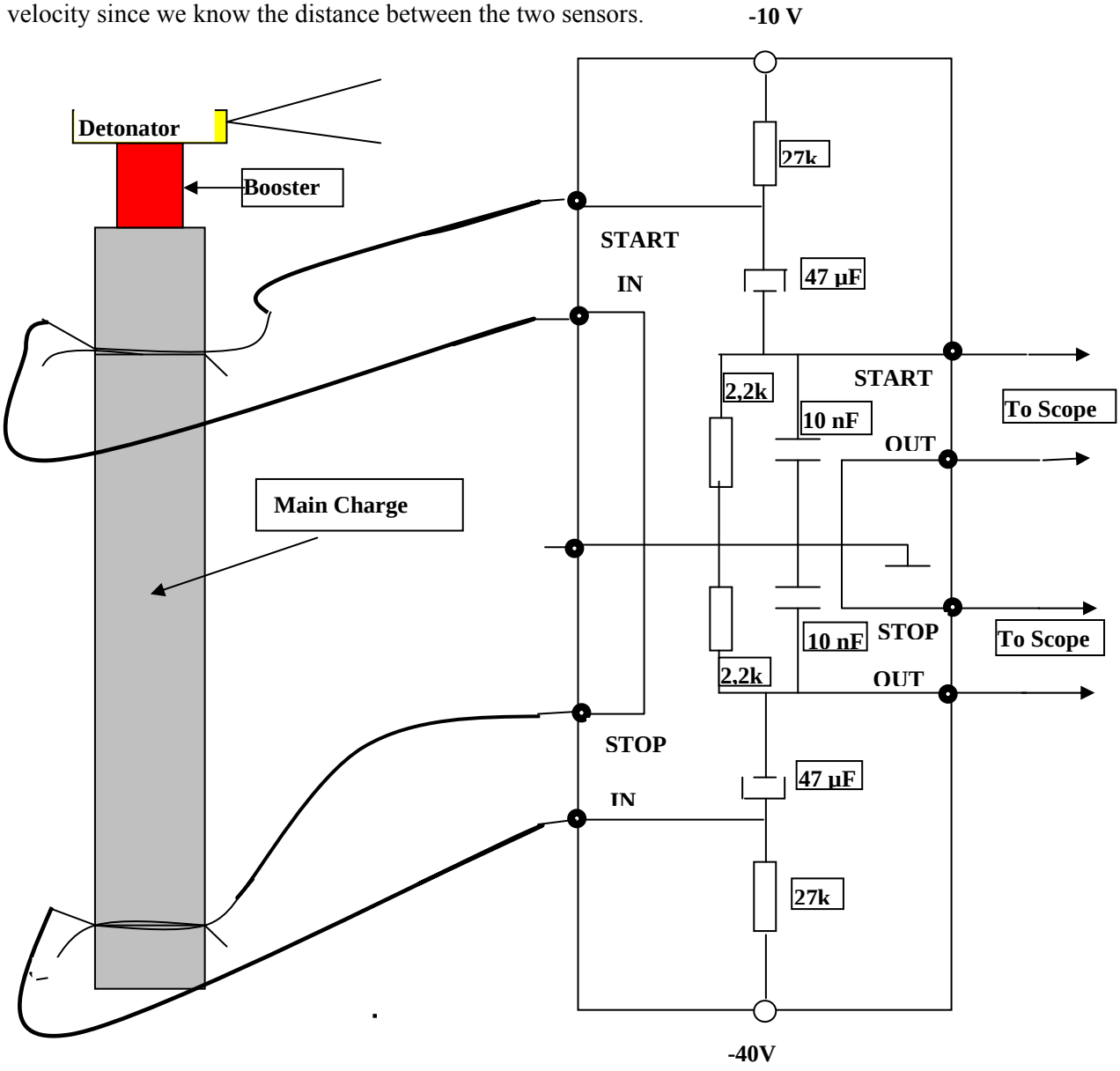

Figure 2.1 Sketch of the instrumentation for measuring the detonation velocity.

2.2 Plate Dent test

The Plate Dent test as described in (3) was performed for all six shots fired for determination of detonation velocity. As witness plates we used round steel plates with diameter 155 mm and thickness of 50 mm of ST-37 steel.

To measure the Dent depth we used a steel bullet with diameter 20 mm and a ring with the same height. To measure the exact depth of the pitting we use a micrometer screw with accuracy of 0.02 mm (Figure 2.2).

Figure 2.2 Picture of the equipment used to measure the Dent depth.

3 Results

3.1 Theoretical Calculations

The performance of a generic composition with RDX content of 88.5 wt% has been calculated by use of Cheetah 2.0 code (1) at TMD (theoretical maximum density) with both the BKWC and BKWS product database. The result is summarized in Table 3.1 and shows some differences in both detonation velocity and pressure for the two product databases. The detonation velocity and pressure obtained with BKWS product database are both higher than for the BKWC database. In general the BKWC (1) product database shall give properties closest to the experimentally measured properties in 3.2 and 3.3. For our compositions the results with regard to detonation pressure determined with BKWC are closer to the experimentally obtained properties, while it for the detonation velocity the BKWS is closest to the experimental results in 3.2.

The C-J Conditions		**BKWS product database**	**BKWC product database**
TMD	**(g/cm^3)**	1.6230	
The pressure	**(GPa)**	25.57	23.22
The volume	**(cc/g)**	0.469	0.465
The density	**(g/cc)**	2.130	2.152
The energy	**(KJ/cc explosive)**	3.04	2.85
Temperature	**(K)**	3622	3727
Shock velocity	**(m/s)**	8134	7630
Particle velocity	**(m/s)**	1937	1875
Speed of sound	**(m/s)**	6197	5755
Gamma		3.199	3.069

Table 3.1 Calculated properties at C-J conditions for 88.5 wt% RDX PBX by use of two different product databases (BKWS and BKWC).

3.2 Detonation velocity

3.2.1 Detonating Cord

To test that time registration equipment functioned as expected it was tested with a detonating cord with length 75.0 cm. The time between the start and the stop signal was 102.8 μs, which gives a detonation velocity of 7296 m/s. This velocity is similar to earlier measurement of 7282 m/s (4, 5) and 7299 m/s in (6) and in addition it confirmed that the cabling and time registration equipment did function as expected. Figure 3.1 shows a picture of the set up for the test of the detonating cord.

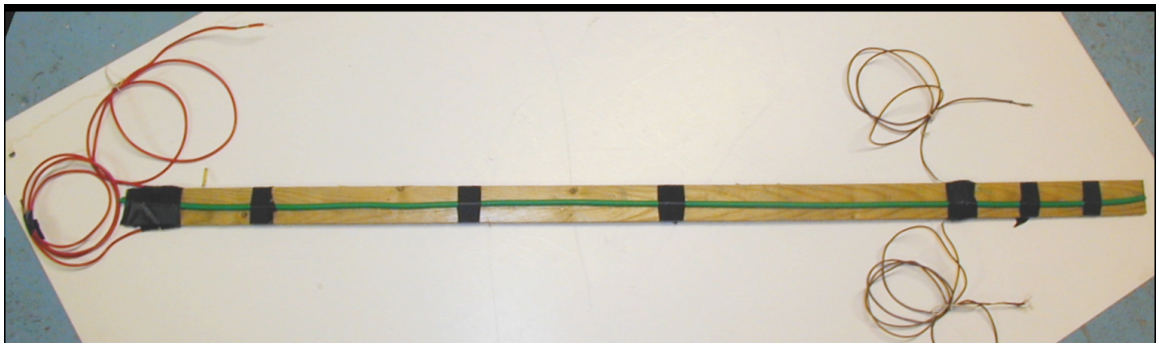

Figure 3.1 Set up for the testing of detonating cord.

Sample Identity	Main Charge length (mm)	Start length (mm)	Time (μs)	Velocity (m/s)
Detonating cord	750.0	200.00	102.8	7296

Table 3.2 Result with regard to detonation velocity for detonating cord.

3.2.2 DPX-9

From the 30 DPX-9 sats 527/09 pellets we received three test charges containing 10 pellets each were produced. The start registration was placed between the second and the third pellet while the stop was placed between the ninth and the tenth pellet. All charges are shown in figure 3.2.

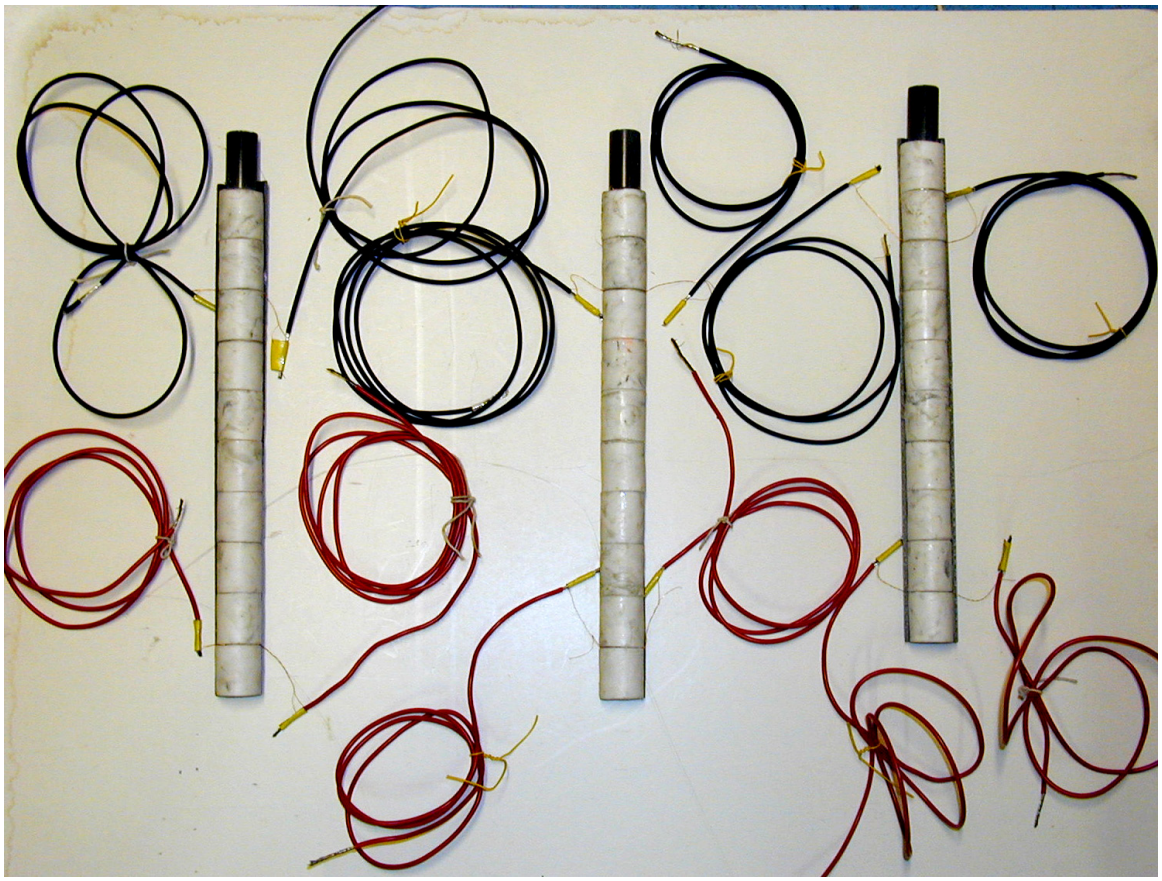

Figure 3.2 Picture of all test charges of DPX-9 sats 527/09 after been assembled.

3.2.2.1 Shot No 1

The first shot with DPX-9 sats 527/09 had a distance between the start and stop sensors of 204.66 mm. For this shot we did not obtain trigging of the start and therefore lost the time registration, however since the charge detonated we got the dent and the pressure is given in 3.3.1

3.2.2.2 Shot No 2

The second shot containing DPX-9 sats 527/09 had a distance between the start and stop sensors of 205.59 mm. Figure 3.3 gives a picture of the time registration on the oscilloscope. As can be seen from the picture both the start sensor and the stop sensor gave good registration and the difference in time between start and stop is 25.4 µs. This gives a detonation velocity of 8094 m/s (Table 3.3).

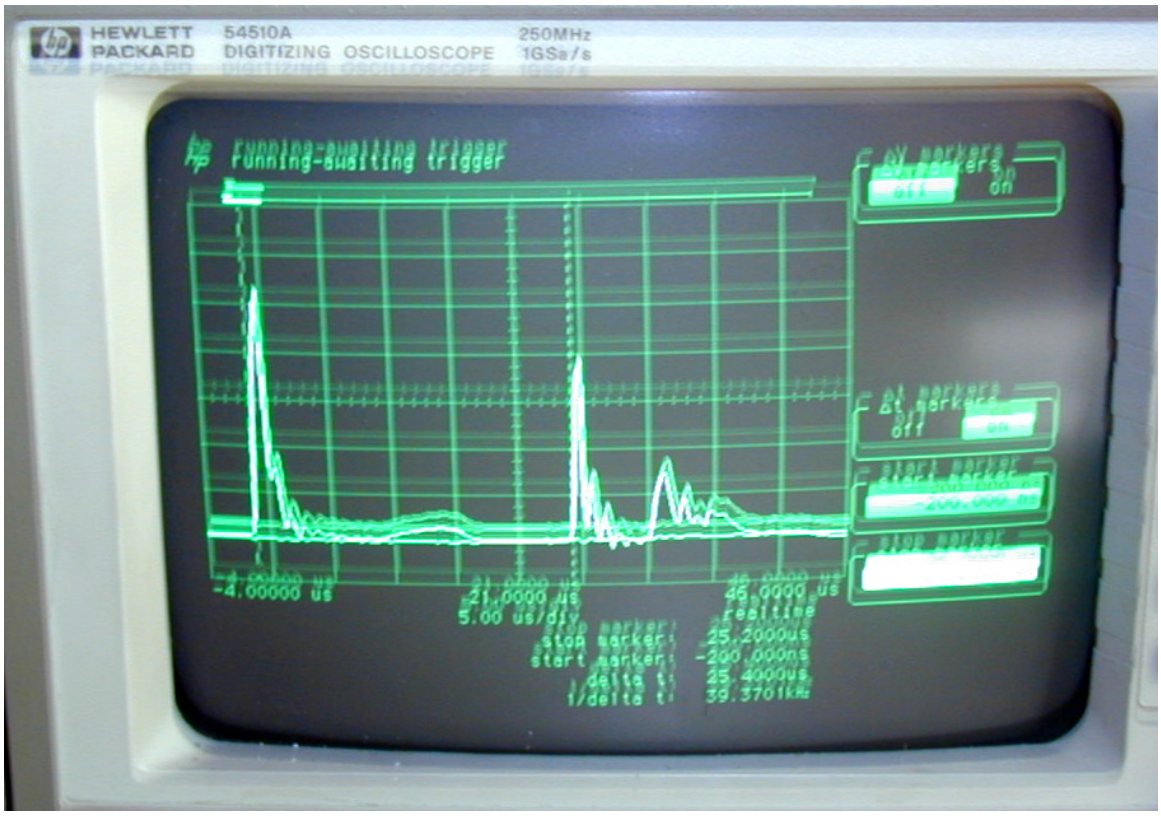

Figure 3.3 Picture of the oscilloscope registration for the second shot with DPX-9 sats 527/09.

3.2.2.3 Shot No 3

The third shot with DPX-9 sats 527/09 had a distance between the start and stop sensors of 207.76 mm.
In figure 3.4 a picture of the charge before firing is given.

Figure 3.5 gives a picture of the time registration on the oscilloscope. As can be seen from the picture both the start sensor and the stop sensor gave good registration and the difference in time between start and stop is 25.1 µs. This gives a detonation velocity of 8277 m/s.

Figure 3.4 Picture of the test upset for shot 3with DPX-9 sats 527/09 showing the Plate Dent witness plate at the bottom of the charge.

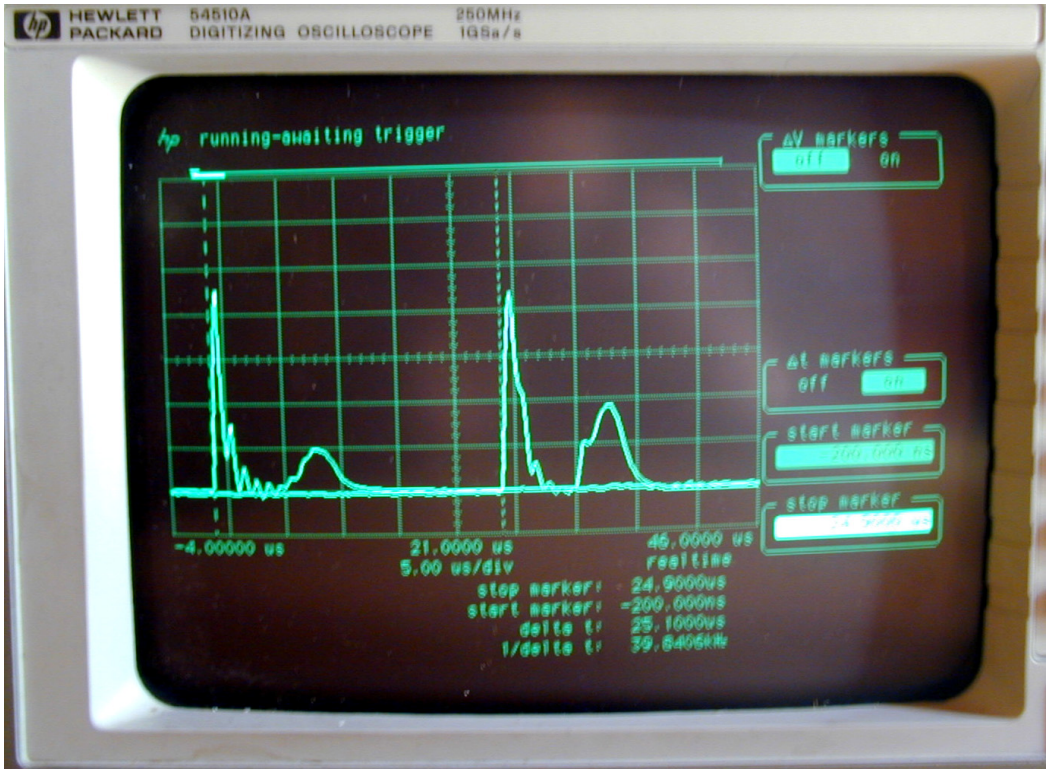

Figure 3.5 Picture of the oscilloscope registration for the third shot with DPX-9 sats 527/09.

3.2.2.4 Summary of detonations velocity determination

Table 3.3 summaries the measured detonation velocities for DPX-9. The average detonation velocity for the two shots where we got registration is 8186 ±130 m/s.

Sample Identity	Main Charge length (mm)	Start length (mm)	Time (µs)	Velocity (m/s)
DPX-9-1	204.66	59.23	-	-
DPX-9-2	205.59	59.55	25.4	8094
DPX-9-3	207.76	59.21	25.1	8277
DPX-9 Average				8186±130

Table 3.3 The table shows detonation velocity results for DPX-9 sats 527/09.

3.2.3 DPX-10

The second composition we tested was DPX-10. From the 30 DPX-10 sats 540/09 pellets we received we produced three test charges containing 10 pellets each. The start registration was placed between the second and the third pellet while the stop was placed between the ninth and the tenth pellet. A picture of all charges is shown in Figure 3.6.

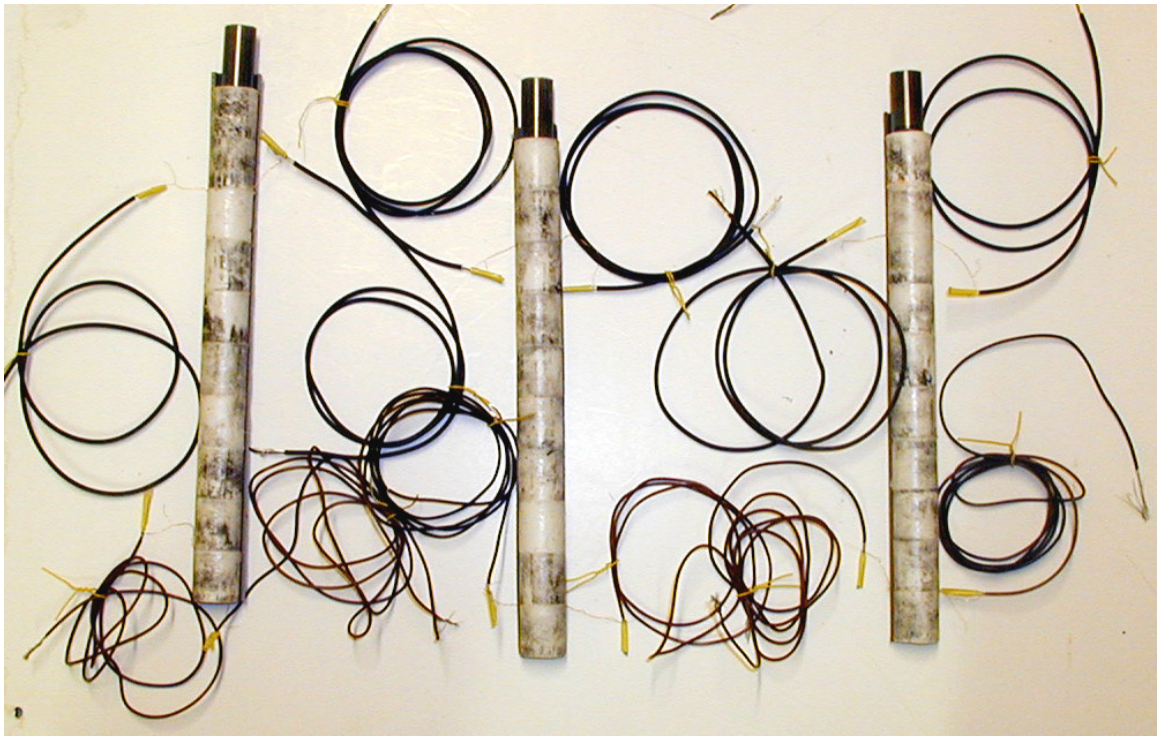

Figure 3.6 Picture of all test charges of DPX-10 sats 540/09 after been assembled.

3.2.3.1 Shot No 1

The first shot with DPX-10 sats 540/09 had a distance between the start and stop sensors of 204.19 mm. For shot 1 with DPX-10 Figure 3.7 gives a picture of the time registration on the used oscilloscope.

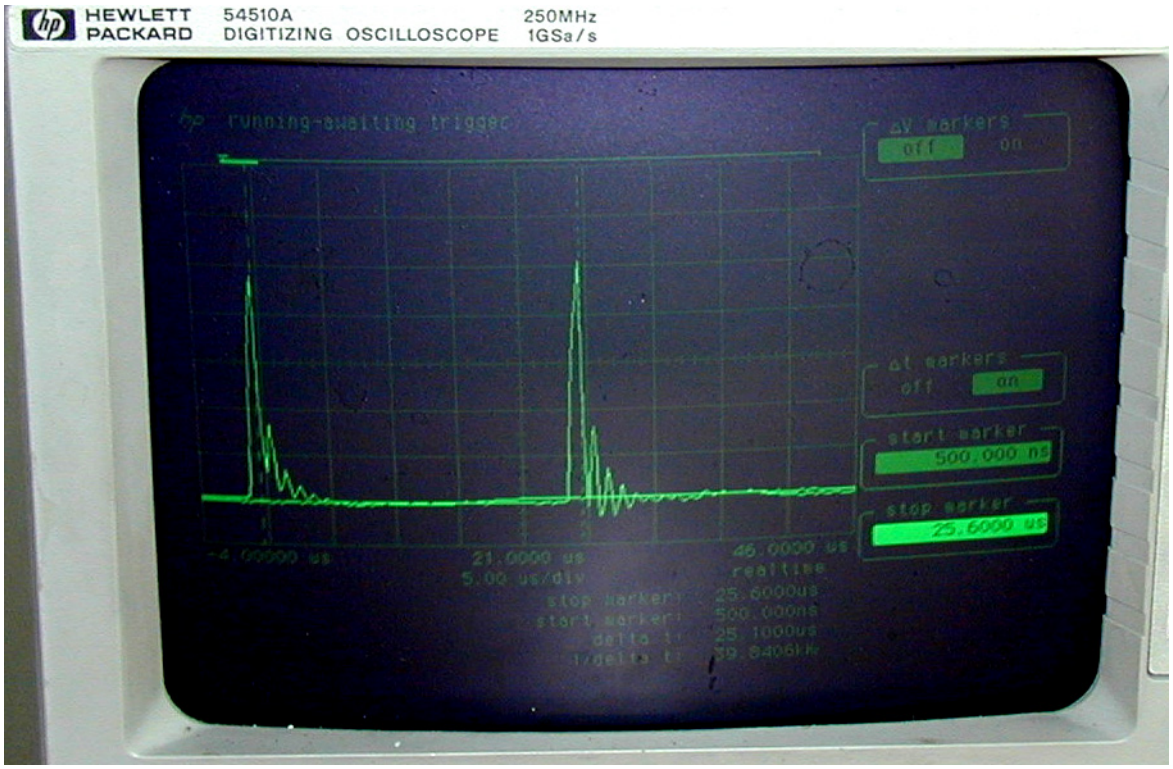

Figure 3.7 Picture of the oscilloscope registration for shot 1 with DPX-10 sats 540/09.

As can be seen from the picture both start sensor and stop sensor gave good registration and the difference in time between start and stop is 25.1 μs. This gives a detonation velocity of 8135 m/s.

3.2.3.2 Shot 2

The second shot with DPX-10 sats 540/09 had a distance between the start and stop sensors of 203.63 mm. Figure 3.8 gives a picture of the time registration on the oscilloscope.
As can be seen from the picture both the start sensor and the stop sensor gave good registration with a difference in time between start and stop of 24.6 μs. This gives a detonation velocity of 8278 m/s.

Figure 3.8 Picture of the oscilloscope registration for the second shot with DPX-10 sats 540/09.

3.2.3.3 Shot No 3

In Figure 3.9 a picture is given of the third charge of DPX-10 before firing. This third shot with DPX-10 sats 540/09 had a distance between the start and stop sensors of 203.63 mm. Figure 3.10 gives a picture of the time registration.

As can be seen from the picture in Figure 3.10 both the start sensor and the stop sensor gave good registration and the difference in time between start and stop is 24.6 µs. This gives a detonation velocity of 8244 m/s.

Figure 3.9 Picture of the test upset for shot 3with DPX-10 sats 540/09 showing the Plate Dent witness plate at the bottom of the charge.

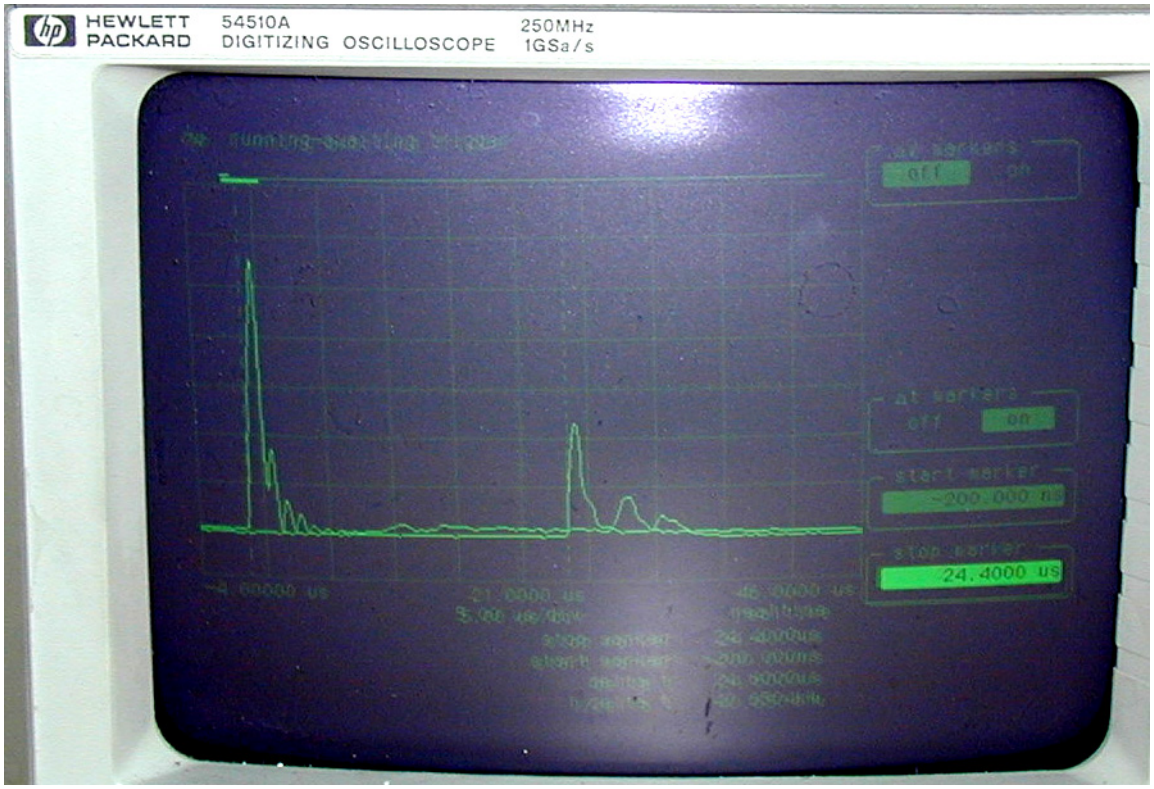

Figure 3.10 Picture of the oscilloscope registration for the third shot with DPX-10 sats 540/09.

3.2.3.4 Summary of detonation velocity measurements

The average detonation velocity for the three shots with DPX-10 sats 540/09 is 8219±75 m/s or 33 m/s higher than obtained for DPX-9. However if the standard deviation is taken into consideration the two results are equal with in the accuracy obtained by 5 firings.

Sample Identity	Main Charge length (mm)	Start length (mm)	Time (μs)	Velocity (m/s)
DPX-10-1	204.19	58.36	25.1	8135
DPX-10-2	203.63	58.36	24.6	8278
DPX-10-3	202.80	58.15	24.6	8244
DPX-10 Average				8219±75

Table 3.4 The table gives detonation velocity results for DPX-10 sats 540/09.

3.3 Plate Dent

The Plate Dent test gives results with respect to pressure performance. The depth of the dent in the witness plate is proportional to the detonation pressure for a given charge diameter (3).

3.3.1 DPX-9

A picture of the three witness plates is given in figure 3.11 for the firings with DPX-9 sats 527/09. And the obtained results are summarized in Table 3.5.

Figure 3.11 Picture of the Plate Dent witness plates for the DPX-9 shots.

For shot 2 a smaller dent is observed than for shot 1 and 3, while the dents for shot 1 and 3 are nearly equal. The average detonation pressure calculated from the dent depth and the charge diameter is 224±18 kbar.

Shot No.	Charge diameter (mm)	Dent Depth (mm)	Calculated detonation Pressure* (kbar)
DPX-9-1	25.22	4.15	237
DPX-9-2	25.26	3.56	203
DPX-9-3	25.07	4.04	232
Average			**224±18**

* Calculated from calibration curves with TNT charges (2)

Table 3.5 Results of DPX-9 sats527/09 in Plate Dent Test.

3.3.2 DPX-10

For the firings with DPX-10 sats 540/09 a picture of the three witness plates is given in figure 3.12. The obtained results are summarized in Table 3.6. As for DPX-9 two shots have almost equal dents while the last shot has a slightly lower dent depth. For the two shots with deepest dent the results are equal to those with the deepest dent for DPX-9. For DPX-10 sats 540/09 calculated dent pressure from measured dent depth and charge diameter gives on average a detonation pressure of 233±11 kbar.

Figure 3.12 Picture of the Plate Dent witness plates for the DPX-10 shots.

Shot No.	Charge diameter (mm)	Dent Depth (mm)	Calculated detonation Pressure* (kbar)
DPX-10-1	25.33	4.18	238
DPX-10-2	25.33	4.22	240
DPX-10-3	25.33	3.87	220
Average			**233±11**

* Calculated from calibration curves with TNT charges (2)

Table 3.6 Results of DPX-10 sats 540/09 in Plate Dent Test.

For DPX-5 Ch. 01/07 we obtained an average dent pressure of 253 kbar (6), and for composition PBXW-11 with 30% Aluminium Ch. 07/05 having a slightly higher HMX content (68.4 wt.%), we obtained a dent depth of 4.56 mm (5). Compared with these properties the results for DPX-9 and DPX-10 are slightly lower than both compared with DPX-5 Ch 01/07 and PBXW-11 with 30% Aluminium ch.07/05.

Appendix A Properties of tested pellets

A.1 DPX-9

Received pellets for determination of detonation velocity and Plate Dent test were all measured with regard to weight and dimensions. These results were used to determination of density. All results are summarized in Table-App 1.

Pellet No	Weight (g)	Height (mm)	Diameter (mm)	Volume (cm^3)	Density (g/cm^3)
1	24.0777	29.14	**25.22**	14.557	1.654
2	24.1023	29.40	25.17	14.629	1.648
3	24.0909	29.09	25.22	14.532	1.658
4	24.1220	28.82	25.21	14.386	1.677
5	24.1160	30.08	25.18	14.979	1.610
6	24.2056	29.33	25.21	14.640	1.653
7	24.1138	28.89	25.22	14.432	1.671
8	23.9719	28.92	25.00	14.196	1.689
9	24.1340	29.15	25.21	14.550	1.659
10	24.1279	29.38	25.21	14.665	1.645
11	24.1796	29.32	**25.26**	14.693	1.646
12	24.1255	29.19	25.24	14.605	1.652
13	23.9798	29.00	25.24	14.510	1.653
14	24.1713	29.27	25.26	14.668	1.648
15	24.0914	28.93	25.28	14.521	1.659
16	24.0870	28.79	25.22	14.382	1.675
17	24.1728	29.52	25.2	14.723	1.642
18	24.1162	29.00	25.23	14.498	1.663
19	24.0718	29.05	25.17	14.454	1.665
20	24.2312	29.20	25.25	14.622	1.657
21	24.1383	29.60	**25.07**	14.611	1.652
22	24.1751	29.28	25.2	14.604	1.655
23	24.0659	28.92	25.21	14.436	1.667
24	24.0617	29.05	25.15	14.432	1.667
25	24.1756	28.92	25.18	14.401	1.679
26	24.1029	28.97	25.37	14.645	1.646
27	24.1512	29.38	25.26	14.723	1.640
28	24.1337	29.17	25.28	14.641	1.648
29	24.1440	29.22	25.16	14.528	1.662
30	24.2100	29.16	25.24	14.590	1.659
Average density					**1.657±0.015**

Table-App. 1 Properties of pressed pellets of DPX-9 used for detonation velocity and Plate Dent measurements.

A.2 DPX-10

Received pellets for determination of detonation velocity and Plate Dent test were all measured with regard to weight and dimensions. These results were used to determination of density. All results are summarized in Table-App 2.

Pellet No	Weight (g)	Height (mm)	Diameter (mm)	Volume (cm^3)	Density (g/cm^3)
1	24.2385	29.52	**25.33**	14.876	1.629
2	24.2895	29.36	25.28	14.737	1.648
3	24.2699	28.60	25.37	14.458	1.679
4	24.2850	29.70	25.33	14.966	1.623
5	24.2307	29.23	25.40	14.811	1.636
6	24.2835	29.95	25.32	15.080	1.610
7	24.3123	29.67	25.28	14.892	1.633
8	24.2609	29.35	25.3	14.755	1.644
9	24.3244	29.32	25.25	14.682	1.657
10	24.2445	29.61	25.26	14.839	1.634
11	24.2881	29.46	**25.33**	14.845	1.636
12	24.2743	29.70	25.29	14.919	1.627
13	24.2714	30.01	25.32	15.111	1.606
14	24.2379	30.19	25.27	15.141	1.601
15	24.2344	29.55	25.34	14.903	1.626
16	24.2507	28.49	25.35	14.379	1.686
17	24.2611	29.71	25.34	14.983	1.619
18	24.2707	29.49	25.31	14.837	1.636
19	24.2741	29.32	25.35	14.798	1.640
20	24.2602	29.85	25.29	14.994	1.618
21	24.2764	29.56	**25.33**	14.896	1.630
22	24.2743	29.72	25.35	15.000	1.618
23	24.2546	29.69	25.27	14.891	1.629
24	23.2398	28.51	25.27	14.299	1.625
25	24.2663	29.88	25.36	15.093	1.608
26	24.6207	30.16	25.30	15.162	1.624
27	24.2685	29.38	25.28	14.747	1.646
28	24.2567	29.77	25.30	14.966	1.621
29	24.2989	29.76	25.32	14.985	1.622
30	24.2606	29.41	25.45	14.961	1.622
Average density					**1.631±0.019**

Table-App. 2 Properties of pressed pellets of DPX-10 used for detonation velocity and Plate Dent measurements.

Appendix B Cheetah calculations of detonation velocity and pressure

B.1 Product database BKWC

B.1.1 Summary output

```
Product library title: bkwc
Reactant library title: # Version 2.0 by P. Clark Souers

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.    TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
dos        11.50   6.34  20.47  -319073   426.66     0.91 C26H50O4
rdx        88.50  93.66  79.53    16496   222.13     1.81 C3H6N6O6
Product library title: bkwc
Reactant library title: # Version 2.0 by P. Clark Souers

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.    TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
dos        11.50   6.34  20.47  -319073   426.66     0.91 C26H50O4
rdx        88.50  93.66  79.53    16496   222.13     1.81 C3H6N6O6

Density  =  1.6230 g/cc   Mixture TMD =  1.6230 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          23.22 GPa
The volume            =          0.465 cc/g
The density           =          2.152 g/cc
The energy            =           2.85 kJ/cc explosive
The temperature       =           3727 K
The shock velocity    =          7.630 mm/us
The particle velocity =          1.875 mm/us
The speed of sound    =          5.755 mm/us
Gamma                 =          3.069

Cylinder runs:              % of standards
  V/V0     Energy    TATB      PETN      HMX     CL-20    TRITON
 (rel.)   (kJ/cc)  1.83g/cc 1.76g/cc 1.89g/cc 2.04g/cc 1.70g/cc
   1.00    -0.88
   2.20    -5.00     103       79       67       55       115
   4.10    -6.15     106       80       69       58       111
   6.50    -6.64     107       80       71       60       109
  10.00    -6.98     107       80       71       61       106
  20.00    -7.38     107       81       72       62       103
  40.00    -7.69     108       81       73       63        99
  80.00    -7.92     108       81       74       64        96
 160.00    -8.11

Freezing occurred at T =     1800.0 K and relative V =   2.150
The mechanical energy of detonation =     -8.410 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -8.410 kJ/cc
JWL Fit results:
E0   =     -8.836 kJ/cc
A    =    694.06 GPa, B    =  8.44 GPa , C     =         1.34 GPa
R[1] =      4.85,     R[2] =  1.06,      omega =         0.34
RMS fitting error =   0.93 %
```

B.1.2 Fulltext output

```
Product library title: bkwc
Executing library command: gas eos, bkw
Executing library command: set, bkw, alpha, 0.499123809964
Executing library command: set, bkw, beta, 0.402655787895
Executing library command: set, bkw, theta, 5441.84607543
Executing library command: set, bkw, kappa, 10.8636743138
Reactant library title:# Version 2.0 by P. Clark Souers

                                The Composition
Name    % wt. % mol % vol.  Heat of  Standard  Standard  Mol.   Formula
                           formation  volume    entropy   wt.
                           (cal/mol) (cc/mol) (cal/K/mol)
dos     11.50  6.34 20.47  -319073   467.83    0.000     426.66  C26H50O4
rdx     88.50 93.66 79.53    16496   122.99    0.000     222.13  C3H6N6O6

Heat of formation =    -20.277 cal/gm
Standard volume   =      0.616 cc/gm
Standard entropy  =      0.000 cal/k/gm
Standard energy   =    -20.292 cal/gm

The elements and percent by mole
     c             18.018
     h             35.524
     o             23.741
     n             22.717
The average mol. wt. = 235.086 g/mol
Input>composition, dos, 11.5, rdx, 88.5, weight
                                The Composition
Name   % wt. % mol % vol.   Heat of  Standard Standard    Mol.   Formula
                           formation  volume   entropy     wt.
                           (cal/mol) (cc/mol)(cal/K/mol)
dos    11.50   6.34  20.47  -319073  467.83    0.000     426.66  C26H50O4
rdx    88.50  93.66  79.53    16496  122.99    0.000     222.13  C3H6N6O6

Heat of formation =    -20.277 cal/gm
Standard volume   =      0.616 cc/gm
Standard entropy  =      0.000 cal/k/gm
Standard energy   =    -20.292 cal/gm

The elements and percent by mole
     c             18.018
     h             35.524
     o             23.741
     n             22.717
The average mol. wt. = 235.086 g/mol
Input>standard run, rho, 1.623035
Too many iterations in the etanewt solver
Failed to find equilibrium.  Will try again.
The hugoniot reference state:
P0 = 1.000000 ATM, V0 = 0.616130 cc/gm, E0 = -20.291838 cal/gm
Using  102733 ATM as a lower bound for the C-J pressure
Using  256834 ATM as an upper bound for the C-J pressure
The C-J point was bracketed in cjbrent
The CJ state was found in 6 iterations
                              The C-J condition
The shock velocity    =   7.62988e+003 m/s
The particle velocity =   1.87510e+003 m/s
The speed of sound    =   5.75478e+003 m/s

P0 =       1 atm, V0 =  0.61613 cc/gm, E0 = -20.29184 cal/gm
```

Reference state = reactants

H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00

P (ATM)	V (CC/GM)	T (K)	H(R) (CAL/GM)	E(R) (CAL/GM)	S(R) (CAL/K/GM)
VGS (CC/GM)	CV (CAL/K/GM)	CP (CAL/K/GM)	ALPHA	BETA	KAPPA
2.29168e+005	4.64711e-001	3.72705e+003	2.99932e+003	4.20188e+002	1.77249e+000
4.13725e-001	6.09490e-001	7.21215e-001	3.17721e+000	1.36108e+000	3.06904e+000

Product concentrations

Name		(mol/kg)	(mol gas/mol explosive)
h2o	Gas	1.865e+001	4.384e+000
n2	Gas	1.195e+001	2.810e+000
co2	Gas	2.466e+000	5.797e-001
co	Gas	1.385e+000	3.255e-001
ch4	Gas	1.041e-002	2.448e-003
ch2o2	Gas	6.817e-003	1.603e-003
c2h4	Gas	4.306e-003	1.012e-003
h2	Gas	2.397e-003	5.635e-004
no	Gas	1.983e-003	4.662e-004
ch3oh	Gas	6.707e-004	1.577e-004
h3n	Gas	6.298e-004	1.480e-004
o2	Gas	1.148e-004	2.699e-005
ch2o	Gas	1.592e-005	3.743e-006
ch3	Gas	4.498e-008	1.057e-008
c2h6	Gas	3.812e-009	8.961e-010
no2	Gas	1.442e-013	3.390e-014
*c	solid	1.508e+001	3.546e+000
Total	Gas	3.448e+001	8.106e+000
Total	Cond.	1.508e+001	3.546e+000

The C-J Adiabat

Reference state = reactants

H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00

P (ATM)	V (CC/GM)	T (K)	H(R) (CAL/GM)	E(R) (CAL/GM)	S(R) (CAL/K/GM)
VGS (CC/GM)	CV (CAL/K/GM)	CP (CAL/K/GM)	ALPHA	BETA	KAPPA
(CAL/K/GM)	(CAL/K/GM)				
9.60826e+004	6.16130e-001	3.00663e+003	1.30466e+003	-1.29020e+002	1.77249e+000
5.59580e-001	5.73012e-001	7.52748e-001	2.88424e+000	1.29568e+000	2.99785e+000

Product concentrations

Name		(mol/kg)	(mol gas/mol explosive)
h2o	Gas	1.802e+001	4.236e+000
n2	Gas	1.194e+001	2.808e+000
co	Gas	3.164e+000	7.439e-001
co2	Gas	1.885e+000	4.432e-001
ch4	Gas	2.430e-001	5.712e-002
h2	Gas	7.685e-002	1.807e-002
c2h4	Gas	3.234e-002	7.603e-003
h3n	Gas	1.548e-002	3.639e-003
ch2o2	Gas	1.227e-002	2.884e-003
ch3oh	Gas	3.927e-003	9.232e-004
ch2o	Gas	4.072e-004	9.572e-005
no	Gas	2.157e-004	5.070e-005
ch3	Gas	8.741e-006	2.055e-006
c2h6	Gas	7.125e-006	1.675e-006
o2	Gas	1.790e-006	4.208e-007
no2	Gas	6.155e-013	1.447e-013
*c	solid	1.359e+001	3.194e+000
Total	Gas	3.540e+001	8.322e+000
Total	Cond.	1.359e+001	3.194e+000

```
                        Reference state = reactants
              H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00

      P           V           T           H(R)        E(R)          S(R)
    (ATM)      (CC/GM)       (K)        (CAL/GM)    (CAL/GM)    (CAL/K/GM)
     VGS         CV          CP         ALPHA        BETA         KAPPA
   (CC/GM)   (CAL/K/GM)   (CAL/K/GM)
1.25896e+004 1.32447e+000 1.80000e+003 -3.23995e+002 -7.27803e+002 1.77249e+000
1.28939e+000 6.55867e-001 9.66443e-001  3.63703e+000  1.96185e+000 2.36360e+000

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
      h2o  Gas   1.248e+001  2.933e+000
       n2  Gas   1.189e+001  2.796e+000
       co  Gas   5.579e+000  1.312e+000
      co2  Gas   3.457e+000  8.127e-001
      ch4  Gas   2.307e+000  5.423e-001
       h2  Gas   1.388e+000  3.262e-001
      h3n  Gas   1.177e-001  2.767e-002
     c2h4  Gas   1.024e-002  2.406e-003
    ch2o2  Gas   5.390e-003  1.267e-003
     c2h6  Gas   2.132e-003  5.012e-004
    ch3oh  Gas   1.779e-003  4.182e-004
     ch2o  Gas   1.744e-003  4.100e-004
      ch3  Gas   5.039e-005  1.184e-005
       no  Gas   1.363e-007  3.204e-008
       o2  Gas   2.506e-011  5.890e-012
      no2  Gas   2.029e-015  4.771e-016
       *c  solid 7.584e+000  1.783e+000
     Total Gas   3.724e+001  8.754e+000
     Total Cond. 7.584e+000  1.783e+000
Freezing at v = 1.324468, t = 1800.000000

                        Reference state = reactants
              H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00
      P           V           T           H(R)        E(R)          S(R)
    (ATM)      (CC/GM)       (K)        (CAL/GM)    (CAL/GM)    (CAL/K/GM)
     VGS         CV          CP         ALPHA        BETA         KAPPA
   (CC/GM)   (CAL/K/GM)   (CAL/K/GM)
1.18971e+004 1.35549e+000 1.78019e+003 -3.46464e+002 -7.36996e+002 1.77249e+000
1.32038e+000 4.07385e-001 4.92039e-001  4.12361e+000  2.10658e+000 2.43219e+000

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*     h2o  Gas   1.248e+001  2.933e+000
*      n2  Gas   1.189e+001  2.796e+000
*      co  Gas   5.579e+000  1.312e+000
*     co2  Gas   3.457e+000  8.127e-001
*     ch4  Gas   2.307e+000  5.423e-001
*      h2  Gas   1.388e+000  3.262e-001
*     h3n  Gas   1.177e-001  2.767e-002
*    c2h4  Gas   1.024e-002  2.406e-003
*   ch2o2  Gas   5.390e-003  1.267e-003
*    c2h6  Gas   2.132e-003  5.012e-004
*   ch3oh  Gas   1.779e-003  4.182e-004
*    ch2o  Gas   1.744e-003  4.100e-004
*     ch3  Gas   5.039e-005  1.184e-005
*      no  Gas   1.363e-007  3.204e-008
*      o2  Gas   2.506e-011  5.890e-012
*     no2  Gas   2.029e-015  4.771e-016
*      *c  solid 7.584e+000  1.783e+000
     Total Gas   3.724e+001  8.754e+000
```

```
     Total Cond. 7.584e+000  1.783e+000

                          Reference state = reactants
               H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00
      P           V           T           H(R)        E(R)          S(R)
    (ATM)      (CC/GM)       (K)        (CAL/GM)    (CAL/GM)    (CAL/K/GM)
     VGS         CV          CP          ALPHA        BETA         KAPPA
   (CC/GM)   (CAL/K/GM)   (CAL/K/GM)
3.10442e+003 2.52613e+000 1.38271e+003 -7.15865e+002 -9.05772e+002 1.77249e+000
2.49073e+000 3.67070e-001 4.43662e-001  4.45913e+000  2.83564e+000 1.92519e+000

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*     h2o  Gas   1.248e+001  2.933e+000
*      n2  Gas   1.189e+001  2.796e+000
*      co  Gas   5.579e+000  1.312e+000
*     co2  Gas   3.457e+000  8.127e-001
*     ch4  Gas   2.307e+000  5.423e-001
*      h2  Gas   1.388e+000  3.262e-001
*     h3n  Gas   1.177e-001  2.767e-002
*    c2h4  Gas   1.024e-002  2.406e-003
*   ch2o2  Gas   5.390e-003  1.267e-003
*    c2h6  Gas   2.132e-003  5.012e-004
*   ch3oh  Gas   1.779e-003  4.182e-004
*    ch2o  Gas   1.744e-003  4.100e-004
*     ch3  Gas   5.039e-005  1.184e-005
*      no  Gas   1.363e-007  3.204e-008
*      o2  Gas   2.506e-011  5.890e-012
*     no2  Gas   2.029e-015  4.771e-016
*      *c  solid 7.584e+000  1.783e+000
     Total Gas   3.724e+001  8.754e+000
     Total Cond. 7.584e+000  1.783e+000


                          Reference state = reactants
               H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00
      P           V           T           H(R)        E(R)          S(R)
    (ATM)      (CC/GM)       (K)        (CAL/GM)    (CAL/GM)    (CAL/K/GM)
     VGS         CV          CP          ALPHA        BETA         KAPPA
   (CC/GM)   (CAL/K/GM)   (CAL/K/GM)
1.35525e+003 4.00484e+000 1.18865e+003 -8.46902e+002 -9.78332e+002 1.77249e+000
3.96941e+000 3.46641e-001 4.20894e-001  4.47711e+000  3.24416e+000 1.68830e+000

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*     h2o  Gas   1.248e+001  2.933e+000
*      n2  Gas   1.189e+001  2.796e+000
*      co  Gas   5.579e+000  1.312e+000
*     co2  Gas   3.457e+000  8.127e-001
*     ch4  Gas   2.307e+000  5.423e-001
*      h2  Gas   1.388e+000  3.262e-001
*     h3n  Gas   1.177e-001  2.767e-002
*    c2h4  Gas   1.024e-002  2.406e-003
*   ch2o2  Gas   5.390e-003  1.267e-003
*    c2h6  Gas   2.132e-003  5.012e-004
*   ch3oh  Gas   1.779e-003  4.182e-004
*    ch2o  Gas   1.744e-003  4.100e-004
*     ch3  Gas   5.039e-005  1.184e-005
*      no  Gas   1.363e-007  3.204e-008
*      o2  Gas   2.506e-011  5.890e-012
*     no2  Gas   2.029e-015  4.771e-016
*      *c  solid 7.584e+000  1.783e+000
     Total Gas   3.724e+001  8.754e+000
```

```
     Total Cond. 7.584e+000  1.783e+000

                          Reference state = reactants
                H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00
      P           V           T           H(R)        E(R)          S(R)
    (ATM)      (CC/GM)       (K)        (CAL/GM)    (CAL/GM)    (CAL/K/GM)
     VGS         CV          CP          ALPHA        BETA         KAPPA
   (CC/GM)   (CAL/K/GM)   (CAL/K/GM)
6.77348e+002 6.16130e+000 1.04634e+003 -9.26812e+002 -1.02787e+003 1.77249e+000
6.12587e+000 3.30641e-001 4.04126e-001  4.38720e+000  3.49430e+000 1.54171e+000

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*     h2o  Gas   1.248e+001  2.933e+000
*      n2  Gas   1.189e+001  2.796e+000
*      co  Gas   5.579e+000  1.312e+000
*     co2  Gas   3.457e+000  8.127e-001
*     ch4  Gas   2.307e+000  5.423e-001
*      h2  Gas   1.388e+000  3.262e-001
*     h3n  Gas   1.177e-001  2.767e-002
*    c2h4  Gas   1.024e-002  2.406e-003
*   ch2o2  Gas   5.390e-003  1.267e-003
*    c2h6  Gas   2.132e-003  5.012e-004
*   ch3oh  Gas   1.779e-003  4.182e-004
*    ch2o  Gas   1.744e-003  4.100e-004
*     ch3  Gas   5.039e-005  1.184e-005
*      no  Gas   1.363e-007  3.204e-008
*      o2  Gas   2.506e-011  5.890e-012
*     no2  Gas   2.029e-015  4.771e-016
*      *c  solid 7.584e+000  1.783e+000
     Total Gas   3.724e+001  8.754e+000
     Total Cond. 7.584e+000  1.783e+000

                          Reference state = reactants
                H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00
      P           V           T           H(R)        E(R)          S(R)
    (ATM)      (CC/GM)       (K)        (CAL/GM)    (CAL/GM)    (CAL/K/GM)
     VGS         CV          CP          ALPHA        BETA         KAPPA
   (CC/GM)   (CAL/K/GM)   (CAL/K/GM)
2.45275e+002 1.23226e+001 8.63031e+002 -1.01410e+003 -1.08728e+003 1.77249e+000
1.22872e+001 3.07845e-001 3.81235e-001  4.14798e+000  3.66253e+000 1.40558e+000

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*     h2o  Gas   1.248e+001  2.933e+000
*      n2  Gas   1.189e+001  2.796e+000
*      co  Gas   5.579e+000  1.312e+000
*     co2  Gas   3.457e+000  8.127e-001
*     ch4  Gas   2.307e+000  5.423e-001
*      h2  Gas   1.388e+000  3.262e-001
*     h3n  Gas   1.177e-001  2.767e-002
*    c2h4  Gas   1.024e-002  2.406e-003
*   ch2o2  Gas   5.390e-003  1.267e-003
*    c2h6  Gas   2.132e-003  5.012e-004
*   ch3oh  Gas   1.779e-003  4.182e-004
*    ch2o  Gas   1.744e-003  4.100e-004
*     ch3  Gas   5.039e-005  1.184e-005
*      no  Gas   1.363e-007  3.204e-008
*      o2  Gas   2.506e-011  5.890e-012
*     no2  Gas   2.029e-015  4.771e-016
*      *c  solid 7.584e+000  1.783e+000
     Total Gas   3.724e+001  8.754e+000
     Total Cond. 7.584e+000  1.783e+000
```

```
                          Reference state = reactants
              H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00
      P           V           T           H(R)        E(R)          S(R)
    (ATM)      (CC/GM)       (K)        (CAL/GM)    (CAL/GM)    (CAL/K/GM)
     VGS         CV          CP         ALPHA        BETA         KAPPA
   (CC/GM)   (CAL/K/GM)   (CAL/K/GM)
9.48962e+001 2.46452e+001 7.14108e+002 -1.07525e+003 -1.13187e+003 1.77249e+000
2.46098e+001 2.86941e-001 3.60563e-001  3.87842e+000  3.63188e+000 1.34322e+000

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*     h2o  Gas   1.248e+001  2.933e+000
*      n2  Gas   1.189e+001  2.796e+000
*      co  Gas   5.579e+000  1.312e+000
*     co2  Gas   3.457e+000  8.127e-001
*     ch4  Gas   2.307e+000  5.423e-001
*      h2  Gas   1.388e+000  3.262e-001
*     h3n  Gas   1.177e-001  2.767e-002
*    c2h4  Gas   1.024e-002  2.406e-003
*   ch2o2  Gas   5.390e-003  1.267e-003
*    c2h6  Gas   2.132e-003  5.012e-004
*   ch3oh  Gas   1.779e-003  4.182e-004
*    ch2o  Gas   1.744e-003  4.100e-004
*     ch3  Gas   5.039e-005  1.184e-005
*      no  Gas   1.363e-007  3.204e-008
*      o2  Gas   2.506e-011  5.890e-012
*     no2  Gas   2.029e-015  4.771e-016
*      *c  solid 7.584e+000  1.783e+000
     Total Gas   3.724e+001  8.754e+000
     Total Cond. 7.584e+000  1.783e+000

                          Reference state = reactants
              H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00
      P           V           T           H(R)        E(R)          S(R)
    (ATM)      (CC/GM)       (K)        (CAL/GM)    (CAL/GM)    (CAL/K/GM)
     VGS         CV          CP         ALPHA        BETA         KAPPA
   (CC/GM)   (CAL/K/GM)   (CAL/K/GM)
3.77612e+001 4.92904e+001 5.88098e+002 -1.12186e+003 -1.16693e+003 1.77249e+000
4.92550e+001 2.67791e-001 3.41600e-001  3.62045e+000  3.49962e+000 1.32027e+000

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*     h2o  Gas   1.248e+001  2.933e+000
*      n2  Gas   1.189e+001  2.796e+000
*      co  Gas   5.579e+000  1.312e+000
*     co2  Gas   3.457e+000  8.127e-001
*     ch4  Gas   2.307e+000  5.423e-001
*      h2  Gas   1.388e+000  3.262e-001
*     h3n  Gas   1.177e-001  2.767e-002
*    c2h4  Gas   1.024e-002  2.406e-003
*   ch2o2  Gas   5.390e-003  1.267e-003
*    c2h6  Gas   2.132e-003  5.012e-004
*   ch3oh  Gas   1.779e-003  4.182e-004
*    ch2o  Gas   1.744e-003  4.100e-004
*     ch3  Gas   5.039e-005  1.184e-005
*      no  Gas   1.363e-007  3.204e-008
*      o2  Gas   2.506e-011  5.890e-012
*     no2  Gas   2.029e-015  4.771e-016
*      *c  solid 7.584e+000  1.783e+000
     Total Gas   3.724e+001  8.754e+000
     Total Cond. 7.584e+000  1.783e+000
```

```
                          Reference state = reactants
                H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00
      P           V           T           H(R)         E(R)          S(R)
    (ATM)      (CC/GM)       (K)        (CAL/GM)     (CAL/GM)    (CAL/K/GM)
     VGS         CV          CP          ALPHA         BETA         KAPPA
   (CC/GM)   (CAL/K/GM)   (CAL/K/GM)
1.51506e+001 9.85807e+001 4.80183e+002 -1.15881e+003 -1.19497e+003 1.77249e+000
9.85454e+001 2.51447e-001 3.25361e-001  3.39880e+000  3.34038e+000 1.31686e+000

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*     h2o  Gas   1.248e+001  2.933e+000
*      n2  Gas   1.189e+001  2.796e+000
*      co  Gas   5.579e+000  1.312e+000
*     co2  Gas   3.457e+000  8.127e-001
*     ch4  Gas   2.307e+000  5.423e-001
*      h2  Gas   1.388e+000  3.262e-001
*     h3n  Gas   1.177e-001  2.767e-002
*    c2h4  Gas   1.024e-002  2.406e-003
*   ch2o2  Gas   5.390e-003  1.267e-003
*    c2h6  Gas   2.132e-003  5.012e-004
*   ch3oh  Gas   1.779e-003  4.182e-004
*    ch2o  Gas   1.744e-003  4.100e-004
*     ch3  Gas   5.039e-005  1.184e-005
*      no  Gas   1.363e-007  3.204e-008
*      o2  Gas   2.506e-011  5.890e-012
*     no2  Gas   2.029e-015  4.771e-016
*      *c  solid 7.584e+000  1.783e+000
     Total Gas   3.724e+001  8.754e+000
     Total Cond. 7.584e+000  1.783e+000

                            The End of the Adiabat
                          Reference state = reactants
                H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00
      P           V           T           H(R)         E(R)          S(R)
    (ATM)      (CC/GM)       (K)        (CAL/GM)     (CAL/GM)    (CAL/K/GM)
     VGS         CV          CP          ALPHA         BETA         KAPPA
   (CC/GM)   (CAL/K/GM)   (CAL/K/GM)
2.02997e+000 4.50359e+002 2.98000e+002 -1.21636e+003 -1.23848e+003 1.77249e+000
4.50324e+002 2.24161e-001 2.98151e-001 3.02919e+000 3.01739e+000 1.33532e+000

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*     h2o  Gas   1.248e+001  2.933e+000
*      n2  Gas   1.189e+001  2.796e+000
*      co  Gas   5.579e+000  1.312e+000
*     co2  Gas   3.457e+000  8.127e-001
*     ch4  Gas   2.307e+000  5.423e-001
*      h2  Gas   1.388e+000  3.262e-001
*     h3n  Gas   1.177e-001  2.767e-002
*    c2h4  Gas   1.024e-002  2.406e-003
*   ch2o2  Gas   5.390e-003  1.267e-003
*    c2h6  Gas   2.132e-003  5.012e-004
*   ch3oh  Gas   1.779e-003  4.182e-004
*    ch2o  Gas   1.744e-003  4.100e-004
*     ch3  Gas   5.039e-005  1.184e-005
*      no  Gas   1.363e-007  3.204e-008
*      o2  Gas   2.506e-011  5.890e-012
*     no2  Gas   2.029e-015  4.771e-016
*      *c  solid 7.584e+000  1.783e+000
     Total Gas   3.724e+001  8.754e+000
     Total Cond. 7.584e+000  1.783e+000
```

The Products at room temperature and pressure
Reference state = reactants
H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00

P (ATM)	V (CC/GM)	T (K)	H(R) (CAL/GM)	E(R) (CAL/GM)	S(R) (CAL/K/GM)
VGS (CC/GM)	CV (CAL/K/GM)	CP (CAL/K/GM)	ALPHA	BETA	KAPPA
1.00000e+000	9.12391e+002	2.98000e+002	-1.21640e+003	-1.23848e+003	1.82489e+000
9.12356e+002	2.24153e-001	2.98151e-001	3.02901e+000	3.02317e+000	1.33271e+000

Product concentrations

	Name		(mol/kg)	(mol gas/mol explosive)
*	h2o	Gas	1.248e+001	2.933e+000
*	n2	Gas	1.189e+001	2.796e+000
*	co	Gas	5.579e+000	1.312e+000
*	co2	Gas	3.457e+000	8.127e-001
*	ch4	Gas	2.307e+000	5.423e-001
*	h2	Gas	1.388e+000	3.262e-001
*	h3n	Gas	1.177e-001	2.767e-002
*	c2h4	Gas	1.024e-002	2.406e-003
*	ch2o2	Gas	5.390e-003	1.267e-003
*	c2h6	Gas	2.132e-003	5.012e-004
*	ch3oh	Gas	1.779e-003	4.182e-004
*	ch2o	Gas	1.744e-003	4.100e-004
*	ch3	Gas	5.039e-005	1.184e-005
*	no	Gas	1.363e-007	3.204e-008
*	o2	Gas	2.506e-011	5.890e-012
*	no2	Gas	2.029e-015	4.771e-016
*	*c	solid	7.584e+000	1.783e+000
	Total	Gas	3.724e+001	8.754e+000
	Total	Cond.	7.584e+000	1.783e+000

The mechanical energy of detonation = -8.410 kJ/cc
The thermal energy of detonation = -0.000 kJ/cc
The total energy of detonation = -8.410 kJ/cc

JWL Tail Fit results:
Initial E0 = -8.859, Final E0 = -8.836 E0(V=infty) = -8.836
C = 1.338, omega = 0.336 Final fitting error = 0.000420

V/V0	Actual E (kJ/cc)	Fit E (kJ/cc)	Actual P (GPa)	Fit P (GPa)
20.000	-7.383	-7.384	0.025	0.024
40.000	-7.686	-7.686	0.010	0.010
80.000	-7.924	-7.925	0.004	0.004
160.000	-8.115	-8.114	0.002	0.002

JWL Fit results:
E0(V=infty) = -8.836
R[1] = 4.845, R[2] = 1.055, omega = 0.336
A = 694.062, B = 8.443, C = 1.338
Final fitting error = 0.009257

V/V0	Actual E (kJ/cc)	Fit E (kJ/cc)	Actual P (GPa)	Fit P (GPa)
0.754	2.853	2.853	23.220	23.717
1.000	-0.876	-0.946	9.736	9.736
2.200	-5.005	-4.996	1.205	1.311
4.100	-6.151	-6.255	0.315	0.315
6.500	-6.644	-6.708	0.137	0.119
10.000	-6.980	-7.002	0.069	0.062
20.000	-7.383	-7.384	0.025	0.024
40.000	-7.686	-7.686	0.010	0.010
80.000	-7.924	-7.925	0.004	0.004

```
   160.000     -8.115     -8.114      0.002      0.002
```

B.2 BKWS Database

B.2.1 Summary output

```
Product library title: bkws library
Reactant library title: # Version 2.0 by P. Clark Souers

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
dos        11.50   6.34  20.47  -319073   426.66     0.91 C26H50O4
rdx        88.50  93.66  79.53    16496   222.13     1.81 C3H6N6O6
Product library title: bkws library
Reactant library title: # Version 2.0 by P. Clark Souers

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
dos        11.50   6.34  20.47  -319073   426.66     0.91 C26H50O4
rdx        88.50  93.66  79.53    16496   222.13     1.81 C3H6N6O6

Density  =  1.6230 g/cc   Mixture TMD =  1.6230 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          25.57 GPa
The volume            =          0.469 cc/g
The density           =          2.130 g/cc
The energy            =           3.04 kJ/cc explosive
The temperature       =           3622 K
The shock velocity    =          8.134 mm/us
The particle velocity =          1.937 mm/us
The speed of sound    =          6.197 mm/us
Gamma                 =          3.199

Cylinder runs:             % of standards
  V/V0     Energy    TATB     PETN      HMX    CL-20   TRITON
 (rel.)   (kJ/cc)  1.83g/cc 1.76g/cc 1.89g/cc 2.04g/cc 1.70g/cc
   1.00    -0.96
   2.20    -5.41     112       85       72       60      124
   4.10    -6.55     113       85       74       62      119
   6.50    -7.04     113       85       75       63      115
  10.00    -7.36     113       85       75       64      112
  20.00    -7.74     113       85       76       65      108
  40.00    -8.02     112       84       77       66      104
  80.00    -8.24     112       84       77       67      100
 160.00    -8.42

Freezing occurred at T =     1800.0 K and relative V =   2.003
The mechanical energy of detonation =     -8.672 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -8.672 kJ/cc
JWL Fit results:
E0   =    -9.076 kJ/cc
A    =   820.01 GPa, B    =    8.72 GPa ,  C     =  1.27 GPa
R[1] =     4.83,     R[2] =    1.05,      omega  =  0.34
RMS fitting error =   1.12 %
```

B.2.2 Fulltext output

```
Product library title: bkws library
Executing library command: gas eos, bkw
Executing library command: set, bkw, alpha, 0.5
Executing library command: set, bkw, beta, 0.298
Executing library command: set, bkw, theta, 6620.
Executing library command: set, bkw, kappa, 10.5
                                The Composition
Name     % wt. % mol % vol. Heat of  Standard   Standard   Mol.  Formula
                           formation  volume     entropy   wt.
                           (cal/mol) (cc/mol)  (cal/K/mol)
dos     11.50  6.34  20.47  -319073   467.83     0.000   426.66  C26H50O4
rdx     88.50 93.66  79.53    16496   122.99     0.000   222.13  C3H6N6O6

Heat of formation =    -20.277 cal/gm
Standard volume   =      0.616 cc/gm
Standard entropy  =      0.000 cal/k/gm
Standard energy   =    -20.292 cal/gm

The elements and percent by mole
     c             18.018
     h             35.524
     o             23.741
     n             22.717
The average mol. wt. = 235.086 g/mol
Input>library file, bkws.chl
Product library title: bkws library
Executing library command: gas eos, bkw
Executing library command: set, bkw, alpha, 0.5
Executing library command: set, bkw, beta, 0.298
Executing library command: set, bkw, theta, 6620.
Executing library command: set, bkw, kappa, 10.5
Input>composition, dos, 11.5, rdx, 88.5, weight
                                The Composition
Name      % wt.   % mol % vol.   Heat of  Standard     Standard     Mol.
Name     % wt. % mol % vol. Heat of  Standard   Standard   Mol.  Formula
                           formation  volume     entropy   wt.
                           (cal/mol) (cc/mol)  (cal/K/mol)
dos     11.50  6.34  20.47  -319073   467.83     0.000   426.66  C26H50O4
rdx     88.50 93.66  79.53    16496   122.99     0.000   222.13  C3H6N6O6

Heat of formation =    -20.277 cal/gm
Standard volume   =      0.616 cc/gm
Standard entropy  =      0.000 cal/k/gm
Standard energy   =    -20.292 cal/gm

The elements and percent by mole
     c             18.018
     h             35.524
     o             23.741
     n             22.717
The average mol. wt. = 235.086 g/mol
Input>gas eos, bkw
Input>standard run, rho, 1.623035
The initial equation error was huge: 117066.170780
Too many iterations in the etanewt solver
Failed to find equilibrium.  Will try again.
The Newton line search was not successful.
Undertaking a gradient line search instead
Too many iterations in the etanewt solver
Failed to find equilibrium.  Will try again.
The initial equation error was huge: 11183.280851
```

```
The hugoniot reference state:
P0 = 1.000000 ATM, V0 = 0.616130 cc/gm, E0 = -20.291838 cal/gm
Using  114832 ATM as a lower bound for the C-J pressure
Using  287080 ATM as an upper bound for the C-J pressure
The C-J point was bracketed in cjbrent
The CJ state was found in 6 iterations
                              The C-J condition
The shock velocity    =   8.13432e+003 m/s
The particle velocity =   1.93699e+003 m/s
The speed of sound    =   6.19733e+003 m/s

P0 =       1 atm, V0 =  0.61613 cc/gm, E0 = -20.29184 cal/gm

                         Reference state = reactants
               H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00
      P           V           T           H(R)        E(R)          S(R)
    (ATM)      (CC/GM)       (K)        (CAL/GM)    (CAL/GM)    (CAL/K/GM)
     VGS         CV          CP          ALPHA        BETA         KAPPA
   (CC/GM)   (CAL/K/GM)   (CAL/K/GM)
2.52384e+005 4.69413e-001 3.62233e+003 3.31754e+003 4.48385e+002 1.72467e+000
4.49476e-001 6.45230e-001 7.58149e-001 3.18316e+000 1.30746e+000 3.19945e+000

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
       n2  Gas   1.102e+001  2.592e+000
      co2  Gas   7.597e+000  1.786e+000
      h2o  Gas   6.369e+000  1.497e+000
      h3n  Gas   1.817e+000  4.271e-001
    ch2o2  Gas   1.563e+000  3.673e-001
      ch4  Gas   1.515e+000  3.563e-001
     c2h6  Gas   1.388e+000  3.263e-001
       h2  Gas   3.532e-001  8.303e-002
    ch3oh  Gas   2.011e-001  4.728e-002
       co  Gas   7.556e-002  1.776e-002
     c2h4  Gas   1.539e-002  3.619e-003
     h4n2  Gas   1.352e-002  3.177e-003
      ch3  Gas   8.941e-003  2.102e-003
       no  Gas   7.070e-003  1.662e-003
     ch2o  Gas   4.077e-003  9.585e-004
      h2n  Gas   2.723e-003  6.401e-004
     h2o2  Gas   2.074e-003  4.875e-004
       ho  Gas   1.178e-003  2.769e-004
     chno  Gas   1.095e-003  2.575e-004
     h2n2  Gas   8.466e-004  1.990e-004
        h  Gas   7.496e-004  1.762e-004
       o2  Gas   7.290e-004  1.714e-004
      cno  Gas   3.921e-004  9.219e-005
     c3h8  Gas   2.003e-004  4.708e-005
        o  Gas   7.508e-005  1.765e-005
      chn  Gas   4.254e-005  1.000e-005
      cho  Gas   4.090e-005  9.616e-006
      ch2  Gas   3.418e-005  8.035e-006
      no2  Gas   2.031e-005  4.775e-006
      hno  Gas   1.525e-005  3.585e-006
      ho2  Gas   1.118e-005  2.629e-006
     c2h2  Gas   9.256e-006  2.176e-006
      n2o  Gas   6.319e-006  1.485e-006
        n  Gas   4.706e-006  1.106e-006
       hn  Gas   3.809e-006  8.955e-007
     c3h6  Gas   2.415e-006  5.677e-007
       cn  Gas   1.517e-006  3.566e-007
       n3  Gas   2.764e-007  6.498e-008
     hno2  Gas   2.484e-007  5.840e-008
```

cn2	Gas	1.665e-007	3.913e-008
no3	Gas	3.604e-008	8.472e-009
c2h	Gas	2.005e-008	4.715e-009
ch	Gas	1.864e-008	4.382e-009
no2h	Gas	8.098e-009	1.904e-009
hno3	Gas	6.237e-009	1.466e-009
c	Gas	2.346e-009	5.514e-010
c2n2	Gas	1.056e-009	2.481e-010
c2h4o	Gas	9.523e-010	2.239e-010
o3	Gas	1.915e-010	4.502e-011
c2n	Gas	1.861e-010	4.374e-011
c2o	Gas	6.178e-011	1.452e-011
c2	Gas	5.206e-011	1.224e-011
n2o4	Gas	2.542e-011	5.976e-012
cnn	Gas	3.709e-012	8.720e-013
n2o3	Gas	1.097e-012	2.578e-013
c3o2	Gas	5.098e-013	1.199e-013
c3	Gas	2.137e-014	5.023e-015
n2o5	Gas	1.498e-016	3.522e-017
c4	Gas	1.230e-023	2.891e-024
c4n2	Gas	1.440e-030	3.385e-031
c5	Gas	8.633e-034	2.029e-034
*c	solid	5.187e+000	1.219e+000
*h2o	liquid	0.000e+000	0.000e+000
Total	Gas	3.196e+001	7.514e+000
Total	Cond.	5.187e+000	1.219e+000

The C-J Adiabat
Reference state = reactants
H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00

P (ATM)	V (CC/GM)	T (K)	H(R) (CAL/GM)	E(R) (CAL/GM)	S(R) (CAL/K/GM)
VGS (CC/GM)	CV (CAL/K/GM)	CP (CAL/K/GM)	ALPHA	BETA	KAPPA
1.07556e+005	6.16130e-001	2.93869e+003	1.46304e+003	-1.41838e+002	1.72467e+000
5.81616e-001	5.79044e-001	7.31598e-001	2.95070e+000	1.28705e+000	3.06959e+000

Product concentrations

Name		(mol/kg)	(mol gas/mol explosive)
n2	Gas	1.129e+001	2.654e+000
h2o	Gas	9.156e+000	2.153e+000
co2	Gas	7.147e+000	1.680e+000
ch4	Gas	2.193e+000	5.156e-001
h3n	Gas	1.322e+000	3.108e-001
h2	Gas	1.275e+000	2.998e-001
co	Gas	5.608e-001	1.318e-001
ch2o2	Gas	4.421e-001	1.039e-001
c2h6	Gas	4.096e-001	9.629e-002
ch3oh	Gas	7.477e-002	1.758e-002
c2h4	Gas	2.021e-002	4.750e-003
ch2o	Gas	9.825e-003	2.310e-003
ch3	Gas	8.685e-003	2.042e-003
chno	Gas	2.730e-003	6.418e-004
h2n	Gas	1.036e-003	2.435e-004
h	Gas	8.514e-004	2.001e-004
no	Gas	6.650e-004	1.563e-004
ho	Gas	6.153e-004	1.447e-004
chn	Gas	6.009e-004	1.413e-004
h4n2	Gas	4.878e-004	1.147e-004
c3h8	Gas	2.748e-004	6.461e-005
cho	Gas	1.423e-004	3.346e-005
c2h2	Gas	6.921e-005	1.627e-005
h2o2	Gas	5.756e-005	1.353e-005

```
     h2n2  Gas   5.540e-005  1.302e-005
      cno  Gas   3.640e-005  8.556e-006
     c3h6  Gas   2.278e-005  5.354e-006
       o2  Gas   1.238e-005  2.911e-006
      ch2  Gas   1.044e-005  2.454e-006
        o  Gas   3.479e-006  8.179e-007
      hno  Gas   3.189e-006  7.497e-007
       hn  Gas   1.112e-006  2.615e-007
       cn  Gas   9.160e-007  2.153e-007
      n2o  Gas   8.463e-007  1.989e-007
      ho2  Gas   4.340e-007  1.020e-007
        n  Gas   3.084e-007  7.250e-008
      no2  Gas   1.784e-007  4.194e-008
      c2h  Gas   5.240e-008  1.232e-008
     hno2  Gas   2.921e-008  6.866e-009
      cn2  Gas   2.559e-008  6.016e-009
     c2n2  Gas   2.034e-008  4.781e-009
       n3  Gas   1.492e-008  3.508e-009
    c2h4o  Gas   8.667e-009  2.038e-009
       ch  Gas   4.061e-009  9.547e-010
     no2h  Gas   3.152e-009  7.410e-010
      c2o  Gas   7.703e-010  1.811e-010
      c2n  Gas   5.441e-010  1.279e-010
     c3o2  Gas   2.057e-010  4.836e-011
        c  Gas   1.656e-010  3.893e-011
     hno3  Gas   2.219e-011  5.216e-012
       c2  Gas   4.039e-012  9.495e-013
      no3  Gas   3.753e-012  8.823e-013
      cnn  Gas   2.871e-012  6.750e-013
       o3  Gas   2.154e-013  5.063e-014
       c3  Gas   4.623e-014  1.087e-014
     n2o3  Gas   2.411e-015  5.668e-016
     n2o4  Gas   1.132e-016  2.661e-017
       c4  Gas   1.099e-021  2.583e-022
     n2o5  Gas   3.978e-022  9.351e-023
     c4n2  Gas   1.062e-023  2.497e-024
       c5  Gas   1.672e-028  3.930e-029
       *c  solid 7.660e+000  1.801e+000
    *h2o liquid 0.000e+000  0.000e+000
     Total Gas   3.392e+001  7.973e+000
     Total Cond. 7.660e+000  1.801e+000

                        Reference state = reactants
              H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00
      P           V           T           H(R)        E(R)          S(R)
    (ATM)      (CC/GM)       (K)        (CAL/GM)    (CAL/GM)    (CAL/K/GM)
     VGS         CV          CP         ALPHA        BETA         KAPPA
   (CC/GM)   (CAL/K/GM)   (CAL/K/GM)
1.52136e+004 1.23401e+000 1.80000e+003 -3.01981e+002 -7.56631e+002 1.72467e+000
1.19987e+000 5.92210e-001 8.44525e-001  3.46044e+000  1.75933e+000 2.53531e+000

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
       n2  Gas   1.175e+001  2.762e+000
      h2o  Gas   9.444e+000  2.220e+000
      co2  Gas   6.367e+000  1.497e+000
      ch4  Gas   2.855e+000  6.711e-001
       h2  Gas   2.778e+000  6.531e-001
       co  Gas   2.760e+000  6.488e-001
      h3n  Gas   4.022e-001  9.455e-002
     c2h6  Gas   3.873e-002  9.105e-003
    ch2o2  Gas   1.826e-002  4.292e-003
     c2h4  Gas   4.365e-003  1.026e-003
```

```
      ch2o  Gas   3.884e-003  9.130e-004
     ch3oh  Gas   3.422e-003  8.044e-004
       chn  Gas   1.902e-003  4.471e-004
      chno  Gas   1.193e-003  2.805e-004
       ch3  Gas   3.280e-004  7.710e-005
      c3h8  Gas   9.996e-005  2.350e-005
      c3h6  Gas   4.062e-005  9.549e-006
      c2h2  Gas   2.338e-005  5.496e-006
         h  Gas   2.126e-005  4.999e-006
       cho  Gas   1.192e-005  2.802e-006
       h2n  Gas   5.485e-006  1.290e-006
        ho  Gas   3.160e-006  7.428e-007
        no  Gas   2.564e-007  6.028e-008
      h4n2  Gas   1.268e-007  2.981e-008
      h2n2  Gas   1.724e-008  4.054e-009
      c2n2  Gas   1.143e-008  2.687e-009
       cno  Gas   6.664e-009  1.567e-009
      c3o2  Gas   5.569e-009  1.309e-009
       ch2  Gas   3.344e-009  7.862e-010
     c2h4o  Gas   2.713e-009  6.377e-010
      h2o2  Gas   1.799e-009  4.228e-010
       hno  Gas   1.555e-009  3.656e-010
        cn  Gas   8.671e-010  2.038e-010
       n2o  Gas   4.204e-010  9.884e-011
        hn  Gas   3.497e-010  8.221e-011
       c2h  Gas   1.622e-010  3.812e-011
        o2  Gas   7.904e-011  1.858e-011
         o  Gas   4.882e-011  1.148e-011
       c2o  Gas   1.569e-011  3.688e-012
         n  Gas   5.455e-012  1.282e-012
       ho2  Gas   4.161e-012  9.781e-013
      hno2  Gas   2.838e-012  6.671e-013
       cn2  Gas   1.586e-012  3.727e-013
      no2h  Gas   1.396e-012  3.283e-013
       c2n  Gas   6.686e-013  1.572e-013
        n3  Gas   3.205e-013  7.533e-014
       no2  Gas   2.283e-013  5.366e-014
        ch  Gas   5.193e-014  1.221e-014
       cnn  Gas   2.288e-016  5.378e-017
         c  Gas   1.266e-016  2.977e-017
      c4n2  Gas   2.864e-018  6.733e-019
      hno3  Gas   1.670e-018  3.926e-019
        c3  Gas   1.543e-018  3.627e-019
        c2  Gas   8.004e-019  1.882e-019
       no3  Gas   2.273e-022  5.344e-023
        o3  Gas   1.082e-022  2.544e-023
      n2o3  Gas   4.069e-024  9.565e-025
        c4  Gas   3.808e-025  8.951e-026
        c5  Gas   1.051e-027  2.472e-028
      n2o4  Gas   6.082e-030  1.430e-030
      n2o5  Gas   2.375e-037  5.584e-038
        *c  solid 6.863e+000  1.613e+000
     *h2o liquid 0.000e+000  0.000e+000
     Total Gas   3.643e+001  8.564e+000
     Total Cond. 6.863e+000  1.613e+000
Freezing at v = 1.234011, t = 1800.000000
                          Reference state = reactants
               H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00
      P           V           T           H(R)        E(R)          S(R)
    (ATM)      (CC/GM)       (K)        (CAL/GM)    (CAL/GM)    (CAL/K/GM)
     VGS         CV          CP          ALPHA        BETA         KAPPA
   (CC/GM)   (CAL/K/GM)   (CAL/K/GM)
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1.20188e+004 1.35549e+000 1.71397e+003 -4.01872e+002 -7.96401e+002 1.72467e+000
1.32124e+000 4.09873e-001 5.03125e-001  3.86470e+000  1.97480e+000 2.46339e+000

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.175e+001  2.762e+000
*      h2o  Gas   9.444e+000  2.220e+000
*      co2  Gas   6.367e+000  1.497e+000
*      ch4  Gas   2.855e+000  6.711e-001
*       h2  Gas   2.778e+000  6.531e-001
*       co  Gas   2.760e+000  6.488e-001
*      h3n  Gas   4.022e-001  9.455e-002
*     c2h6  Gas   3.873e-002  9.105e-003
*    ch2o2  Gas   1.826e-002  4.292e-003
*     c2h4  Gas   4.365e-003  1.026e-003
*     ch2o  Gas   3.884e-003  9.130e-004
*    ch3oh  Gas   3.422e-003  8.044e-004
*      chn  Gas   1.902e-003  4.471e-004
*     chno  Gas   1.193e-003  2.805e-004
*      ch3  Gas   3.280e-004  7.710e-005
*     c3h8  Gas   9.996e-005  2.350e-005
*     c3h6  Gas   4.062e-005  9.549e-006
*     c2h2  Gas   2.338e-005  5.496e-006
*        h  Gas   2.126e-005  4.999e-006
*      cho  Gas   1.192e-005  2.802e-006
*      h2n  Gas   5.485e-006  1.290e-006
*       ho  Gas   3.160e-006  7.428e-007
*       no  Gas   2.564e-007  6.028e-008
*     h4n2  Gas   1.268e-007  2.981e-008
*     h2n2  Gas   1.724e-008  4.054e-009
*     c2n2  Gas   1.143e-008  2.687e-009
*      cno  Gas   6.664e-009  1.567e-009
*     c3o2  Gas   5.569e-009  1.309e-009
*      ch2  Gas   3.344e-009  7.862e-010
*    c2h4o  Gas   2.713e-009  6.377e-010
*     h2o2  Gas   1.799e-009  4.228e-010
*      hno  Gas   1.555e-009  3.656e-010
*       cn  Gas   8.671e-010  2.038e-010
*      n2o  Gas   4.204e-010  9.884e-011
*       hn  Gas   3.497e-010  8.221e-011
*      c2h  Gas   1.622e-010  3.812e-011
*       o2  Gas   7.904e-011  1.858e-011
*        o  Gas   4.882e-011  1.148e-011
*      c2o  Gas   1.569e-011  3.688e-012
*        n  Gas   5.455e-012  1.282e-012
*      ho2  Gas   4.161e-012  9.781e-013
*     hno2  Gas   2.838e-012  6.671e-013
*      cn2  Gas   1.586e-012  3.727e-013
*     no2h  Gas   1.396e-012  3.283e-013
*      c2n  Gas   6.686e-013  1.572e-013
*       n3  Gas   3.205e-013  7.533e-014
*      no2  Gas   2.283e-013  5.366e-014
*       ch  Gas   5.193e-014  1.221e-014
*      cnn  Gas   2.288e-016  5.378e-017
*        c  Gas   1.266e-016  2.977e-017
*     c4n2  Gas   2.864e-018  6.733e-019
*     hno3  Gas   1.670e-018  3.926e-019
*       c3  Gas   1.543e-018  3.627e-019
*       c2  Gas   8.004e-019  1.882e-019
*      no3  Gas   2.273e-022  5.344e-023
*       o3  Gas   1.082e-022  2.544e-023
*     n2o3  Gas   4.069e-024  9.565e-025
*       c4  Gas   3.808e-025  8.951e-026
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*      c5  Gas   1.051e-027  2.472e-028
*    n2o4  Gas   6.082e-030  1.430e-030
*    n2o5  Gas   2.375e-037  5.584e-038
*      *c  solid 6.863e+000  1.613e+000
*    *h2o liquid 0.000e+000  0.000e+000
     Total Gas   3.643e+001  8.564e+000
     Total Cond. 6.863e+000  1.613e+000

                          Reference state = reactants
               H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00
      P           V           T           H(R)        E(R)          S(R)
    (ATM)       (CC/GM)       (K)        (CAL/GM)    (CAL/GM)    (CAL/K/GM)
     VGS         CV          CP          ALPHA        BETA         KAPPA
   (CC/GM)   (CAL/K/GM)   (CAL/K/GM)
3.06197e+003 2.52613e+000 1.31239e+003 -7.77907e+002 -9.65218e+002 1.72467e+000
2.49163e+000 3.68425e-001 4.48251e-001  4.33995e+000  2.71433e+000 1.96732e+000

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.175e+001  2.762e+000
*      h2o  Gas   9.444e+000  2.220e+000
*      co2  Gas   6.367e+000  1.497e+000
*      ch4  Gas   2.855e+000  6.711e-001
*       h2  Gas   2.778e+000  6.531e-001
*       co  Gas   2.760e+000  6.488e-001
*      h3n  Gas   4.022e-001  9.455e-002
*     c2h6  Gas   3.873e-002  9.105e-003
*    ch2o2  Gas   1.826e-002  4.292e-003
*     c2h4  Gas   4.365e-003  1.026e-003
*     ch2o  Gas   3.884e-003  9.130e-004
*    ch3oh  Gas   3.422e-003  8.044e-004
*      chn  Gas   1.902e-003  4.471e-004
*     chno  Gas   1.193e-003  2.805e-004
*      ch3  Gas   3.280e-004  7.710e-005
*     c3h8  Gas   9.996e-005  2.350e-005
*     c3h6  Gas   4.062e-005  9.549e-006
*     c2h2  Gas   2.338e-005  5.496e-006
*        h  Gas   2.126e-005  4.999e-006
*      cho  Gas   1.192e-005  2.802e-006
*      h2n  Gas   5.485e-006  1.290e-006
*       ho  Gas   3.160e-006  7.428e-007
*       no  Gas   2.564e-007  6.028e-008
*     h4n2  Gas   1.268e-007  2.981e-008
*     h2n2  Gas   1.724e-008  4.054e-009
*     c2n2  Gas   1.143e-008  2.687e-009
*      cno  Gas   6.664e-009  1.567e-009
*     c3o2  Gas   5.569e-009  1.309e-009
*      ch2  Gas   3.344e-009  7.862e-010
*    c2h4o  Gas   2.713e-009  6.377e-010
*     h2o2  Gas   1.799e-009  4.228e-010
*      hno  Gas   1.555e-009  3.656e-010
*       cn  Gas   8.671e-010  2.038e-010
*      n2o  Gas   4.204e-010  9.884e-011
*       hn  Gas   3.497e-010  8.221e-011
*      c2h  Gas   1.622e-010  3.812e-011
*       o2  Gas   7.904e-011  1.858e-011
*        o  Gas   4.882e-011  1.148e-011
*      c2o  Gas   1.569e-011  3.688e-012
*        n  Gas   5.455e-012  1.282e-012
*      ho2  Gas   4.161e-012  9.781e-013
*     hno2  Gas   2.838e-012  6.671e-013
*      cn2  Gas   1.586e-012  3.727e-013
*     no2h  Gas   1.396e-012  3.283e-013
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*      c2n  Gas   6.686e-013  1.572e-013
*       n3  Gas   3.205e-013  7.533e-014
*      no2  Gas   2.283e-013  5.366e-014
*       ch  Gas   5.193e-014  1.221e-014
*      cnn  Gas   2.288e-016  5.378e-017
*        c  Gas   1.266e-016  2.977e-017
*     c4n2  Gas   2.864e-018  6.733e-019
*     hno3  Gas   1.670e-018  3.926e-019
*       c3  Gas   1.543e-018  3.627e-019
*       c2  Gas   8.004e-019  1.882e-019
*      no3  Gas   2.273e-022  5.344e-023
*       o3  Gas   1.082e-022  2.544e-023
*     n2o3  Gas   4.069e-024  9.565e-025
*       c4  Gas   3.808e-025  8.951e-026
*       c5  Gas   1.051e-027  2.472e-028
*     n2o4  Gas   6.082e-030  1.430e-030
*     n2o5  Gas   2.375e-037  5.584e-038
*       *c  solid 6.863e+000  1.613e+000
*     *h2o liquid 0.000e+000  0.000e+000
      Total Gas   3.643e+001  8.564e+000
      Total Cond. 6.863e+000  1.613e+000

                          Reference state = reactants
                H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00
      P           V           T           H(R)        E(R)          S(R)
    (ATM)      (CC/GM)       (K)        (CAL/GM)    (CAL/GM)    (CAL/K/GM)
     VGS         CV          CP          ALPHA        BETA         KAPPA
   (CC/GM)   (CAL/K/GM)   (CAL/K/GM)
1.31177e+003 4.00484e+000 1.12199e+003 -9.08933e+002 -1.03615e+003 1.72467e+000
3.97032e+000 3.47234e-001 4.22513e-001  4.44768e+000  3.15488e+000 1.72675e+000

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.175e+001  2.762e+000
*      h2o  Gas   9.444e+000  2.220e+000
*      co2  Gas   6.367e+000  1.497e+000
*      ch4  Gas   2.855e+000  6.711e-001
*       h2  Gas   2.778e+000  6.531e-001
*       co  Gas   2.760e+000  6.488e-001
*      h3n  Gas   4.022e-001  9.455e-002
*     c2h6  Gas   3.873e-002  9.105e-003
*    ch2o2  Gas   1.826e-002  4.292e-003
*     c2h4  Gas   4.365e-003  1.026e-003
*     ch2o  Gas   3.884e-003  9.130e-004
*    ch3oh  Gas   3.422e-003  8.044e-004
*      chn  Gas   1.902e-003  4.471e-004
*     chno  Gas   1.193e-003  2.805e-004
*      ch3  Gas   3.280e-004  7.710e-005
*     c3h8  Gas   9.996e-005  2.350e-005
*     c3h6  Gas   4.062e-005  9.549e-006
*     c2h2  Gas   2.338e-005  5.496e-006
*        h  Gas   2.126e-005  4.999e-006
*      cho  Gas   1.192e-005  2.802e-006
*      h2n  Gas   5.485e-006  1.290e-006
*       ho  Gas   3.160e-006  7.428e-007
*       no  Gas   2.564e-007  6.028e-008
*     h4n2  Gas   1.268e-007  2.981e-008
*     h2n2  Gas   1.724e-008  4.054e-009
*     c2n2  Gas   1.143e-008  2.687e-009
*      cno  Gas   6.664e-009  1.567e-009
*     c3o2  Gas   5.569e-009  1.309e-009
*      ch2  Gas   3.344e-009  7.862e-010
*    c2h4o  Gas   2.713e-009  6.377e-010
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```
*     h2o2  Gas    1.799e-009  4.228e-010
*      hno  Gas    1.555e-009  3.656e-010
*       cn  Gas    8.671e-010  2.038e-010
*      n2o  Gas    4.204e-010  9.884e-011
*       hn  Gas    3.497e-010  8.221e-011
*      c2h  Gas    1.622e-010  3.812e-011
*       o2  Gas    7.904e-011  1.858e-011
*        o  Gas    4.882e-011  1.148e-011
*      c2o  Gas    1.569e-011  3.688e-012
*        n  Gas    5.455e-012  1.282e-012
*      ho2  Gas    4.161e-012  9.781e-013
*     hno2  Gas    2.838e-012  6.671e-013
*      cn2  Gas    1.586e-012  3.727e-013
*     no2h  Gas    1.396e-012  3.283e-013
*      c2n  Gas    6.686e-013  1.572e-013
*       n3  Gas    3.205e-013  7.533e-014
*      no2  Gas    2.283e-013  5.366e-014
*       ch  Gas    5.193e-014  1.221e-014
*      cnn  Gas    2.288e-016  5.378e-017
*        c  Gas    1.266e-016  2.977e-017
*     c4n2  Gas    2.864e-018  6.733e-019
*     hno3  Gas    1.670e-018  3.926e-019
*       c3  Gas    1.543e-018  3.627e-019
*       c2  Gas    8.004e-019  1.882e-019
*      no3  Gas    2.273e-022  5.344e-023
*       o3  Gas    1.082e-022  2.544e-023
*     n2o3  Gas    4.069e-024  9.565e-025
*       c4  Gas    3.808e-025  8.951e-026
*       c5  Gas    1.051e-027  2.472e-028
*     n2o4  Gas    6.082e-030  1.430e-030
*     n2o5  Gas    2.375e-037  5.584e-038
*       *c  solid  6.863e+000  1.613e+000
*     *h2o liquid  0.000e+000  0.000e+000
      Total Gas    3.643e+001  8.564e+000
      Total Cond.  6.863e+000  1.613e+000

                          Reference state = reactants
                H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00
      P           V           T           H(R)         E(R)          S(R)
    (ATM)      (CC/GM)       (K)        (CAL/GM)     (CAL/GM)    (CAL/K/GM)
     VGS         CV          CP          ALPHA         BETA         KAPPA
   (CC/GM)   (CAL/K/GM)   (CAL/K/GM)
6.45875e+002 6.16130e+000 9.84934e+002 -9.87378e+002 -1.08374e+003 1.72467e+000
6.12678e+000 3.30662e-001 4.03962e-001  4.41149e+000  3.44153e+000 1.57241e+000

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas    1.175e+001  2.762e+000
*      h2o  Gas    9.444e+000  2.220e+000
*      co2  Gas    6.367e+000  1.497e+000
*      ch4  Gas    2.855e+000  6.711e-001
*       h2  Gas    2.778e+000  6.531e-001
*       co  Gas    2.760e+000  6.488e-001
*      h3n  Gas    4.022e-001  9.455e-002
*     c2h6  Gas    3.873e-002  9.105e-003
*    ch2o2  Gas    1.826e-002  4.292e-003
*     c2h4  Gas    4.365e-003  1.026e-003
*     ch2o  Gas    3.884e-003  9.130e-004
*    ch3oh  Gas    3.422e-003  8.044e-004
*      chn  Gas    1.902e-003  4.471e-004
*     chno  Gas    1.193e-003  2.805e-004
*      ch3  Gas    3.280e-004  7.710e-005
*     c3h8  Gas    9.996e-005  2.350e-005
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```
*     c3h6  Gas   4.062e-005  9.549e-006
*     c2h2  Gas   2.338e-005  5.496e-006
*        h  Gas   2.126e-005  4.999e-006
*      cho  Gas   1.192e-005  2.802e-006
*      h2n  Gas   5.485e-006  1.290e-006
*       ho  Gas   3.160e-006  7.428e-007
*       no  Gas   2.564e-007  6.028e-008
*     h4n2  Gas   1.268e-007  2.981e-008
*     h2n2  Gas   1.724e-008  4.054e-009
*     c2n2  Gas   1.143e-008  2.687e-009
*      cno  Gas   6.664e-009  1.567e-009
*     c3o2  Gas   5.569e-009  1.309e-009
*      ch2  Gas   3.344e-009  7.862e-010
*    c2h4o  Gas   2.713e-009  6.377e-010
*     h2o2  Gas   1.799e-009  4.228e-010
*      hno  Gas   1.555e-009  3.656e-010
*       cn  Gas   8.671e-010  2.038e-010
*      n2o  Gas   4.204e-010  9.884e-011
*       hn  Gas   3.497e-010  8.221e-011
*      c2h  Gas   1.622e-010  3.812e-011
*       o2  Gas   7.904e-011  1.858e-011
*        o  Gas   4.882e-011  1.148e-011
*      c2o  Gas   1.569e-011  3.688e-012
*        n  Gas   5.455e-012  1.282e-012
*      ho2  Gas   4.161e-012  9.781e-013
*     hno2  Gas   2.838e-012  6.671e-013
*      cn2  Gas   1.586e-012  3.727e-013
*     no2h  Gas   1.396e-012  3.283e-013
*      c2n  Gas   6.686e-013  1.572e-013
*       n3  Gas   3.205e-013  7.533e-014
*      no2  Gas   2.283e-013  5.366e-014
*       ch  Gas   5.193e-014  1.221e-014
*      cnn  Gas   2.288e-016  5.378e-017
*        c  Gas   1.266e-016  2.977e-017
*     c4n2  Gas   2.864e-018  6.733e-019
*     hno3  Gas   1.670e-018  3.926e-019
*       c3  Gas   1.543e-018  3.627e-019
*       c2  Gas   8.004e-019  1.882e-019
*      no3  Gas   2.273e-022  5.344e-023
*       o3  Gas   1.082e-022  2.544e-023
*     n2o3  Gas   4.069e-024  9.565e-025
*       c4  Gas   3.808e-025  8.951e-026
*       c5  Gas   1.051e-027  2.472e-028
*     n2o4  Gas   6.082e-030  1.430e-030
*     n2o5  Gas   2.375e-037  5.584e-038
*       *c  solid 6.863e+000  1.613e+000
*     *h2o liquid 0.000e+000  0.000e+000
      Total Gas   3.643e+001  8.564e+000
      Total Cond. 6.863e+000  1.613e+000

                          Reference state = reactants
                H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00
      P           V           T           H(R)        E(R)          S(R)
    (ATM)      (CC/GM)       (K)        (CAL/GM)    (CAL/GM)    (CAL/K/GM)
     VGS         CV          CP          ALPHA        BETA         KAPPA
   (CC/GM)   (CAL/K/GM)   (CAL/K/GM)
2.30034e+002 1.23226e+001 8.11218e+002 -1.07127e+003 -1.13990e+003 1.72467e+000
1.22881e+001 3.07217e-001 3.79487e-001  4.20845e+000  3.66003e+000 1.42306e+000

Product concentrations
          Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.175e+001  2.762e+000
*      h2o  Gas   9.444e+000  2.220e+000
```

```
*      co2  Gas   6.367e+000  1.497e+000
*      ch4  Gas   2.855e+000  6.711e-001
*       h2  Gas   2.778e+000  6.531e-001
*       co  Gas   2.760e+000  6.488e-001
*      h3n  Gas   4.022e-001  9.455e-002
*     c2h6  Gas   3.873e-002  9.105e-003
*    ch2o2  Gas   1.826e-002  4.292e-003
*     c2h4  Gas   4.365e-003  1.026e-003
*     ch2o  Gas   3.884e-003  9.130e-004
*    ch3oh  Gas   3.422e-003  8.044e-004
*      chn  Gas   1.902e-003  4.471e-004
*     chno  Gas   1.193e-003  2.805e-004
*      ch3  Gas   3.280e-004  7.710e-005
*     c3h8  Gas   9.996e-005  2.350e-005
*     c3h6  Gas   4.062e-005  9.549e-006
*     c2h2  Gas   2.338e-005  5.496e-006
*        h  Gas   2.126e-005  4.999e-006
*      cho  Gas   1.192e-005  2.802e-006
*      h2n  Gas   5.485e-006  1.290e-006
*       ho  Gas   3.160e-006  7.428e-007
*       no  Gas   2.564e-007  6.028e-008
*     h4n2  Gas   1.268e-007  2.981e-008
*     h2n2  Gas   1.724e-008  4.054e-009
*     c2n2  Gas   1.143e-008  2.687e-009
*      cno  Gas   6.664e-009  1.567e-009
*     c3o2  Gas   5.569e-009  1.309e-009
*      ch2  Gas   3.344e-009  7.862e-010
*    c2h4o  Gas   2.713e-009  6.377e-010
*     h2o2  Gas   1.799e-009  4.228e-010
*      hno  Gas   1.555e-009  3.656e-010
*       cn  Gas   8.671e-010  2.038e-010
*      n2o  Gas   4.204e-010  9.884e-011
*       hn  Gas   3.497e-010  8.221e-011
*      c2h  Gas   1.622e-010  3.812e-011
*       o2  Gas   7.904e-011  1.858e-011
*        o  Gas   4.882e-011  1.148e-011
*      c2o  Gas   1.569e-011  3.688e-012
*        n  Gas   5.455e-012  1.282e-012
*      ho2  Gas   4.161e-012  9.781e-013
*     hno2  Gas   2.838e-012  6.671e-013
*      cn2  Gas   1.586e-012  3.727e-013
*     no2h  Gas   1.396e-012  3.283e-013
*      c2n  Gas   6.686e-013  1.572e-013
*       n3  Gas   3.205e-013  7.533e-014
*      no2  Gas   2.283e-013  5.366e-014
*       ch  Gas   5.193e-014  1.221e-014
*      cnn  Gas   2.288e-016  5.378e-017
*        c  Gas   1.266e-016  2.977e-017
*     c4n2  Gas   2.864e-018  6.733e-019
*     hno3  Gas   1.670e-018  3.926e-019
*       c3  Gas   1.543e-018  3.627e-019
*       c2  Gas   8.004e-019  1.882e-019
*      no3  Gas   2.273e-022  5.344e-023
*       o3  Gas   1.082e-022  2.544e-023
*     n2o3  Gas   4.069e-024  9.565e-025
*       c4  Gas   3.808e-025  8.951e-026
*       c5  Gas   1.051e-027  2.472e-028
*     n2o4  Gas   6.082e-030  1.430e-030
*     n2o5  Gas   2.375e-037  5.584e-038
*       *c  solid 6.863e+000  1.613e+000
*     *h2o liquid 0.000e+000  0.000e+000
      Total Gas   3.643e+001  8.564e+000
      Total Cond. 6.863e+000  1.613e+000
```

Reference state = reactants

H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00

P (ATM)	V (CC/GM)	T (K)	H(R) (CAL/GM)	E(R) (CAL/GM)	S(R) (CAL/K/GM)
VGS (CC/GM)	CV (CAL/K/GM)	CP (CAL/K/GM)	ALPHA	BETA	KAPPA
8.82445e+001	2.46452e+001	6.71729e+002	-1.12888e+003	-1.18153e+003	1.72467e+000
2.46107e+001	2.85925e-001	3.58096e-001	3.94416e+000	3.65959e+000	1.35102e+000

Product concentrations

	Name		(mol/kg)	(mol gas/mol explosive)
*	n2	Gas	1.175e+001	2.762e+000
*	h2o	Gas	9.444e+000	2.220e+000
*	co2	Gas	6.367e+000	1.497e+000
*	ch4	Gas	2.855e+000	6.711e-001
*	h2	Gas	2.778e+000	6.531e-001
*	co	Gas	2.760e+000	6.488e-001
*	h3n	Gas	4.022e-001	9.455e-002
*	c2h6	Gas	3.873e-002	9.105e-003
*	ch2o2	Gas	1.826e-002	4.292e-003
*	c2h4	Gas	4.365e-003	1.026e-003
*	ch2o	Gas	3.884e-003	9.130e-004
*	ch3oh	Gas	3.422e-003	8.044e-004
*	chn	Gas	1.902e-003	4.471e-004
*	chno	Gas	1.193e-003	2.805e-004
*	ch3	Gas	3.280e-004	7.710e-005
*	c3h8	Gas	9.996e-005	2.350e-005
*	c3h6	Gas	4.062e-005	9.549e-006
*	c2h2	Gas	2.338e-005	5.496e-006
*	h	Gas	2.126e-005	4.999e-006
*	cho	Gas	1.192e-005	2.802e-006
*	h2n	Gas	5.485e-006	1.290e-006
*	ho	Gas	3.160e-006	7.428e-007
*	no	Gas	2.564e-007	6.028e-008
*	h4n2	Gas	1.268e-007	2.981e-008
*	h2n2	Gas	1.724e-008	4.054e-009
*	c2n2	Gas	1.143e-008	2.687e-009
*	cno	Gas	6.664e-009	1.567e-009
*	c3o2	Gas	5.569e-009	1.309e-009
*	ch2	Gas	3.344e-009	7.862e-010
*	c2h4o	Gas	2.713e-009	6.377e-010
*	h2o2	Gas	1.799e-009	4.228e-010
*	hno	Gas	1.555e-009	3.656e-010
*	cn	Gas	8.671e-010	2.038e-010
*	n2o	Gas	4.204e-010	9.884e-011
*	hn	Gas	3.497e-010	8.221e-011
*	c2h	Gas	1.622e-010	3.812e-011
*	o2	Gas	7.904e-011	1.858e-011
*	o	Gas	4.882e-011	1.148e-011
*	c2o	Gas	1.569e-011	3.688e-012
*	n	Gas	5.455e-012	1.282e-012
*	ho2	Gas	4.161e-012	9.781e-013
*	hno2	Gas	2.838e-012	6.671e-013
*	cn2	Gas	1.586e-012	3.727e-013
*	no2h	Gas	1.396e-012	3.283e-013
*	c2n	Gas	6.686e-013	1.572e-013
*	n3	Gas	3.205e-013	7.533e-014
*	no2	Gas	2.283e-013	5.366e-014
*	ch	Gas	5.193e-014	1.221e-014
*	cnn	Gas	2.288e-016	5.378e-017
*	c	Gas	1.266e-016	2.977e-017
*	c4n2	Gas	2.864e-018	6.733e-019

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*     hno3  Gas   1.670e-018  3.926e-019
*       c3  Gas   1.543e-018  3.627e-019
*       c2  Gas   8.004e-019  1.882e-019
*      no3  Gas   2.273e-022  5.344e-023
*       o3  Gas   1.082e-022  2.544e-023
*     n2o3  Gas   4.069e-024  9.565e-025
*       c4  Gas   3.808e-025  8.951e-026
*       c5  Gas   1.051e-027  2.472e-028
*     n2o4  Gas   6.082e-030  1.430e-030
*     n2o5  Gas   2.375e-037  5.584e-038
*       *c  solid 6.863e+000  1.613e+000
*     *h2o liquid 0.000e+000  0.000e+000
      Total Gas   3.643e+001  8.564e+000
      Total Cond. 6.863e+000  1.613e+000

                          Reference state = reactants
                H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00
       P           V           T           H(R)        E(R)          S(R)
    (ATM)       (CC/GM)       (K)        (CAL/GM)    (CAL/GM)    (CAL/K/GM)
      VGS         CV          CP          ALPHA        BETA         KAPPA
   (CC/GM)   (CAL/K/GM)   (CAL/K/GM)
3.50029e+001 4.92904e+001 5.54264e+002 -1.17230e+003 -1.21407e+003 1.72467e+000
4.92560e+001 2.66542e-001 3.38792e-001  3.68201e+000  3.54109e+000 1.32219e+000

Product concentrations
          Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.175e+001  2.762e+000
*      h2o  Gas   9.444e+000  2.220e+000
*      co2  Gas   6.367e+000  1.497e+000
*      ch4  Gas   2.855e+000  6.711e-001
*       h2  Gas   2.778e+000  6.531e-001
*       co  Gas   2.760e+000  6.488e-001
*      h3n  Gas   4.022e-001  9.455e-002
*     c2h6  Gas   3.873e-002  9.105e-003
*    ch2o2  Gas   1.826e-002  4.292e-003
*     c2h4  Gas   4.365e-003  1.026e-003
*     ch2o  Gas   3.884e-003  9.130e-004
*    ch3oh  Gas   3.422e-003  8.044e-004
*      chn  Gas   1.902e-003  4.471e-004
*     chno  Gas   1.193e-003  2.805e-004
*      ch3  Gas   3.280e-004  7.710e-005
*     c3h8  Gas   9.996e-005  2.350e-005
*     c3h6  Gas   4.062e-005  9.549e-006
*     c2h2  Gas   2.338e-005  5.496e-006
*        h  Gas   2.126e-005  4.999e-006
*      cho  Gas   1.192e-005  2.802e-006
*      h2n  Gas   5.485e-006  1.290e-006
*       ho  Gas   3.160e-006  7.428e-007
*       no  Gas   2.564e-007  6.028e-008
*     h4n2  Gas   1.268e-007  2.981e-008
*     h2n2  Gas   1.724e-008  4.054e-009
*     c2n2  Gas   1.143e-008  2.687e-009
*      cno  Gas   6.664e-009  1.567e-009
*     c3o2  Gas   5.569e-009  1.309e-009
*      ch2  Gas   3.344e-009  7.862e-010
*    c2h4o  Gas   2.713e-009  6.377e-010
*     h2o2  Gas   1.799e-009  4.228e-010
*      hno  Gas   1.555e-009  3.656e-010
*       cn  Gas   8.671e-010  2.038e-010
*      n2o  Gas   4.204e-010  9.884e-011
*       hn  Gas   3.497e-010  8.221e-011
*      c2h  Gas   1.622e-010  3.812e-011
*       o2  Gas   7.904e-011  1.858e-011
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*       o  Gas   4.882e-011  1.148e-011
*     c2o  Gas   1.569e-011  3.688e-012
*       n  Gas   5.455e-012  1.282e-012
*     ho2  Gas   4.161e-012  9.781e-013
*    hno2  Gas   2.838e-012  6.671e-013
*     cn2  Gas   1.586e-012  3.727e-013
*    no2h  Gas   1.396e-012  3.283e-013
*     c2n  Gas   6.686e-013  1.572e-013
*      n3  Gas   3.205e-013  7.533e-014
*     no2  Gas   2.283e-013  5.366e-014
*      ch  Gas   5.193e-014  1.221e-014
*     cnn  Gas   2.288e-016  5.378e-017
*       c  Gas   1.266e-016  2.977e-017
*    c4n2  Gas   2.864e-018  6.733e-019
*    hno3  Gas   1.670e-018  3.926e-019
*      c3  Gas   1.543e-018  3.627e-019
*      c2  Gas   8.004e-019  1.882e-019
*     no3  Gas   2.273e-022  5.344e-023
*      o3  Gas   1.082e-022  2.544e-023
*    n2o3  Gas   4.069e-024  9.565e-025
*      c4  Gas   3.808e-025  8.951e-026
*      c5  Gas   1.051e-027  2.472e-028
*    n2o4  Gas   6.082e-030  1.430e-030
*    n2o5  Gas   2.375e-037  5.584e-038
*      *c  solid 6.863e+000  1.613e+000
*    *h2o liquid 0.000e+000  0.000e+000
     Total Gas   3.643e+001  8.564e+000
     Total Cond. 6.863e+000  1.613e+000

                          Reference state = reactants
               H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00
      P           V           T           H(R)        E(R)          S(R)
    (ATM)       (CC/GM)       (K)        (CAL/GM)    (CAL/GM)    (CAL/K/GM)
     VGS         CV          CP          ALPHA        BETA         KAPPA
   (CC/GM)   (CAL/K/GM)   (CAL/K/GM)
1.40422e+001 9.85807e+001 4.53714e+002 -1.20654e+003 -1.24005e+003 1.72467e+000
9.85464e+001 2.49907e-001 3.22227e-001  3.45271e+000  3.38432e+000 1.31569e+000

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.175e+001  2.762e+000
*      h2o  Gas   9.444e+000  2.220e+000
*      co2  Gas   6.367e+000  1.497e+000
*      ch4  Gas   2.855e+000  6.711e-001
*       h2  Gas   2.778e+000  6.531e-001
*       co  Gas   2.760e+000  6.488e-001
*      h3n  Gas   4.022e-001  9.455e-002
*     c2h6  Gas   3.873e-002  9.105e-003
*    ch2o2  Gas   1.826e-002  4.292e-003
*     c2h4  Gas   4.365e-003  1.026e-003
*     ch2o  Gas   3.884e-003  9.130e-004
*    ch3oh  Gas   3.422e-003  8.044e-004
*      chn  Gas   1.902e-003  4.471e-004
*     chno  Gas   1.193e-003  2.805e-004
*      ch3  Gas   3.280e-004  7.710e-005
*     c3h8  Gas   9.996e-005  2.350e-005
*     c3h6  Gas   4.062e-005  9.549e-006
*     c2h2  Gas   2.338e-005  5.496e-006
*        h  Gas   2.126e-005  4.999e-006
*      cho  Gas   1.192e-005  2.802e-006
*      h2n  Gas   5.485e-006  1.290e-006
*       ho  Gas   3.160e-006  7.428e-007
*       no  Gas   2.564e-007  6.028e-008
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*     h4n2  Gas   1.268e-007  2.981e-008
*     h2n2  Gas   1.724e-008  4.054e-009
*     c2n2  Gas   1.143e-008  2.687e-009
*      cno  Gas   6.664e-009  1.567e-009
*     c3o2  Gas   5.569e-009  1.309e-009
*      ch2  Gas   3.344e-009  7.862e-010
*    c2h4o  Gas   2.713e-009  6.377e-010
*     h2o2  Gas   1.799e-009  4.228e-010
*      hno  Gas   1.555e-009  3.656e-010
*       cn  Gas   8.671e-010  2.038e-010
*      n2o  Gas   4.204e-010  9.884e-011
*       hn  Gas   3.497e-010  8.221e-011
*      c2h  Gas   1.622e-010  3.812e-011
*       o2  Gas   7.904e-011  1.858e-011
*        o  Gas   4.882e-011  1.148e-011
*      c2o  Gas   1.569e-011  3.688e-012
*        n  Gas   5.455e-012  1.282e-012
*      ho2  Gas   4.161e-012  9.781e-013
*     hno2  Gas   2.838e-012  6.671e-013
*      cn2  Gas   1.586e-012  3.727e-013
*     no2h  Gas   1.396e-012  3.283e-013
*      c2n  Gas   6.686e-013  1.572e-013
*       n3  Gas   3.205e-013  7.533e-014
*      no2  Gas   2.283e-013  5.366e-014
*       ch  Gas   5.193e-014  1.221e-014
*      cnn  Gas   2.288e-016  5.378e-017
*        c  Gas   1.266e-016  2.977e-017
*     c4n2  Gas   2.864e-018  6.733e-019
*     hno3  Gas   1.670e-018  3.926e-019
*       c3  Gas   1.543e-018  3.627e-019
*       c2  Gas   8.004e-019  1.882e-019
*      no3  Gas   2.273e-022  5.344e-023
*       o3  Gas   1.082e-022  2.544e-023
*     n2o3  Gas   4.069e-024  9.565e-025
*       c4  Gas   3.808e-025  8.951e-026
*       c5  Gas   1.051e-027  2.472e-028
*     n2o4  Gas   6.082e-030  1.430e-030
*     n2o5  Gas   2.375e-037  5.584e-038
*       *c  solid 6.863e+000  1.613e+000
*     *h2o liquid 0.000e+000  0.000e+000
      Total Gas   3.643e+001  8.564e+000
      Total Cond. 6.863e+000  1.613e+000

                          The End of the Adiabat
                       Reference state = reactants
                H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00
      P           V           T           H(R)        E(R)          S(R)
    (ATM)      (CC/GM)       (K)        (CAL/GM)    (CAL/GM)    (CAL/K/GM)
     VGS         CV          CP          ALPHA        BETA         KAPPA
   (CC/GM)   (CAL/K/GM)   (CAL/K/GM)
2.33702e+000 3.83203e+002 2.98000e+002 -1.25534e+003 -1.27702e+003 1.72467e+000
3.83169e+002 2.22448e-001 2.94826e-001  3.07296e+000  3.05677e+000 1.33244e+000

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.175e+001  2.762e+000
*      h2o  Gas   9.444e+000  2.220e+000
*      co2  Gas   6.367e+000  1.497e+000
*      ch4  Gas   2.855e+000  6.711e-001
*       h2  Gas   2.778e+000  6.531e-001
*       co  Gas   2.760e+000  6.488e-001
*      h3n  Gas   4.022e-001  9.455e-002
*     c2h6  Gas   3.873e-002  9.105e-003
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```
*    ch2o2  Gas    1.826e-002  4.292e-003
*     c2h4  Gas    4.365e-003  1.026e-003
*     ch2o  Gas    3.884e-003  9.130e-004
*    ch3oh  Gas    3.422e-003  8.044e-004
*      chn  Gas    1.902e-003  4.471e-004
*     chno  Gas    1.193e-003  2.805e-004
*      ch3  Gas    3.280e-004  7.710e-005
*     c3h8  Gas    9.996e-005  2.350e-005
*     c3h6  Gas    4.062e-005  9.549e-006
*     c2h2  Gas    2.338e-005  5.496e-006
*        h  Gas    2.126e-005  4.999e-006
*      cho  Gas    1.192e-005  2.802e-006
*      h2n  Gas    5.485e-006  1.290e-006
*       ho  Gas    3.160e-006  7.428e-007
*       no  Gas    2.564e-007  6.028e-008
*     h4n2  Gas    1.268e-007  2.981e-008
*     h2n2  Gas    1.724e-008  4.054e-009
*     c2n2  Gas    1.143e-008  2.687e-009
*      cno  Gas    6.664e-009  1.567e-009
*     c3o2  Gas    5.569e-009  1.309e-009
*      ch2  Gas    3.344e-009  7.862e-010
*    c2h4o  Gas    2.713e-009  6.377e-010
*     h2o2  Gas    1.799e-009  4.228e-010
*      hno  Gas    1.555e-009  3.656e-010
*       cn  Gas    8.671e-010  2.038e-010
*      n2o  Gas    4.204e-010  9.884e-011
*       hn  Gas    3.497e-010  8.221e-011
*      c2h  Gas    1.622e-010  3.812e-011
*       o2  Gas    7.904e-011  1.858e-011
*        o  Gas    4.882e-011  1.148e-011
*      c2o  Gas    1.569e-011  3.688e-012
*        n  Gas    5.455e-012  1.282e-012
*      ho2  Gas    4.161e-012  9.781e-013
*     hno2  Gas    2.838e-012  6.671e-013
*      cn2  Gas    1.586e-012  3.727e-013
*     no2h  Gas    1.396e-012  3.283e-013
*      c2n  Gas    6.686e-013  1.572e-013
*       n3  Gas    3.205e-013  7.533e-014
*      no2  Gas    2.283e-013  5.366e-014
*       ch  Gas    5.193e-014  1.221e-014
*      cnn  Gas    2.288e-016  5.378e-017
*        c  Gas    1.266e-016  2.977e-017
*     c4n2  Gas    2.864e-018  6.733e-019
*     hno3  Gas    1.670e-018  3.926e-019
*       c3  Gas    1.543e-018  3.627e-019
*       c2  Gas    8.004e-019  1.882e-019
*      no3  Gas    2.273e-022  5.344e-023
*       o3  Gas    1.082e-022  2.544e-023
*     n2o3  Gas    4.069e-024  9.565e-025
*       c4  Gas    3.808e-025  8.951e-026
*       c5  Gas    1.051e-027  2.472e-028
*     n2o4  Gas    6.082e-030  1.430e-030
*     n2o5  Gas    2.375e-037  5.584e-038
*       *c  solid  6.863e+000  1.613e+000
*     *h2o liquid  0.000e+000  0.000e+000
      Total Gas    3.643e+001  8.564e+000
      Total Cond.  6.863e+000  1.613e+000

                The Products at room temperature and pressure
                          Reference state = reactants
                H(R) = H--20.28, E(R) = E--20.29, S(R) = S- 0.00
      P           V           T           H(R)        E(R)          S(R)
    (ATM)      (CC/GM)       (K)        (CAL/GM)    (CAL/GM)    (CAL/K/GM)
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     VGS         CV           CP          ALPHA         BETA         KAPPA
   (CC/GM)   (CAL/K/GM)   (CAL/K/GM)
1.00000e+000 8.92829e+002 2.98000e+002 -1.25541e+003 -1.27702e+003 1.78612e+000
8.92794e+002 2.22439e-001 2.94825e-001  3.07275e+000  3.06578e+000 1.32846e+000

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.175e+001  2.762e+000
*      h2o  Gas   9.444e+000  2.220e+000
*      co2  Gas   6.367e+000  1.497e+000
*      ch4  Gas   2.855e+000  6.711e-001
*       h2  Gas   2.778e+000  6.531e-001
*       co  Gas   2.760e+000  6.488e-001
*      h3n  Gas   4.022e-001  9.455e-002
*     c2h6  Gas   3.873e-002  9.105e-003
*    ch2o2  Gas   1.826e-002  4.292e-003
*     c2h4  Gas   4.365e-003  1.026e-003
*     ch2o  Gas   3.884e-003  9.130e-004
*    ch3oh  Gas   3.422e-003  8.044e-004
*      chn  Gas   1.902e-003  4.471e-004
*     chno  Gas   1.193e-003  2.805e-004
*      ch3  Gas   3.280e-004  7.710e-005
*     c3h8  Gas   9.996e-005  2.350e-005
*     c3h6  Gas   4.062e-005  9.549e-006
*     c2h2  Gas   2.338e-005  5.496e-006
*        h  Gas   2.126e-005  4.999e-006
*      cho  Gas   1.192e-005  2.802e-006
*      h2n  Gas   5.485e-006  1.290e-006
*       ho  Gas   3.160e-006  7.428e-007
*       no  Gas   2.564e-007  6.028e-008
*     h4n2  Gas   1.268e-007  2.981e-008
*     h2n2  Gas   1.724e-008  4.054e-009
*     c2n2  Gas   1.143e-008  2.687e-009
*      cno  Gas   6.664e-009  1.567e-009
*     c3o2  Gas   5.569e-009  1.309e-009
*      ch2  Gas   3.344e-009  7.862e-010
*    c2h4o  Gas   2.713e-009  6.377e-010
*     h2o2  Gas   1.799e-009  4.228e-010
*      hno  Gas   1.555e-009  3.656e-010
*       cn  Gas   8.671e-010  2.038e-010
*      n2o  Gas   4.204e-010  9.884e-011
*       hn  Gas   3.497e-010  8.221e-011
*      c2h  Gas   1.622e-010  3.812e-011
*       o2  Gas   7.904e-011  1.858e-011
*        o  Gas   4.882e-011  1.148e-011
*      c2o  Gas   1.569e-011  3.688e-012
*        n  Gas   5.455e-012  1.282e-012
*      ho2  Gas   4.161e-012  9.781e-013
*     hno2  Gas   2.838e-012  6.671e-013
*      cn2  Gas   1.586e-012  3.727e-013
*     no2h  Gas   1.396e-012  3.283e-013
*      c2n  Gas   6.686e-013  1.572e-013
*       n3  Gas   3.205e-013  7.533e-014
*      no2  Gas   2.283e-013  5.366e-014
*       ch  Gas   5.193e-014  1.221e-014
*      cnn  Gas   2.288e-016  5.378e-017
*        c  Gas   1.266e-016  2.977e-017
*     c4n2  Gas   2.864e-018  6.733e-019
*     hno3  Gas   1.670e-018  3.926e-019
*       c3  Gas   1.543e-018  3.627e-019
*       c2  Gas   8.004e-019  1.882e-019
*      no3  Gas   2.273e-022  5.344e-023
*       o3  Gas   1.082e-022  2.544e-023
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*    n2o3  Gas   4.069e-024  9.565e-025
*      c4  Gas   3.808e-025  8.951e-026
*      c5  Gas   1.051e-027  2.472e-028
*    n2o4  Gas   6.082e-030  1.430e-030
*    n2o5  Gas   2.375e-037  5.584e-038
*      *c  solid 6.863e+000  1.613e+000
*    *h2o liquid 0.000e+000  0.000e+000
     Total Gas   3.643e+001  8.564e+000
     Total Cond. 6.863e+000  1.613e+000

The mechanical energy of detonation =     -8.672 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -8.672 kJ/cc

JWL Tail Fit results:
Initial  E0 =     -9.115, Final E0 =     -9.076
E0(V=infty) =     -9.076
C =      1.272,  omega =      0.342
Final fitting error = 0.000528

     V/V0     Actual E     Fit E    Actual P      Fit P
              (kJ/cc)     (kJ/cc)    (GPa)        (GPa)
    20.000     -7.741     -7.741      0.023      0.023
    40.000     -8.024     -8.023      0.009      0.009
    80.000     -8.244     -8.245      0.004      0.004
   160.000     -8.421     -8.421      0.001      0.001

JWL Fit results:
E0(V=infty) =     -9.076
R[1] =   4.828,    R[2] =  1.048,    omega = 0.342
A    = 820.010,    B    =  8.722,    C     = 1.272
Final fitting error = 0.011206

     V/V0     Actual E     Fit E    Actual P      Fit P
              (kJ/cc)     (kJ/cc)    (GPa)        (GPa)

     0.762      3.045      3.045     25.573     26.483
     1.000     -0.963     -1.078     10.898     10.896
     2.200     -5.408     -5.402      1.218      1.331
     4.100     -6.555     -6.667      0.310      0.310
     6.500     -7.036     -7.106      0.133      0.113
    10.000     -7.359     -7.384      0.065      0.058
    20.000     -7.741     -7.741      0.023      0.023
    40.000     -8.024     -8.023      0.009      0.009
    80.000     -8.244     -8.245      0.004      0.004
   160.000     -8.421     -8.421      0.001      0.001
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