Shock sensitivity testing of Octols

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Approved by

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English summary

Octol 60/40 and 70/30 (HMX/TNT) have been tested with regard to shock sensitivity in Intermediate Scale GAP test. Both compositions were cast filled into the test tubes. An average density of 98.1% of TMD was obtained for the fillings with Octol 60/40 and 98.2 % of TMD for the fillings with Octol 70/30.

The shock sensitivity for Octol 60/40 was found to be 14.5 kbar and for Octol 70/30 16.0 kbar, indicating that Octol 60/40 is slightly more shock sensitive than Octol 70/30.

Sammendrag

Oktol 60/40 og Oktol 70/30 (HMX/TNT) har blitt testet med hensyn på sjokkfølsomhet i Intermediate Scale GAP test. Begge komposisjonene ble smeltestøpt i test rørene. En gjennomsnittlig tetthet på 98.1% av TMD ble oppnådd for fyllingene med Oktol 60/40 og 98.2% av TMD for fyllingene med Oktol 70/30.

Sjokkfølsomheten ble funnet å være 14.5 kbar for Oktol 60/40 og 16.0 kbar for Oktol 70/30. Et resultat som gir Oktol 60/40 en noe høyere sjokkfølsomhet enn Oktol 70/30.

Contents

1 Introduction

Octols containing TNT and HMX have been used in various combinations for a long range of fillings. TNT can, with its moderate melting point of 80.8 ^{o}C, be filled into warheads by a melt cast process. One disadvantage with the TNT is the change in volume when it goes from solid to liquid. The density of molten TNT is 1.47 g/cm^3 while solid TNT has a density of 1.654 g/cm^3 (1). Octols containing TNT as binder can be melt cast filled or pressed filled. The fillings we have tested are melt cast.

Octols have relatively high energy content and can be used in shaped charges with good results. The drawbacks of Octols are the low melting point of TNT and in general that they are more sensitive than more modern PBX compositions containing an inert binder and HMX. The requirement for new munitions to day in several NATO countries are that they shall fulfill the requirement in STANAG 4443. This requirement will in the future require that many new and existing munitions have to use explosives filling with reduced shock sensitivity.

In this report we have tested two Octols 60/40 (HMX/TNT) and 70/30 (HMX/TNT) with regard to chock sensitivity in Intermediate Scale Gap test (2). In addition some standard thermochemical calculations by use of Cheetah 2.0 Code (3) have been performed.

2 Experimentally

2.1 Sample preparation

All Intermediate Scale Gap test tubes were melt cast filled at Nammo Raufoss AS.

2.2 Intermediate Scale Gap Test

The Intermediate Scale Gap test was carried out according to the STANAG 4488 edition 2 (2) except for the thickness of the cards. We did use ethyl acetate cards with thickness 0.254 mm instead of 0.19 +0.02/-0.01mm recommended in the STANAG. As booster explosive we used HWC containing RDX/wax/graphite (94.5/4.5/1). The control report for the booster explosive lot 08/02 is given in the Appendix A.

3 Results

3.1 OCTOL 70/30

Table 3.1 gives properties of the tubes before and after they were filled with Octol 70/30. The obtained average density for the fillings of 1.787±0.005 g/cm^3 or 98.1% of TMD (1.8220 g/cm^3) is relatively good. The variation in density of the different tubes is as the standard deviation (±0.005) indicates small.

Tube No	Weight (g)	Inner diameter Top (cm)	Inner diameter Bottom (cm)	Height (cm)	Volume (cm^3)	Filling Octol	Weight tube +Explosive (g)	Weight Explosive (g)	Density (g/cm^3)
1	907.06	3.945	3.940	20.108	245.472	70/30	1344.20	437.14	1.781
2	916.51	3.938	3.930	20.198	245.509	70/30	1354.90	438.39	1.786
3	886.34	3.955	3.956	20.032	246.160	70/30	1325.70	439.36	1.785
4	900.37	3.938	3.940	20.004	243.769	70/30	1335.65	435.28	1.786
5	908.21	3.926	3.932	20.104	243.745	70/30	1345.00	436.79	1.792
6	908.23	3.936	3.931	20.090	244.134	70/30	1344.20	435.97	1.786
7	899.74	3.940	3.943	20.001	244.042	70/30	1334.25	434.51	1.780
8	883.02	3.945	3.948	19.992	244.552	70/30	1322.75	439.73	1.798
9	878.43	3.970	3.965	20.066	248.076	70/30	1320.65	442.22	1.783
10	880.48	3.958	3.958	20.007	246.163	70/30	1321.05	440.57	1.790
	Average density (g/cm^3)								**1.787±0.005**

Table 3.1 Densities of Octol fillings tested in Intermediate Scale GAP Test.

Figure 3.1 Picture of shot No 1 after it was assembled.

Figure 3.1 is a picture of the test unit after it has been assembled. For the first shot we started with a barrier thickness of 200 cards. After initiation with a detonator No 8 the main charge did undergo a full detonation as the hole in the witness plate shows. Figure 3.2 shows a picture of the recovered witness plate. Fragments from the tube or the explosive filling rests was not recovered.

For the next shot we increased the barrier thickness to 220 cards. Figure 3.3 shows the witness plate with a hole. The reaction is therefore a detonation. For shot No 3 we increased the barrier thickness to 240 cards. In Figure 3.4 the witness plate and the recovered rest of the tube are shown, indicating that no reaction had taken place.

Shot No 4 was a repetition of shot No 3 and the result was identical. For the following shots the barrier thickness was successively reduced until detonation was obtained. The results are summarized in Table 3.2. Figure 3.12 shows a plot of the test results.

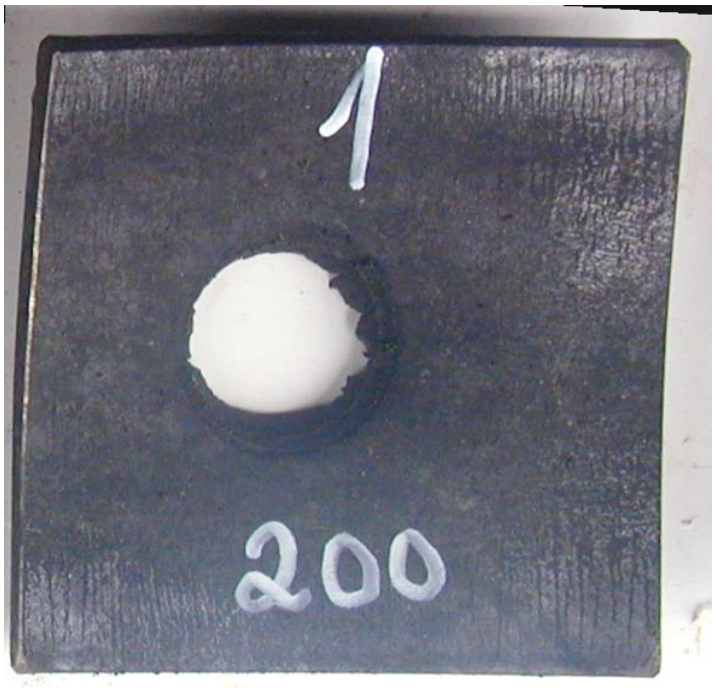

Figure 3.2 Shot No 1, tube No 1, barrier thickness 200 cards, detonation.

Figure 3.3 Shot No 2, tube No 2, barrier thickness 220 cards, detonation.

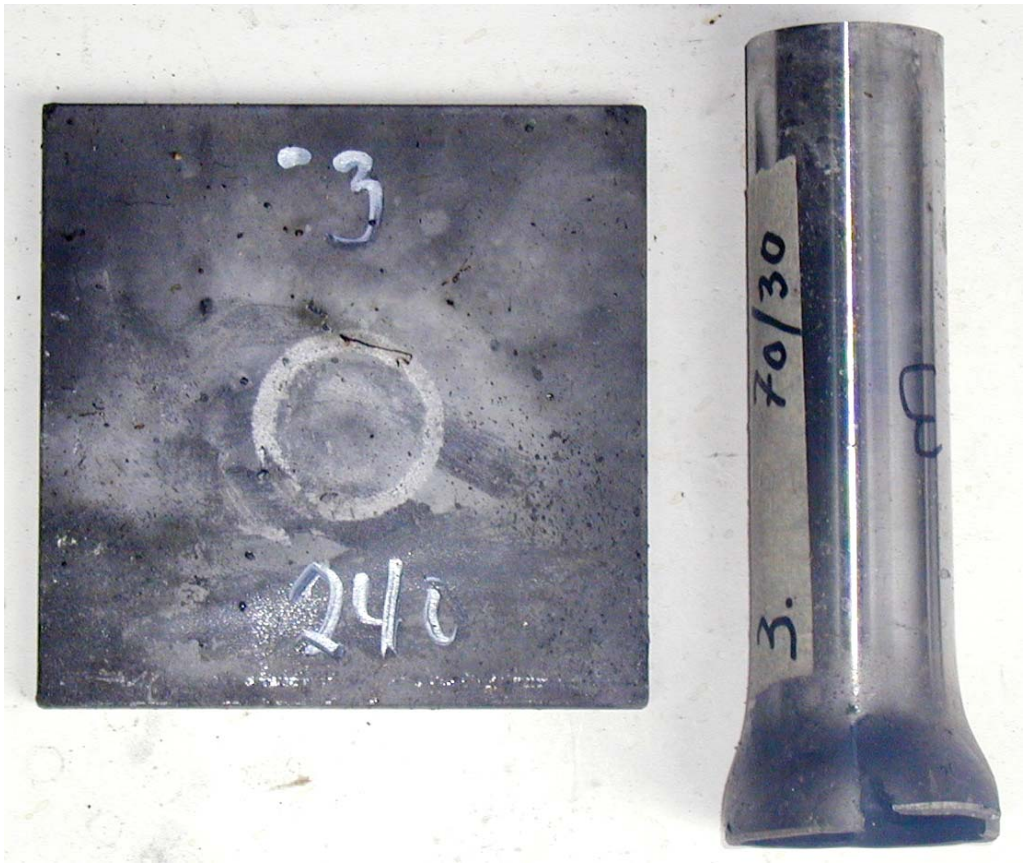

Figure 3.4 Shot No 3, tube No 3, barrier 240 cards, no reaction.

Figure 3.5 Shot No 4, tube No 4, barrier 240 cards, no reaction.

Figure 3.6 Shot No 5, tube No 5, barrier 220 cards, no reaction.

Figure 3.7 Shot No 6, tube No 6, barrier 220 cards, no reaction

Figure 3.8 Shot No 7, tube No 8, barrier 210 cards, no reaction.

Figure 3.9 Shot No 8, tube No 9, barrier 200 cards, no reaction.

Figure 3.10 Shot No 9, tube No 10, barrier 200 cards, detonation.

Figure 3.11 Shot No 10, tube No 7, barrier 200 cards, no reaction.

Shot No.	Tube No.	Barrier Thickness (Cards)	Barrier Thickness (mm)	Reaction
1	1	200	50.8	Detonation
2	2	220	55.88	Detonation
3	3	240	60.96	No Reaction
4	4	240	60.96	No Reaction
5	5	220	55.88	No Reaction
6	6	220	55.88	No Reaction
7	8	210	53.34	No Reaction
8	9	200	50.8	No Reaction
9	10	200	50.8	Detonation
10	7	200	50.8	No Reaction

Table 3.2 Summary of the results of the firings in Card GAP-test of Octol 70/30.

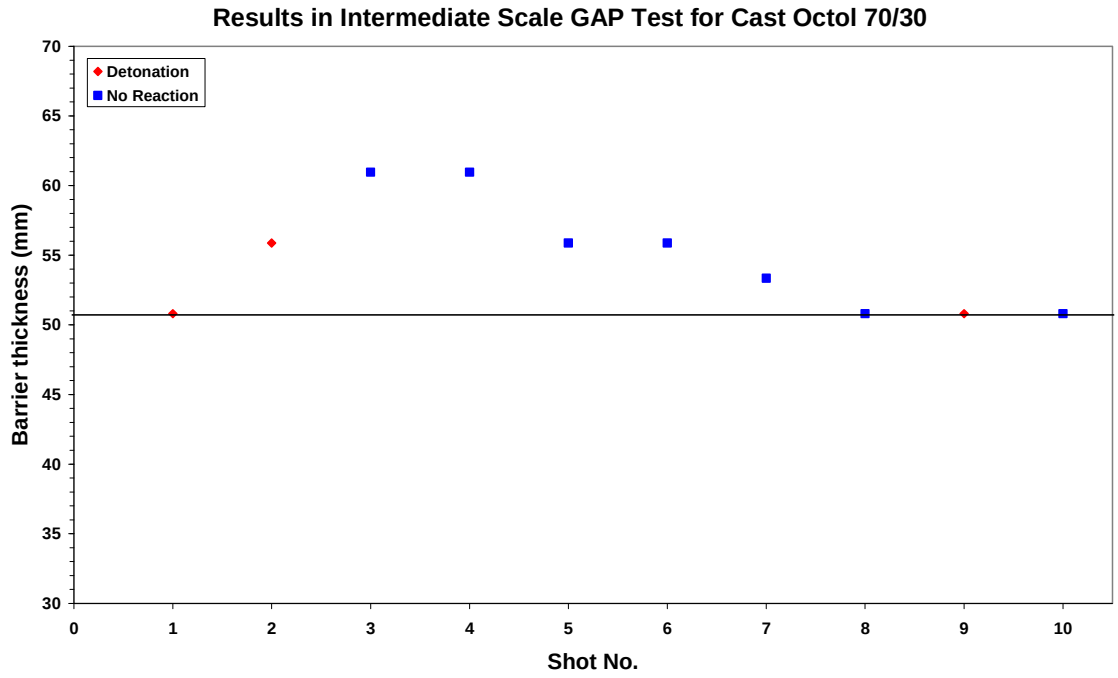

Figure 3.12 Plot of the results in Intermediate Scale Gap test for Octol 70/30.

Out of the 10 tubes tested only 3 went to full detonation. At the largest barrier thickness (240 cards) we did test two tubes with no reaction. At the next barrier thickness 220 cards we obtained full detonation for one out of three tubes. With 210 cards we had only one shot which did not react. At the lowest barrier thickness of 200 cards we tested 4 tubes. Two gave full detonation while two gave no reaction. Our conclusion is that the 50% point with respect to shock initiation of the tested quality of Octol 70/30 is 200 cards.

3.2 Octol 60/40

3.2.1 Density of filling

The tubes with Octol 60/40 were as the tubes with Octol 70/30 melt cast filled at Nammo Raufoss ASA. Table 3.3 gives properties of the tubes before and after they were filled. Average obtained density is 1.7662±0.007 g/cm^3. Octol 60/40 have theoretically a density of 1.7960 g/cm^3. The average filling density of our tubes is therefore 98.1%TMD or of equal quality as the filling of Octol 70/30 obtained in 3.1.1.

Tube No	Weight (g)	Inner Diameter Top (cm)	Inner Diameter Bottom (cm)	Height (cm)	Volume (cm^3)	Filling Octol	Weight tube + Explosive (g)	Weight Explosive (g)	Density (g/cm^3)
11	879.67	3.943	3.946	20.075	245.318	60/40	1315.10	435.43	1.775
12	880.28	3.951	3.965	19.995	246.016	60/40	1312.15	431.87	1.755
13	884.44	3.950	3.950	20.075	246.003	60/40	1319.15	434.71	1.767
14	910.18	3.944	3.943	20.138	245.963	60/40	1341.20	431.02	1.752
15	877.83	3.968	3.963	20.022	247.282	60/40	1312.45	434.62	1.758
16	877.30	3.959	3.950	19.979	245.384	60/40	1309.25	431.95	1.760
17	880.37	3.968	3.962	20.002	246.973	60/40	1313.90	433.53	1.755
18	871.00	3.961	3.959	19.988	246.178	60/40	1305.20	434.20	1.764
19	867.11	3.960	3.968	20.009	246.935	60/40	1304.10	436.99	1.770
20	887.08	3.956	3.953	20.043	246.170	60/40	1321.95	434.87	1.767
	Average density (g/cm^3)								**1.762±0.007**

Table 3.3 Densities of Octol 60/40 fillings tested in Intermediate Scale GAP test.

3.2.2 Intermediate Scale Gap Test

10 tubes were tested in Intermediate Scale Gap test. For the first shot we used a barrier thickness of 200 cards. This shot did not react as shown by the witness plate and the recovered rest of the shot given in Figure 3.13. Therefore we for the second shot, shot No. 12, decreased the number of cards to 180. As the picture of the witness plate in Figure 3.14 shows, this shot went to full detonation. Shot No 13 was fired with the same barrier thickness as shot No. 12. The obtained reaction was the same, full detonation. For the following shots we successively increased the number of cards up to 215 for shots No 18 and 19 for which we obtained not reaction. Figures 3.15 to 3.21 give pictures of recovered witness plates and rests of tubes and explosive fillings. Table 3.4 summarizes the obtained results for all 10 tubes. Figure 3.22 gives a plot of the reactions for every shot.

Figure 3.13 Shot No 11, tube No 11, barrier 200 cards, no reaction.

Figure 3.14 Shot No 12, tube No 12, barrier 180 cards, detonation.

Figure 3.15 Shot No 13, tube No 13, barrier 180 cards, detonation.

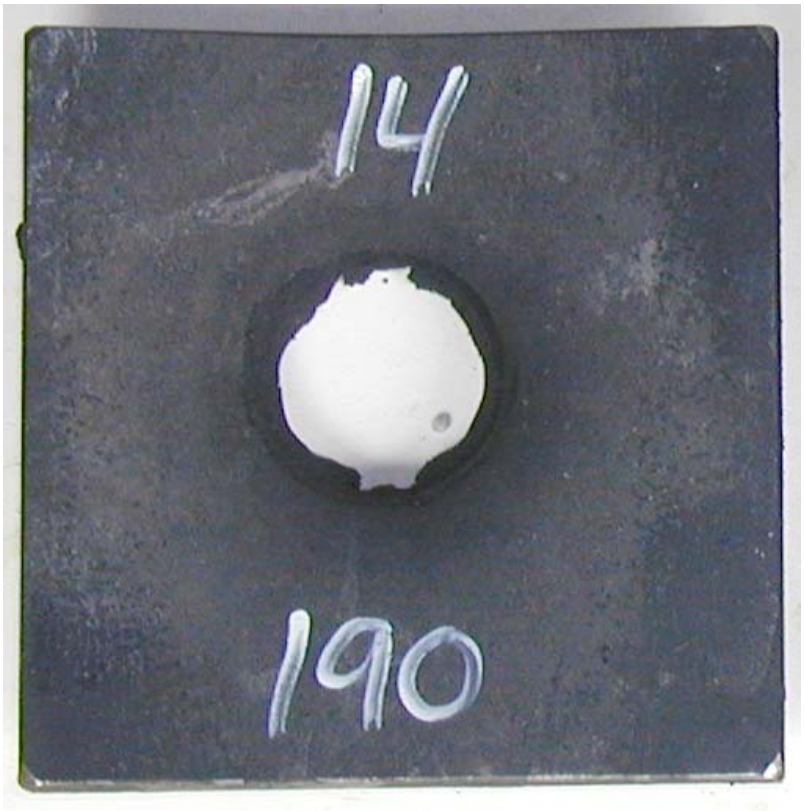

Figure 3.16 Shot No 14, tube No 14, barrier 190 cards, detonation.

Figure 3.17 Shot No 15, tube No 15, barrier 200 cards, detonation.

Figure 3.18 Shot No 16, tube No 16, barrier 200 cards, detonation.

Figure 3.19 Shot No 17, tube No 17, barrier 200 cards, detonation.

Figure 3.20 Shot No 18, tube No 18, barrier 215 cards, no reaction.

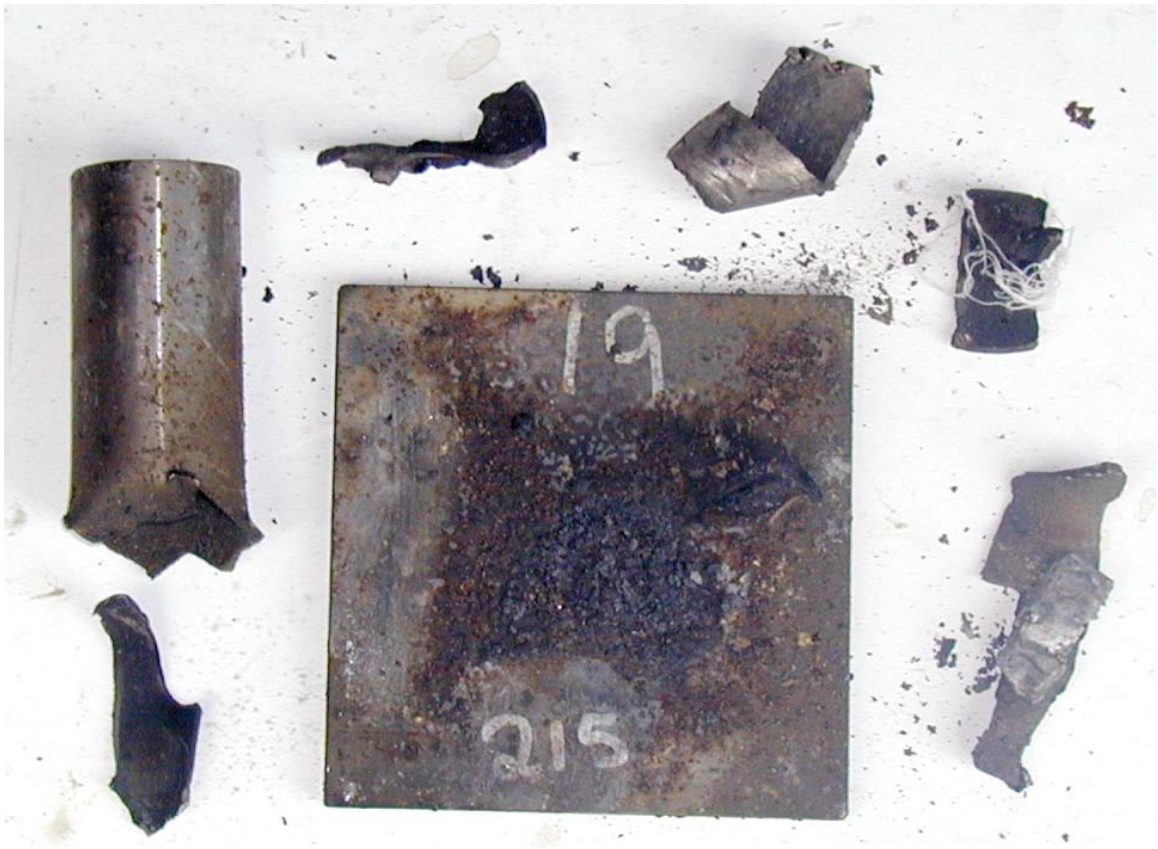

Figure 3.21 Shot No 19, tube No 19, barrier 215 cards, no reaction.

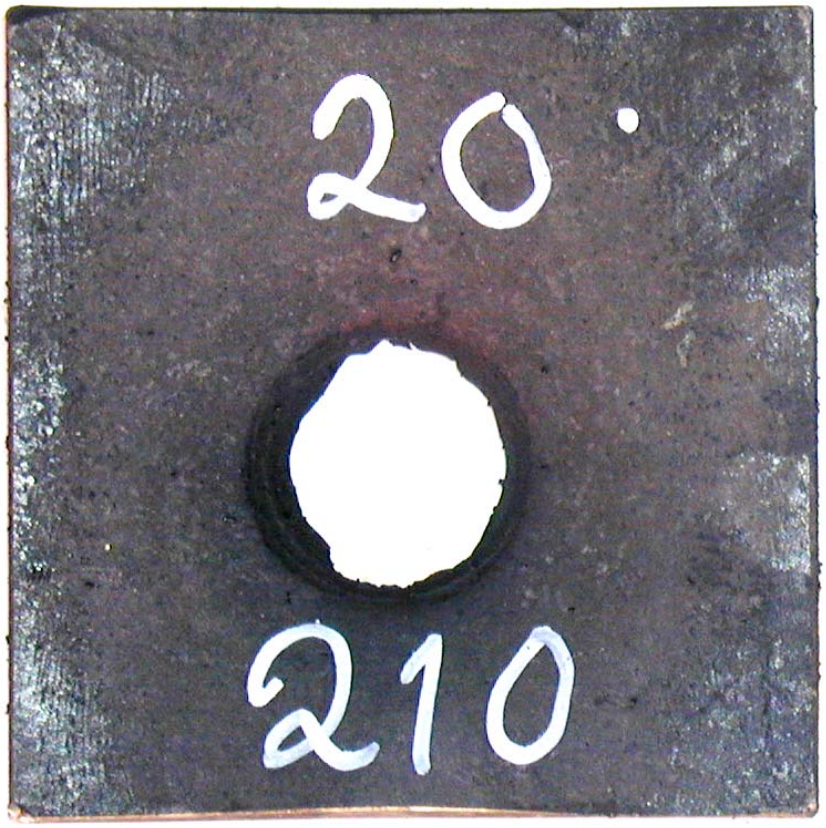

Figure 3.22 Shot No 20, tube No 20, barrier 210 cards, detonation.

Shot No.	Tube No.	Barrier Thickness (Cards)	Barrier Thickness (mm)	Reaction
11	11	200	50.8	No Reaction
12	12	180	45.72	Detonation
13	13	180	45.72	Detonation
14	14	190	48.26	Detonation
15	15	200	50.8	Detonation
16	16	200	50.8	Detonation
17	17	200	50.8	Detonation
18	18	215	54.61	No Reaction
19	19	215	54.61	No Reaction
20	20	210	53.34	Detonation

Table 3.4 Results in Intermediate Scale Gap Test for Octol 60/40.

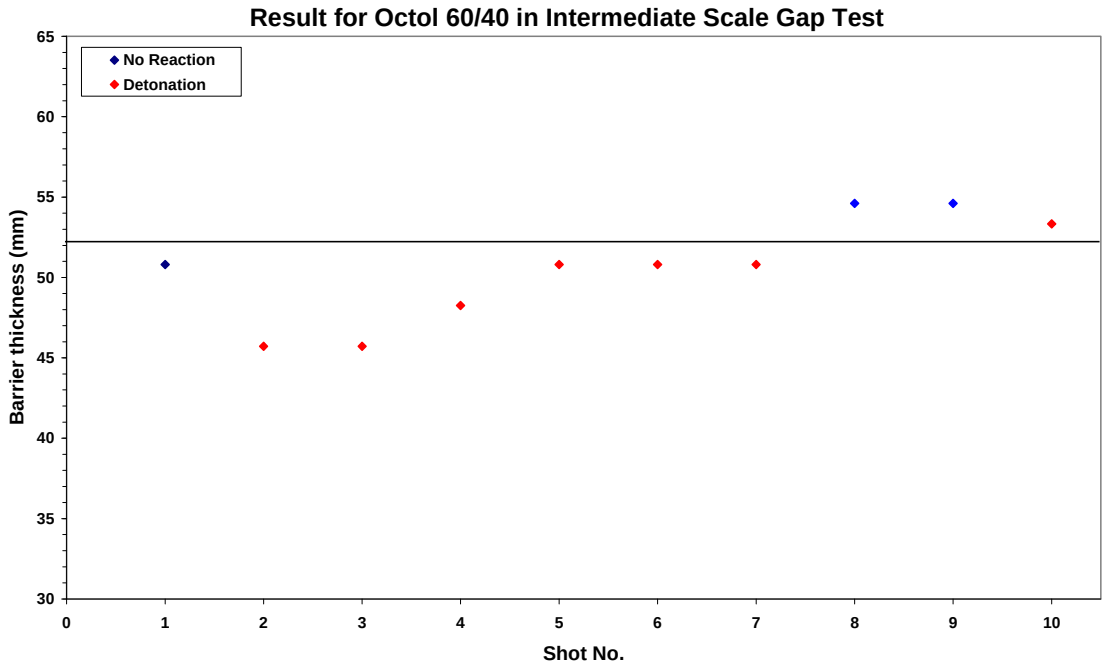

Figure 3.23 Plot of the results in Intermediate Scale Gap test for Octol 60/40.

From Table 3.4 and Figure 3.23 we see that we did get more detonation reactions than no reactions. At a barrier thickness of 215 cards (54.6 mm) we tested two charges and both gave no reaction. At the barrier thickness of 200 cards (50.8 mm) 3 of 4 charges did react with a full detonation response. These results have been used to find the 50% point with respect to shock initiation of the tested quality of Octol 60/40. The obtained barrier thickness is 208 cards.

3.3 The sensitivity as shock pressure

To obtain the shock sensitivity as pressure we have used the calibration data of the test given in STANAG 4488(2). These data have been reproduced in Figure 3.24.

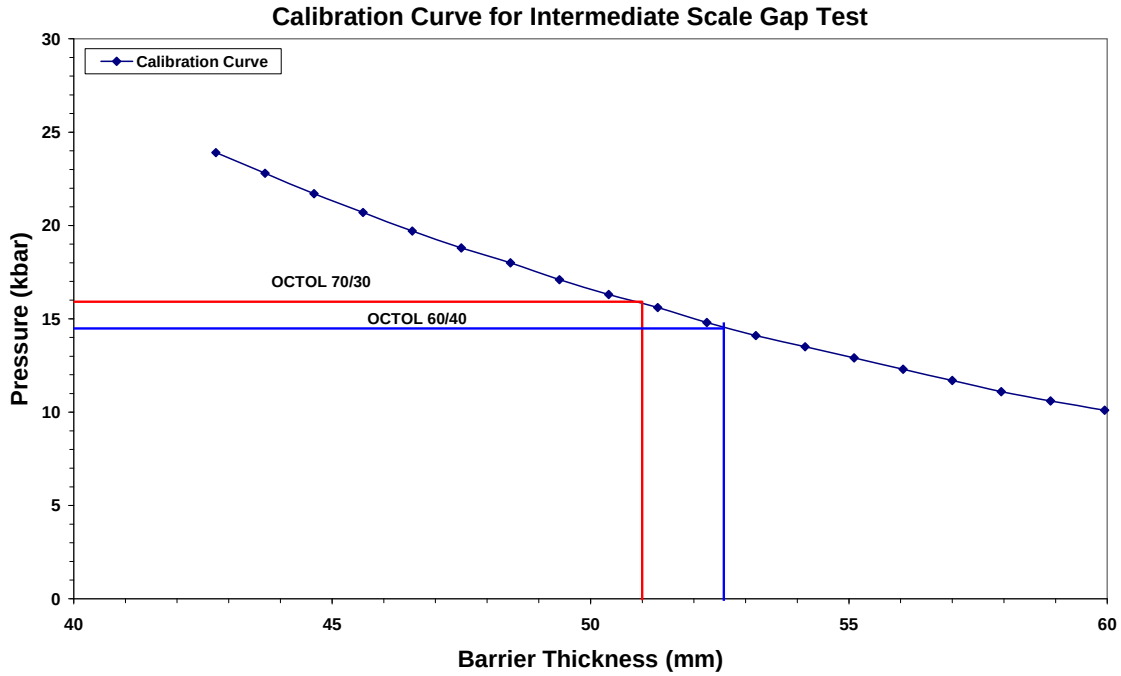

Figure 3.24 Pressure as function of barrier thickness for two 80 g HWC pellets.

From figure 3.24 the obtained result for Octol 70/30 with a barrier thickness of 51 mm is equal in pressure to 16 kbar. For Octol 60/40 and a barrier thickness of 52.5 mm correspond in pressure to 14.5 kbar. These results indicate that the tested quality of Octol 60/40 is slightly more sensitive to shock initiation than tested quality of Octol 70/30.

3.4 Theoretical properties

Theoretical calculations with Cheetah 2.0 Code (3) have been carried out for both Octol 60/40 and Octol 70/30 and the results are given in Appendix A and Appendix B respectively. We have carried out calculations with both the BKWC and BKWS product data bases.

Table 3.5 summarize the properties given by standard runs for both compositions and product data bases. Octol 70/30 gives approximately 2 GPa higher detonation pressure than Octol 60/40 in addition to approximately 250 m/s higher detonation velocity. For Octol 70/30 the detonation energy is approximately 4% higher than for Octol 60/40. However, both the detonation pressure and detonation velocity for both Octol compounds are significantly lower than for press filled compositions that contain HMX as the main component. In Table 3.5 comparable properties are given for PBXN-5 a composition with 95 wt.% HMX.

Properties at C-J condition	**Octol 60/40 TMD= 1.7960 g/cm^3**		**Octol 70/30 TMD= 1.8220 g/cm^3**		**PBXN-5***
	BKWC	***BKWS***	***BKWC***	***BKWS***	***BKWC***
Pressure (GPa)	30.16	30.21	32.29	32.05	36.64
Volume (cc/g)	0.418	0.426	0.413	0.421	0.400
Density (g/cc)	2.391	2.349	2.421	2.378	2.502
Energy (kJ/cc)	3.75	3.56	3.99	3.74	4.39
Temperature (K)	3998	3948	4033	3979	3987
Shock velocity (m/s)	8214	8454	8463	8677	8966
Particle velocity (m/s)	2045	1990	2094	2027	2147
Speed of sound (m/s)	6169	6464	6370	6649	6819
Gamma	3.017	3.249	3.042	3.280	3.176
Freezing at 1800 K gives					
Total energy of detonation (kJ/cc)	**-9.584**	**-9.904**	**-9.949**	**-10.253**	**-10.702**

*HMX/Viton (95/5) + 0.5wt.% Graphite added.

Table 3.5 Properties of Octol 40/60 and 70/30 calculated by Cheetah 2.0 Code.

Appendix A Octol 60/40

A.1 Complete printout BKWS Product Library

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The Composition
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Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
HMX	60.00	53.50	56.57	17866	155.47	0.000	296.17	$C_4H_8N_8O_8$
TNT	40.00	46.50	43.43	-15057	137.32	0.000	227.13	$C_7H_5N_3O_6$

```
Heat of formation =       9.677 cal/gm
Standard volume   =       0.557 cc/gm
Standard entropy  =       0.000 cal/k/gm
Standard energy   =       9.663 cal/gm

The elements and percent by mole
     c              21.803
     h              26.692
     n              22.933
     o              28.571
The average mol. wt. = 264.065 g/mol
Input>standard run, rho, 1.795982
The hugoniot reference state:
P0 = 1.000000 ATM, V0 = 0.556798 cc/gm, E0 = 9.663045 cal/gm
Using  135598 ATM as a lower bound for the C-J pressure
Using  338994 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    =   8.45382e+003 m/s
The particle velocity =   1.98977e+003 m/s
The speed of sound    =   6.46405e+003 m/s

P0 =       1 atm, V0 =  0.55680 cc/gm, E0 =   9.66304 cal/gm

                          Reference state = reactants
                H(R) = H- 9.68, E(R) = E- 9.66, S(R) = S- 0.00

          P           V         T       H(R)       E(R)       S(R)      VGS
       (ATM)       (CC/GM)     (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)  298156.0      0.4257   3947.8   3547.34     473.15     1.607     0.4005

Product concentrations
         Name    (mol/kg) (mol gas/mol explosive)
       n2  Gas   1.013e+001  2.675e+000
      co2  Gas   9.050e+000  2.390e+000
      h2o  Gas   4.400e+000  1.162e+000
    ch2o2  Gas   2.000e+000  5.282e-001
      h3n  Gas   1.172e+000  3.096e-001
     c2h6  Gas   7.549e-001  1.993e-001
      ch4  Gas   7.350e-001  1.941e-001
       h2  Gas   1.955e-001  5.163e-002
    ch3oh  Gas   1.676e-001  4.426e-002
       co  Gas   6.568e-002  1.734e-002
     h4n2  Gas   1.792e-002  4.732e-003
       no  Gas   1.607e-002  4.243e-003
     c2h4  Gas   1.019e-002  2.691e-003
      ch3  Gas   7.269e-003  1.920e-003
```

h2o2	Gas	4.940e-003	1.304e-003
ch2o	Gas	3.563e-003	9.409e-004
h2n	Gas	3.128e-003	8.260e-004
o2	Gas	2.713e-003	7.163e-004
ho	Gas	1.667e-003	4.402e-004
h2n2	Gas	1.415e-003	3.735e-004
chno	Gas	1.203e-003	3.178e-004
cno	Gas	1.076e-003	2.841e-004
h	Gas	7.749e-004	2.046e-004
o	Gas	2.233e-004	5.898e-005
no2	Gas	9.805e-005	2.589e-005
c3h8	Gas	8.237e-005	2.175e-005
ch2	Gas	5.263e-005	1.390e-005
cho	Gas	4.905e-005	1.295e-005
ho2	Gas	3.600e-005	9.507e-006
chn	Gas	3.343e-005	8.829e-006
hno	Gas	3.055e-005	8.066e-006
n2o	Gas	1.604e-005	4.235e-006
n	Gas	1.290e-005	3.406e-006
c2h2	Gas	8.124e-006	2.145e-006
hn	Gas	6.863e-006	1.812e-006
cn	Gas	3.107e-006	8.204e-007
c3h6	Gas	1.102e-006	2.910e-007
n3	Gas	9.147e-007	2.415e-007
hno2	Gas	7.155e-007	1.889e-007
no3	Gas	5.726e-007	1.512e-007
cn2	Gas	4.953e-007	1.308e-007
ch	Gas	4.795e-008	1.266e-008
hno3	Gas	4.408e-008	1.164e-008
c2h	Gas	3.288e-008	8.683e-009
no2h	Gas	2.049e-008	5.412e-009
c	Gas	9.135e-009	2.412e-009
o3	Gas	2.319e-009	6.123e-010
c2n2	Gas	1.448e-009	3.822e-010
n2o4	Gas	1.125e-009	2.972e-010
c2h4o	Gas	7.985e-010	2.108e-010
c2n	Gas	4.296e-010	1.134e-010
c2	Gas	2.587e-010	6.831e-011
c2o	Gas	1.181e-010	3.119e-011
n2o3	Gas	1.492e-011	3.940e-012
cnn	Gas	1.143e-011	3.017e-012
c3o2	Gas	6.403e-013	1.691e-013
c3	Gas	7.011e-014	1.851e-014
n2o5	Gas	1.308e-014	3.453e-015
c4	Gas	4.103e-023	1.083e-023
c4n2	Gas	8.882e-031	2.346e-031
c5	Gas	1.384e-033	3.654e-034
*c	solid	6.869e+000	1.814e+000
*h2o	liquid	0.000e+000	0.000e+000
Total	Gas	2.874e+001	7.590e+000
Total	Cond.	6.869e+000	1.814e+000

The C-J Adiabat

Reference state = reactants
H(R) = H- 9.68, E(R) = E- 9.66, 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)
1.)	126975.0	0.5568	3205.3	1562.72	-149.47	1.607	0.5195

Product concentrations

Name		(mol/kg)	(mol gas/mol explosive)
n2	Gas	1.031e+001	2.721e+000
co2	Gas	9.076e+000	2.397e+000
h2o	Gas	6.695e+000	1.768e+000
ch4	Gas	1.109e+000	2.928e-001
h3n	Gas	8.693e-001	2.295e-001

h2	Gas	7.869e-001	2.078e-001
ch2o2	Gas	6.232e-001	1.646e-001
co	Gas	5.939e-001	1.568e-001
c2h6	Gas	2.269e-001	5.992e-002
ch3oh	Gas	6.848e-002	1.808e-002
c2h4	Gas	1.576e-002	4.162e-003
ch2o	Gas	1.053e-002	2.781e-003
ch3	Gas	8.800e-003	2.324e-003
chno	Gas	3.652e-003	9.643e-004
no	Gas	1.879e-003	4.961e-004
h2n	Gas	1.446e-003	3.819e-004
ho	Gas	1.140e-003	3.010e-004
h	Gas	1.131e-003	2.987e-004
h4n2	Gas	6.952e-004	1.836e-004
chn	Gas	6.188e-004	1.634e-004
cho	Gas	2.426e-004	6.407e-005
h2o2	Gas	1.745e-004	4.609e-005
cno	Gas	1.329e-004	3.509e-005
c3h8	Gas	1.301e-004	3.435e-005
h2n2	Gas	1.075e-004	2.838e-005
c2h2	Gas	8.681e-005	2.292e-005
o2	Gas	6.129e-005	1.618e-005
ch2	Gas	2.356e-005	6.222e-006
o	Gas	1.462e-005	3.860e-006
c3h6	Gas	1.399e-005	3.694e-006
hno	Gas	8.575e-006	2.264e-006
hn	Gas	2.832e-006	7.479e-007
cn	Gas	2.779e-006	7.340e-007
n2o	Gas	2.710e-006	7.155e-007
ho2	Gas	1.992e-006	5.259e-007
n	Gas	1.198e-006	3.163e-007
no2	Gas	1.160e-006	3.062e-007
c2h	Gas	1.455e-007	3.843e-008
hno2	Gas	1.177e-007	3.107e-008
cn2	Gas	1.125e-007	2.970e-008
n3	Gas	6.615e-008	1.747e-008
c2n2	Gas	4.306e-008	1.137e-008
ch	Gas	1.800e-008	4.754e-009
no2h	Gas	1.174e-008	3.100e-009
c2h4o	Gas	1.070e-008	2.825e-009
c2o	Gas	2.743e-009	7.244e-010
c2n	Gas	2.285e-009	6.034e-010
c	Gas	1.161e-009	3.065e-010
c3o2	Gas	4.872e-010	1.286e-010
hno3	Gas	2.262e-010	5.974e-011
no3	Gas	8.793e-011	2.322e-011
c2	Gas	4.072e-011	1.075e-011
cnn	Gas	1.564e-011	4.129e-012
o3	Gas	4.550e-012	1.202e-012
c3	Gas	3.454e-013	9.122e-014
n2o3	Gas	5.634e-014	1.488e-014
n2o4	Gas	7.780e-015	2.054e-015
n2o5	Gas	6.796e-020	1.795e-020
c4	Gas	1.157e-020	3.056e-021
c4n2	Gas	2.236e-023	5.905e-024
c5	Gas	1.196e-027	3.159e-028
*c	solid	8.451e+000	2.232e+000
*h2o	liquid	0.000e+000	0.000e+000
Total	Gas	3.040e+001	8.028e+000
Total	Cond.	8.451e+000	2.232e+000

Reference state = reactants
H(R) = H- 9.68, E(R) = E- 9.66, 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)

1.)	13680.5	1.2250	1811.6	-433.65	-839.49	1.607	1.1886

Product concentrations

Name		(mol/kg)	(mol gas/mol explosive)
n2	Gas	1.063e+001	2.808e+000
co2	Gas	7.950e+000	2.099e+000
h2o	Gas	7.158e+000	1.890e+000
co	Gas	3.675e+000	9.704e-001
h2	Gas	2.032e+000	5.365e-001
ch4	Gas	1.454e+000	3.840e-001
h3n	Gas	2.224e-001	5.874e-002
ch2o2	Gas	1.638e-002	4.325e-003
c2h6	Gas	1.421e-002	3.751e-003
ch2o	Gas	3.634e-003	9.595e-004
c2h4	Gas	2.643e-003	6.980e-004
chn	Gas	2.131e-003	5.627e-004
ch3oh	Gas	1.990e-003	5.255e-004
chno	Gas	1.328e-003	3.506e-004
ch3	Gas	2.302e-004	6.079e-005
c3h8	Gas	3.221e-005	8.505e-006
c2h2	Gas	2.491e-005	6.578e-006
c3h6	Gas	2.189e-005	5.781e-006
h	Gas	2.045e-005	5.399e-006
cho	Gas	1.525e-005	4.026e-006
h2n	Gas	4.165e-006	1.100e-006
ho	Gas	3.368e-006	8.893e-007
no	Gas	2.972e-007	7.848e-008
h4n2	Gas	5.891e-008	1.556e-008
c2n2	Gas	1.912e-008	5.050e-009
c3o2	Gas	1.579e-008	4.171e-009
h2n2	Gas	1.209e-008	3.194e-009
cno	Gas	8.734e-009	2.306e-009
ch2	Gas	3.128e-009	8.260e-010
c2h4o	Gas	2.403e-009	6.346e-010
hno	Gas	1.675e-009	4.423e-010
h2o2	Gas	1.624e-009	4.289e-010
cn	Gas	1.189e-009	3.140e-010
n2o	Gas	5.076e-010	1.340e-010
hn	Gas	3.585e-010	9.466e-011
c2h	Gas	2.322e-010	6.132e-011
o2	Gas	1.035e-010	2.732e-011
o	Gas	6.223e-011	1.643e-011
c2o	Gas	3.376e-011	8.915e-012
n	Gas	6.381e-012	1.685e-012
ho2	Gas	5.031e-012	1.329e-012
hno2	Gas	3.518e-012	9.290e-013
cn2	Gas	2.107e-012	5.565e-013
no2h	Gas	1.876e-012	4.954e-013
c2n	Gas	1.221e-012	3.223e-013
n3	Gas	3.624e-013	9.570e-014
no2	Gas	2.992e-013	7.901e-014
ch	Gas	6.667e-014	1.761e-014
cnn	Gas	3.764e-016	9.941e-017
c	Gas	1.942e-016	5.129e-017
c4n2	Gas	1.617e-017	4.270e-018
c3	Gas	3.570e-018	9.428e-019
hno3	Gas	2.182e-018	5.761e-019
c2	Gas	1.454e-018	3.840e-019
no3	Gas	3.242e-022	8.561e-023
o3	Gas	1.900e-022	5.017e-023
n2o3	Gas	7.372e-024	1.947e-024
c4	Gas	1.421e-024	3.752e-025
c5	Gas	7.107e-027	1.877e-027
n2o4	Gas	9.585e-030	2.531e-030
n2o5	Gas	5.118e-037	1.351e-037
*c	solid	7.292e+000	1.926e+000
*h2o	liquid	0.000e+000	0.000e+000
Total	Gas	3.317e+001	8.758e+000

Total Cond. 7.292e+000 1.926e+000

Reference state = reactants
H(R) = H- 9.68, E(R) = E- 9.66, 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)
1.)	13292.2	1.2391	1800.0	-445.24	-844.09	1.607	1.2028

Product concentrations

Name		(mol/kg)	(mol gas/mol explosive)
n2	Gas	1.063e+001	2.808e+000
co2	Gas	7.948e+000	2.099e+000
h2o	Gas	7.152e+000	1.889e+000
co	Gas	3.688e+000	9.738e-001
h2	Gas	2.035e+000	5.373e-001
ch4	Gas	1.460e+000	3.854e-001
h3n	Gas	2.187e-001	5.775e-002
ch2o2	Gas	1.566e-002	4.135e-003
c2h6	Gas	1.382e-002	3.649e-003
ch2o	Gas	3.522e-003	9.301e-004
c2h4	Gas	2.553e-003	6.742e-004
chn	Gas	2.095e-003	5.531e-004
ch3oh	Gas	1.900e-003	5.018e-004
chno	Gas	1.285e-003	3.394e-004
ch3	Gas	2.156e-004	5.694e-005
c3h8	Gas	3.142e-005	8.297e-006
c2h2	Gas	2.361e-005	6.235e-006
c3h6	Gas	2.141e-005	5.653e-006
h	Gas	1.898e-005	5.011e-006
cho	Gas	1.421e-005	3.752e-006
h2n	Gas	3.795e-006	1.002e-006
ho	Gas	3.055e-006	8.068e-007
no	Gas	2.616e-007	6.907e-008
h4n2	Gas	5.222e-008	1.379e-008
c2n2	Gas	1.795e-008	4.739e-009
c3o2	Gas	1.535e-008	4.054e-009
h2n2	Gas	1.065e-008	2.812e-009
cno	Gas	7.554e-009	1.995e-009
ch2	Gas	2.696e-009	7.120e-010
c2h4o	Gas	2.267e-009	5.987e-010
hno	Gas	1.463e-009	3.864e-010
h2o2	Gas	1.385e-009	3.658e-010
cn	Gas	1.034e-009	2.730e-010
n2o	Gas	4.457e-010	1.177e-010
hn	Gas	3.089e-010	8.157e-011
c2h	Gas	2.025e-010	5.347e-011
o2	Gas	8.593e-011	2.269e-011
o	Gas	5.178e-011	1.367e-011
c2o	Gas	2.986e-011	7.885e-012
n	Gas	5.297e-012	1.399e-012
ho2	Gas	4.161e-012	1.099e-012
hno2	Gas	2.996e-012	7.911e-013
cn2	Gas	1.764e-012	4.658e-013
no2h	Gas	1.619e-012	4.274e-013
c2n	Gas	1.039e-012	2.744e-013
n3	Gas	3.015e-013	7.962e-014
no2	Gas	2.421e-013	6.393e-014
ch	Gas	5.396e-014	1.425e-014
cnn	Gas	3.087e-016	8.152e-017
c	Gas	1.507e-016	3.979e-017
c4n2	Gas	1.626e-017	4.294e-018
c3	Gas	2.827e-018	7.465e-019
hno3	Gas	1.687e-018	4.454e-019
c2	Gas	1.092e-018	2.884e-019
no3	Gas	2.278e-022	6.016e-023
o3	Gas	1.347e-022	3.558e-023
n2o3	Gas	5.283e-024	1.395e-024
c4	Gas	1.113e-024	2.940e-025

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       c5  Gas   6.054e-027  1.599e-027
     n2o4  Gas   6.086e-030  1.607e-030
     n2o5  Gas   2.975e-037  7.857e-038
       *c  solid 7.278e+000  1.922e+000
     *h2o liquid 0.000e+000  0.000e+000

     Total Gas   3.318e+001  8.761e+000
     Total Cond. 7.278e+000  1.922e+000

                          Reference state = reactants
                H(R) = H- 9.68, E(R) = E- 9.66, S(R) = S- 0.00

          P          V         T       H(R)      E(R)      S(R)      VGS
       (ATM)      (CC/GM)     (K)    (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)  3365.0      2.2829   1373.4   -824.22  -1010.25    1.607    2.2463

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*      n2  Gas   1.063e+001  2.808e+000
*     co2  Gas   7.948e+000  2.099e+000
*     h2o  Gas   7.152e+000  1.889e+000
*      co  Gas   3.688e+000  9.738e-001
*      h2  Gas   2.035e+000  5.373e-001
*     ch4  Gas   1.460e+000  3.854e-001
*     h3n  Gas   2.187e-001  5.775e-002
*   ch2o2  Gas   1.566e-002  4.135e-003
*    c2h6  Gas   1.382e-002  3.649e-003
*    ch2o  Gas   3.522e-003  9.301e-004
*    c2h4  Gas   2.553e-003  6.742e-004
*     chn  Gas   2.095e-003  5.531e-004
*   ch3oh  Gas   1.900e-003  5.018e-004
*    chno  Gas   1.285e-003  3.394e-004
*     ch3  Gas   2.156e-004  5.694e-005
*    c3h8  Gas   3.142e-005  8.297e-006
*    c2h2  Gas   2.361e-005  6.235e-006
*    c3h6  Gas   2.141e-005  5.653e-006
*       h  Gas   1.898e-005  5.011e-006
*     cho  Gas   1.421e-005  3.752e-006
*     h2n  Gas   3.795e-006  1.002e-006
*      ho  Gas   3.055e-006  8.068e-007
*      no  Gas   2.616e-007  6.907e-008
*    h4n2  Gas   5.222e-008  1.379e-008
*    c2n2  Gas   1.795e-008  4.739e-009
*    c3o2  Gas   1.535e-008  4.054e-009
*    h2n2  Gas   1.065e-008  2.812e-009
*     cno  Gas   7.554e-009  1.995e-009
*     ch2  Gas   2.696e-009  7.120e-010
*   c2h4o  Gas   2.267e-009  5.987e-010
*     hno  Gas   1.463e-009  3.864e-010
*    h2o2  Gas   1.385e-009  3.658e-010
*      cn  Gas   1.034e-009  2.730e-010
*     n2o  Gas   4.457e-010  1.177e-010
*      hn  Gas   3.089e-010  8.157e-011
*     c2h  Gas   2.025e-010  5.347e-011
*      o2  Gas   8.593e-011  2.269e-011
*       o  Gas   5.178e-011  1.367e-011
*     c2o  Gas   2.986e-011  7.885e-012
*       n  Gas   5.297e-012  1.399e-012
*     ho2  Gas   4.161e-012  1.099e-012
*    hno2  Gas   2.996e-012  7.911e-013
*     cn2  Gas   1.764e-012  4.658e-013
*    no2h  Gas   1.619e-012  4.274e-013
*     c2n  Gas   1.039e-012  2.744e-013
*      n3  Gas   3.015e-013  7.962e-014
*     no2  Gas   2.421e-013  6.393e-014
*      ch  Gas   5.396e-014  1.425e-014
*     cnn  Gas   3.087e-016  8.152e-017
*       c  Gas   1.507e-016  3.979e-017
*    c4n2  Gas   1.626e-017  4.294e-018
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*       c3  Gas   2.827e-018  7.465e-019
*     hno3  Gas   1.687e-018  4.454e-019
*       c2  Gas   1.092e-018  2.884e-019
*      no3  Gas   2.278e-022  6.016e-023
*       o3  Gas   1.347e-022  3.558e-023
*     n2o3  Gas   5.283e-024  1.395e-024
*       c4  Gas   1.113e-024  2.940e-025
*       c5  Gas   6.054e-027  1.599e-027
*     n2o4  Gas   6.086e-030  1.607e-030
*     n2o5  Gas   2.975e-037  7.857e-038
*       *c  solid 7.278e+000  1.922e+000
*     *h2o liquid 0.000e+000  0.000e+000

      Total Gas   3.318e+001  8.761e+000
      Total Cond. 7.278e+000  1.922e+000

                          Reference state = reactants
                H(R) = H- 9.68, E(R) = E- 9.66, S(R) = S- 0.00

          P           V         T       H(R)       E(R)       S(R)      VGS
       (ATM)       (CC/GM)     (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)    1419.0      3.6192   1171.1   -955.77  -1080.13    1.607    3.5826

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.063e+001  2.808e+000
*      co2  Gas   7.948e+000  2.099e+000
*      h2o  Gas   7.152e+000  1.889e+000
*       co  Gas   3.688e+000  9.738e-001
*       h2  Gas   2.035e+000  5.373e-001
*      ch4  Gas   1.460e+000  3.854e-001
*      h3n  Gas   2.187e-001  5.775e-002
*    ch2o2  Gas   1.566e-002  4.135e-003
*     c2h6  Gas   1.382e-002  3.649e-003
*     ch2o  Gas   3.522e-003  9.301e-004
*     c2h4  Gas   2.553e-003  6.742e-004
*      chn  Gas   2.095e-003  5.531e-004
*    ch3oh  Gas   1.900e-003  5.018e-004
*     chno  Gas   1.285e-003  3.394e-004
*      ch3  Gas   2.156e-004  5.694e-005
*     c3h8  Gas   3.142e-005  8.297e-006
*     c2h2  Gas   2.361e-005  6.235e-006
*     c3h6  Gas   2.141e-005  5.653e-006
*        h  Gas   1.898e-005  5.011e-006
*      cho  Gas   1.421e-005  3.752e-006
*      h2n  Gas   3.795e-006  1.002e-006
*       ho  Gas   3.055e-006  8.068e-007
*       no  Gas   2.616e-007  6.907e-008
*     h4n2  Gas   5.222e-008  1.379e-008
*     c2n2  Gas   1.795e-008  4.739e-009
*     c3o2  Gas   1.535e-008  4.054e-009
*     h2n2  Gas   1.065e-008  2.812e-009
*      cno  Gas   7.554e-009  1.995e-009
*      ch2  Gas   2.696e-009  7.120e-010
*    c2h4o  Gas   2.267e-009  5.987e-010
*      hno  Gas   1.463e-009  3.864e-010
*     h2o2  Gas   1.385e-009  3.658e-010
*       cn  Gas   1.034e-009  2.730e-010
*      n2o  Gas   4.457e-010  1.177e-010
*       hn  Gas   3.089e-010  8.157e-011
*      c2h  Gas   2.025e-010  5.347e-011
*       o2  Gas   8.593e-011  2.269e-011
*        o  Gas   5.178e-011  1.367e-011
*      c2o  Gas   2.986e-011  7.885e-012
*        n  Gas   5.297e-012  1.399e-012
*      ho2  Gas   4.161e-012  1.099e-012
*     hno2  Gas   2.996e-012  7.911e-013
*      cn2  Gas   1.764e-012  4.658e-013
*     no2h  Gas   1.619e-012  4.274e-013
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*      c2n  Gas   1.039e-012  2.744e-013
*       n3  Gas   3.015e-013  7.962e-014
*      no2  Gas   2.421e-013  6.393e-014
*       ch  Gas   5.396e-014  1.425e-014
*      cnn  Gas   3.087e-016  8.152e-017
*        c  Gas   1.507e-016  3.979e-017
*     c4n2  Gas   1.626e-017  4.294e-018
*       c3  Gas   2.827e-018  7.465e-019
*     hno3  Gas   1.687e-018  4.454e-019
*       c2  Gas   1.092e-018  2.884e-019
*      no3  Gas   2.278e-022  6.016e-023
*       o3  Gas   1.347e-022  3.558e-023
*     n2o3  Gas   5.283e-024  1.395e-024
*       c4  Gas   1.113e-024  2.940e-025
*       c5  Gas   6.054e-027  1.599e-027
*     n2o4  Gas   6.086e-030  1.607e-030
*     n2o5  Gas   2.975e-037  7.857e-038
*       *c  solid 7.278e+000  1.922e+000
*     *h2o liquid 0.000e+000  0.000e+000

      Total Gas   3.318e+001  8.761e+000
      Total Cond. 7.278e+000  1.922e+000

                              Reference state = reactants
                    H(R) = H- 9.68, E(R) = E- 9.66, S(R) = S- 0.00

          P           V         T       H(R)       E(R)       S(R)      VGS
       (ATM)       (CC/GM)     (K)     (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)    692.2       5.5680   1027.6   -1033.10   -1126.43    1.607     5.5314

Product concentrations
          Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.063e+001  2.808e+000
*      co2  Gas   7.948e+000  2.099e+000
*      h2o  Gas   7.152e+000  1.889e+000
*       co  Gas   3.688e+000  9.738e-001
*       h2  Gas   2.035e+000  5.373e-001
*      ch4  Gas   1.460e+000  3.854e-001
*      h3n  Gas   2.187e-001  5.775e-002
*    ch2o2  Gas   1.566e-002  4.135e-003
*     c2h6  Gas   1.382e-002  3.649e-003
*     ch2o  Gas   3.522e-003  9.301e-004
*     c2h4  Gas   2.553e-003  6.742e-004
*      chn  Gas   2.095e-003  5.531e-004
*    ch3oh  Gas   1.900e-003  5.018e-004
*     chno  Gas   1.285e-003  3.394e-004
*      ch3  Gas   2.156e-004  5.694e-005
*     c3h8  Gas   3.142e-005  8.297e-006
*     c2h2  Gas   2.361e-005  6.235e-006
*     c3h6  Gas   2.141e-005  5.653e-006
*        h  Gas   1.898e-005  5.011e-006
*      cho  Gas   1.421e-005  3.752e-006
*      h2n  Gas   3.795e-006  1.002e-006
*       ho  Gas   3.055e-006  8.068e-007
*       no  Gas   2.616e-007  6.907e-008
*     h4n2  Gas   5.222e-008  1.379e-008
*     c2n2  Gas   1.795e-008  4.739e-009
*     c3o2  Gas   1.535e-008  4.054e-009
*     h2n2  Gas   1.065e-008  2.812e-009
*      cno  Gas   7.554e-009  1.995e-009
*      ch2  Gas   2.696e-009  7.120e-010
*    c2h4o  Gas   2.267e-009  5.987e-010
*      hno  Gas   1.463e-009  3.864e-010
*     h2o2  Gas   1.385e-009  3.658e-010
*       cn  Gas   1.034e-009  2.730e-010
*      n2o  Gas   4.457e-010  1.177e-010
*       hn  Gas   3.089e-010  8.157e-011
*      c2h  Gas   2.025e-010  5.347e-011
*       o2  Gas   8.593e-011  2.269e-011
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*       o  Gas   5.178e-011  1.367e-011
*     c2o  Gas   2.986e-011  7.885e-012
*       n  Gas   5.297e-012  1.399e-012
*     ho2  Gas   4.161e-012  1.099e-012
*    hno2  Gas   2.996e-012  7.911e-013
*     cn2  Gas   1.764e-012  4.658e-013
*    no2h  Gas   1.619e-012  4.274e-013
*     c2n  Gas   1.039e-012  2.744e-013
*      n3  Gas   3.015e-013  7.962e-014
*     no2  Gas   2.421e-013  6.393e-014
*      ch  Gas   5.396e-014  1.425e-014
*     cnn  Gas   3.087e-016  8.152e-017
*       c  Gas   1.507e-016  3.979e-017
*    c4n2  Gas   1.626e-017  4.294e-018
*      c3  Gas   2.827e-018  7.465e-019
*    hno3  Gas   1.687e-018  4.454e-019
*      c2  Gas   1.092e-018  2.884e-019
*     no3  Gas   2.278e-022  6.016e-023
*      o3  Gas   1.347e-022  3.558e-023
*    n2o3  Gas   5.283e-024  1.395e-024
*      c4  Gas   1.113e-024  2.940e-025
*      c5  Gas   6.054e-027  1.599e-027
*    n2o4  Gas   6.086e-030  1.607e-030
*    n2o5  Gas   2.975e-037  7.857e-038
*      *c  solid 7.278e+000  1.922e+000
*    *h2o liquid 0.000e+000  0.000e+000

     Total Gas   3.318e+001  8.761e+000
     Total Cond. 7.278e+000  1.922e+000


                          Reference state = reactants
                H(R) = H- 9.68, E(R) = E- 9.66, S(R) = S- 0.00

          P           V          T       H(R)       E(R)       S(R)      VGS
        (ATM)       (CC/GM)     (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)    244.8      11.1360    848.0  -1114.61   -1180.62    1.607    11.0994

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*      n2  Gas   1.063e+001  2.808e+000
*     co2  Gas   7.948e+000  2.099e+000
*     h2o  Gas   7.152e+000  1.889e+000
*      co  Gas   3.688e+000  9.738e-001
*      h2  Gas   2.035e+000  5.373e-001
*     ch4  Gas   1.460e+000  3.854e-001
*     h3n  Gas   2.187e-001  5.775e-002
*   ch2o2  Gas   1.566e-002  4.135e-003
*    c2h6  Gas   1.382e-002  3.649e-003
*    ch2o  Gas   3.522e-003  9.301e-004
*    c2h4  Gas   2.553e-003  6.742e-004
*     chn  Gas   2.095e-003  5.531e-004
*   ch3oh  Gas   1.900e-003  5.018e-004
*    chno  Gas   1.285e-003  3.394e-004
*     ch3  Gas   2.156e-004  5.694e-005
*    c3h8  Gas   3.142e-005  8.297e-006
*    c2h2  Gas   2.361e-005  6.235e-006
*    c3h6  Gas   2.141e-005  5.653e-006
*       h  Gas   1.898e-005  5.011e-006
*     cho  Gas   1.421e-005  3.752e-006
*     h2n  Gas   3.795e-006  1.002e-006
*      ho  Gas   3.055e-006  8.068e-007
*      no  Gas   2.616e-007  6.907e-008
*    h4n2  Gas   5.222e-008  1.379e-008
*    c2n2  Gas   1.795e-008  4.739e-009
*    c3o2  Gas   1.535e-008  4.054e-009
*    h2n2  Gas   1.065e-008  2.812e-009
*     cno  Gas   7.554e-009  1.995e-009
*     ch2  Gas   2.696e-009  7.120e-010
```

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*    c2h4o  Gas    2.267e-009  5.987e-010
*      hno  Gas    1.463e-009  3.864e-010
*     h2o2  Gas    1.385e-009  3.658e-010
*       cn  Gas    1.034e-009  2.730e-010
*      n2o  Gas    4.457e-010  1.177e-010
*       hn  Gas    3.089e-010  8.157e-011
*      c2h  Gas    2.025e-010  5.347e-011
*       o2  Gas    8.593e-011  2.269e-011
*        o  Gas    5.178e-011  1.367e-011
*      c2o  Gas    2.986e-011  7.885e-012
*        n  Gas    5.297e-012  1.399e-012
*      ho2  Gas    4.161e-012  1.099e-012
*     hno2  Gas    2.996e-012  7.911e-013
*      cn2  Gas    1.764e-012  4.658e-013
*     no2h  Gas    1.619e-012  4.274e-013
*      c2n  Gas    1.039e-012  2.744e-013
*       n3  Gas    3.015e-013  7.962e-014
*      no2  Gas    2.421e-013  6.393e-014
*       ch  Gas    5.396e-014  1.425e-014
*      cnn  Gas    3.087e-016  8.152e-017
*        c  Gas    1.507e-016  3.979e-017
*     c4n2  Gas    1.626e-017  4.294e-018
*       c3  Gas    2.827e-018  7.465e-019
*     hno3  Gas    1.687e-018  4.454e-019
*       c2  Gas    1.092e-018  2.884e-019
*      no3  Gas    2.278e-022  6.016e-023
*       o3  Gas    1.347e-022  3.558e-023
*     n2o3  Gas    5.283e-024  1.395e-024
*       c4  Gas    1.113e-024  2.940e-025
*       c5  Gas    6.054e-027  1.599e-027
*     n2o4  Gas    6.086e-030  1.607e-030
*     n2o5  Gas    2.975e-037  7.857e-038
*       *c  solid  7.278e+000  1.922e+000
*     *h2o liquid  0.000e+000  0.000e+000

      Total Gas    3.318e+001  8.761e+000
      Total Cond.  7.278e+000  1.922e+000

                          Reference state = reactants
                 H(R) = H- 9.68, E(R) = E- 9.66, S(R) = S- 0.00

          P          V         T       H(R)       E(R)       S(R)      VGS
       (ATM)      (CC/GM)     (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)    93.9     22.2719    705.2  -1170.02   -1220.63     1.607    22.2354

Product concentrations
         Name    (mol/kg) (mol gas/mol explosive)
*       n2  Gas    1.063e+001  2.808e+000
*      co2  Gas    7.948e+000  2.099e+000
*      h2o  Gas    7.152e+000  1.889e+000
*       co  Gas    3.688e+000  9.738e-001
*       h2  Gas    2.035e+000  5.373e-001
*      ch4  Gas    1.460e+000  3.854e-001
*      h3n  Gas    2.187e-001  5.775e-002
*    ch2o2  Gas    1.566e-002  4.135e-003
*     c2h6  Gas    1.382e-002  3.649e-003
*     ch2o  Gas    3.522e-003  9.301e-004
*     c2h4  Gas    2.553e-003  6.742e-004
*      chn  Gas    2.095e-003  5.531e-004
*    ch3oh  Gas    1.900e-003  5.018e-004
*     chno  Gas    1.285e-003  3.394e-004
*      ch3  Gas    2.156e-004  5.694e-005
*     c3h8  Gas    3.142e-005  8.297e-006
*     c2h2  Gas    2.361e-005  6.235e-006
*     c3h6  Gas    2.141e-005  5.653e-006
*        h  Gas    1.898e-005  5.011e-006
*      cho  Gas    1.421e-005  3.752e-006
*      h2n  Gas    3.795e-006  1.002e-006
*       ho  Gas    3.055e-006  8.068e-007
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*       no  Gas   2.616e-007  6.907e-008
*     h4n2  Gas   5.222e-008  1.379e-008
*     c2n2  Gas   1.795e-008  4.739e-009
*     c3o2  Gas   1.535e-008  4.054e-009
*     h2n2  Gas   1.065e-008  2.812e-009
*      cno  Gas   7.554e-009  1.995e-009
*      ch2  Gas   2.696e-009  7.120e-010
*    c2h4o  Gas   2.267e-009  5.987e-010
*      hno  Gas   1.463e-009  3.864e-010
*     h2o2  Gas   1.385e-009  3.658e-010
*       cn  Gas   1.034e-009  2.730e-010
*      n2o  Gas   4.457e-010  1.177e-010
*       hn  Gas   3.089e-010  8.157e-011
*      c2h  Gas   2.025e-010  5.347e-011
*       o2  Gas   8.593e-011  2.269e-011
*        o  Gas   5.178e-011  1.367e-011
*      c2o  Gas   2.986e-011  7.885e-012
*        n  Gas   5.297e-012  1.399e-012
*      ho2  Gas   4.161e-012  1.099e-012
*     hno2  Gas   2.996e-012  7.911e-013
*      cn2  Gas   1.764e-012  4.658e-013
*     no2h  Gas   1.619e-012  4.274e-013
*      c2n  Gas   1.039e-012  2.744e-013
*       n3  Gas   3.015e-013  7.962e-014
*      no2  Gas   2.421e-013  6.393e-014
*       ch  Gas   5.396e-014  1.425e-014
*      cnn  Gas   3.087e-016  8.152e-017
*        c  Gas   1.507e-016  3.979e-017
*     c4n2  Gas   1.626e-017  4.294e-018
*       c3  Gas   2.827e-018  7.465e-019
*     hno3  Gas   1.687e-018  4.454e-019
*       c2  Gas   1.092e-018  2.884e-019
*      no3  Gas   2.278e-022  6.016e-023
*       o3  Gas   1.347e-022  3.558e-023
*     n2o3  Gas   5.283e-024  1.395e-024
*       c4  Gas   1.113e-024  2.940e-025
*       c5  Gas   6.054e-027  1.599e-027
*     n2o4  Gas   6.086e-030  1.607e-030
*     n2o5  Gas   2.975e-037  7.857e-038
*       *c  solid 7.278e+000  1.922e+000
*     *h2o liquid 0.000e+000  0.000e+000

      Total Gas   3.318e+001  8.761e+000
      Total Cond. 7.278e+000  1.922e+000

                          Reference state = reactants
                 H(R) = H- 9.68, E(R) = E- 9.66, S(R) = S- 0.00

          P           V         T       H(R)       E(R)       S(R)      VGS
       (ATM)      (CC/GM)      (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)    37.4     44.5439    585.4  -1211.66  -1251.94    1.607   44.5074

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.063e+001  2.808e+000
*      co2  Gas   7.948e+000  2.099e+000
*      h2o  Gas   7.152e+000  1.889e+000
*       co  Gas   3.688e+000  9.738e-001
*       h2  Gas   2.035e+000  5.373e-001
*      ch4  Gas   1.460e+000  3.854e-001
*      h3n  Gas   2.187e-001  5.775e-002
*    ch2o2  Gas   1.566e-002  4.135e-003
*     c2h6  Gas   1.382e-002  3.649e-003
*     ch2o  Gas   3.522e-003  9.301e-004
*     c2h4  Gas   2.553e-003  6.742e-004
*      chn  Gas   2.095e-003  5.531e-004
*    ch3oh  Gas   1.900e-003  5.018e-004
*     chno  Gas   1.285e-003  3.394e-004
*      ch3  Gas   2.156e-004  5.694e-005
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*     c3h8  Gas   3.142e-005  8.297e-006
*     c2h2  Gas   2.361e-005  6.235e-006
*     c3h6  Gas   2.141e-005  5.653e-006
*        h  Gas   1.898e-005  5.011e-006
*      cho  Gas   1.421e-005  3.752e-006
*      h2n  Gas   3.795e-006  1.002e-006
*       ho  Gas   3.055e-006  8.068e-007
*       no  Gas   2.616e-007  6.907e-008
*     h4n2  Gas   5.222e-008  1.379e-008
*     c2n2  Gas   1.795e-008  4.739e-009
*     c3o2  Gas   1.535e-008  4.054e-009
*     h2n2  Gas   1.065e-008  2.812e-009
*      cno  Gas   7.554e-009  1.995e-009
*      ch2  Gas   2.696e-009  7.120e-010
*    c2h4o  Gas   2.267e-009  5.987e-010
*      hno  Gas   1.463e-009  3.864e-010
*     h2o2  Gas   1.385e-009  3.658e-010
*       cn  Gas   1.034e-009  2.730e-010
*      n2o  Gas   4.457e-010  1.177e-010
*       hn  Gas   3.089e-010  8.157e-011
*      c2h  Gas   2.025e-010  5.347e-011
*       o2  Gas   8.593e-011  2.269e-011
*        o  Gas   5.178e-011  1.367e-011
*      c2o  Gas   2.986e-011  7.885e-012
*        n  Gas   5.297e-012  1.399e-012
*      ho2  Gas   4.161e-012  1.099e-012
*     hno2  Gas   2.996e-012  7.911e-013
*      cn2  Gas   1.764e-012  4.658e-013
*     no2h  Gas   1.619e-012  4.274e-013
*      c2n  Gas   1.039e-012  2.744e-013
*       n3  Gas   3.015e-013  7.962e-014
*      no2  Gas   2.421e-013  6.393e-014
*       ch  Gas   5.396e-014  1.425e-014
*      cnn  Gas   3.087e-016  8.152e-017
*        c  Gas   1.507e-016  3.979e-017
*     c4n2  Gas   1.626e-017  4.294e-018
*       c3  Gas   2.827e-018  7.465e-019
*     hno3  Gas   1.687e-018  4.454e-019
*       c2  Gas   1.092e-018  2.884e-019
*      no3  Gas   2.278e-022  6.016e-023
*       o3  Gas   1.347e-022  3.558e-023
*     n2o3  Gas   5.283e-024  1.395e-024
*       c4  Gas   1.113e-024  2.940e-025
*       c5  Gas   6.054e-027  1.599e-027
*     n2o4  Gas   6.086e-030  1.607e-030
*     n2o5  Gas   2.975e-037  7.857e-038
*       *c  solid 7.278e+000  1.922e+000
*     *h2o liquid 0.000e+000  0.000e+000

      Total Gas   3.318e+001  8.761e+000
      Total Cond. 7.278e+000  1.922e+000

                          Reference state = reactants
                 H(R) = H- 9.68, E(R) = E- 9.66, S(R) = S- 0.00

          P          V         T       H(R)      E(R)      S(R)      VGS
       (ATM)      (CC/GM)     (K)    (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)    15.1     89.0878    482.5  -1244.57  -1277.07    1.607   89.0513

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.063e+001  2.808e+000
*      co2  Gas   7.948e+000  2.099e+000
*      h2o  Gas   7.152e+000  1.889e+000
*       co  Gas   3.688e+000  9.738e-001
*       h2  Gas   2.035e+000  5.373e-001
*      ch4  Gas   1.460e+000  3.854e-001
*      h3n  Gas   2.187e-001  5.775e-002
*    ch2o2  Gas   1.566e-002  4.135e-003
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*     c2h6  Gas    1.382e-002  3.649e-003
*     ch2o  Gas    3.522e-003  9.301e-004
*     c2h4  Gas    2.553e-003  6.742e-004
*      chn  Gas    2.095e-003  5.531e-004
*    ch3oh  Gas    1.900e-003  5.018e-004
*     chno  Gas    1.285e-003  3.394e-004
*      ch3  Gas    2.156e-004  5.694e-005
*     c3h8  Gas    3.142e-005  8.297e-006
*     c2h2  Gas    2.361e-005  6.235e-006
*     c3h6  Gas    2.141e-005  5.653e-006
*        h  Gas    1.898e-005  5.011e-006
*      cho  Gas    1.421e-005  3.752e-006
*      h2n  Gas    3.795e-006  1.002e-006
*       ho  Gas    3.055e-006  8.068e-007
*       no  Gas    2.616e-007  6.907e-008
*     h4n2  Gas    5.222e-008  1.379e-008
*     c2n2  Gas    1.795e-008  4.739e-009
*     c3o2  Gas    1.535e-008  4.054e-009
*     h2n2  Gas    1.065e-008  2.812e-009
*      cno  Gas    7.554e-009  1.995e-009
*      ch2  Gas    2.696e-009  7.120e-010
*    c2h4o  Gas    2.267e-009  5.987e-010
*      hno  Gas    1.463e-009  3.864e-010
*     h2o2  Gas    1.385e-009  3.658e-010
*       cn  Gas    1.034e-009  2.730e-010
*      n2o  Gas    4.457e-010  1.177e-010
*       hn  Gas    3.089e-010  8.157e-011
*      c2h  Gas    2.025e-010  5.347e-011
*       o2  Gas    8.593e-011  2.269e-011
*        o  Gas    5.178e-011  1.367e-011
*      c2o  Gas    2.986e-011  7.885e-012
*        n  Gas    5.297e-012  1.399e-012
*      ho2  Gas    4.161e-012  1.099e-012
*     hno2  Gas    2.996e-012  7.911e-013
*      cn2  Gas    1.764e-012  4.658e-013
*     no2h  Gas    1.619e-012  4.274e-013
*      c2n  Gas    1.039e-012  2.744e-013
*       n3  Gas    3.015e-013  7.962e-014
*      no2  Gas    2.421e-013  6.393e-014
*       ch  Gas    5.396e-014  1.425e-014
*      cnn  Gas    3.087e-016  8.152e-017
*        c  Gas    1.507e-016  3.979e-017
*     c4n2  Gas    1.626e-017  4.294e-018
*       c3  Gas    2.827e-018  7.465e-019
*     hno3  Gas    1.687e-018  4.454e-019
*       c2  Gas    1.092e-018  2.884e-019
*      no3  Gas    2.278e-022  6.016e-023
*       o3  Gas    1.347e-022  3.558e-023
*     n2o3  Gas    5.283e-024  1.395e-024
*       c4  Gas    1.113e-024  2.940e-025
*       c5  Gas    6.054e-027  1.599e-027
*     n2o4  Gas    6.086e-030  1.607e-030
*     n2o5  Gas    2.975e-037  7.857e-038
*       *c  solid  7.278e+000  1.922e+000
*     *h2o liquid  0.000e+000  0.000e+000

      Total Gas    3.318e+001  8.761e+000
      Total Cond.  7.278e+000  1.922e+000

                          The End of the Adiabat

                          Reference state = reactants
                H(R) = H- 9.68, E(R) = E- 9.66, S(R) = S- 0.00

          P           V         T       H(R)       E(R)       S(R)      VGS
       (ATM)       (CC/GM)     (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)     1.9     438.6719    298.0   -1298.25   -1317.97     1.607   438.6354

Product concentrations
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	Name		(mol/kg)	(mol gas/mol explosive)
*	n2	Gas	1.063e+001	2.808e+000
*	co2	Gas	7.948e+000	2.099e+000
*	h2o	Gas	7.152e+000	1.889e+000
*	co	Gas	3.688e+000	9.738e-001
*	h2	Gas	2.035e+000	5.373e-001
*	ch4	Gas	1.460e+000	3.854e-001
*	h3n	Gas	2.187e-001	5.775e-002
*	ch2o2	Gas	1.566e-002	4.135e-003
*	c2h6	Gas	1.382e-002	3.649e-003
*	ch2o	Gas	3.522e-003	9.301e-004
*	c2h4	Gas	2.553e-003	6.742e-004
*	chn	Gas	2.095e-003	5.531e-004
*	ch3oh	Gas	1.900e-003	5.018e-004
*	chno	Gas	1.285e-003	3.394e-004
*	ch3	Gas	2.156e-004	5.694e-005
*	c3h8	Gas	3.142e-005	8.297e-006
*	c2h2	Gas	2.361e-005	6.235e-006
*	c3h6	Gas	2.141e-005	5.653e-006
*	h	Gas	1.898e-005	5.011e-006
*	cho	Gas	1.421e-005	3.752e-006
*	h2n	Gas	3.795e-006	1.002e-006
*	ho	Gas	3.055e-006	8.068e-007
*	no	Gas	2.616e-007	6.907e-008
*	h4n2	Gas	5.222e-008	1.379e-008
*	c2n2	Gas	1.795e-008	4.739e-009
*	c3o2	Gas	1.535e-008	4.054e-009
*	h2n2	Gas	1.065e-008	2.812e-009
*	cno	Gas	7.554e-009	1.995e-009
*	ch2	Gas	2.696e-009	7.120e-010
*	c2h4o	Gas	2.267e-009	5.987e-010
*	hno	Gas	1.463e-009	3.864e-010
*	h2o2	Gas	1.385e-009	3.658e-010
*	cn	Gas	1.034e-009	2.730e-010
*	n2o	Gas	4.457e-010	1.177e-010
*	hn	Gas	3.089e-010	8.157e-011
*	c2h	Gas	2.025e-010	5.347e-011
*	o2	Gas	8.593e-011	2.269e-011
*	o	Gas	5.178e-011	1.367e-011
*	c2o	Gas	2.986e-011	7.885e-012
*	n	Gas	5.297e-012	1.399e-012
*	ho2	Gas	4.161e-012	1.099e-012
*	hno2	Gas	2.996e-012	7.911e-013
*	cn2	Gas	1.764e-012	4.658e-013
*	no2h	Gas	1.619e-012	4.274e-013
*	c2n	Gas	1.039e-012	2.744e-013
*	n3	Gas	3.015e-013	7.962e-014
*	no2	Gas	2.421e-013	6.393e-014
*	ch	Gas	5.396e-014	1.425e-014
*	cnn	Gas	3.087e-016	8.152e-017
*	c	Gas	1.507e-016	3.979e-017
*	c4n2	Gas	1.626e-017	4.294e-018
*	c3	Gas	2.827e-018	7.465e-019
*	hno3	Gas	1.687e-018	4.454e-019
*	c2	Gas	1.092e-018	2.884e-019
*	no3	Gas	2.278e-022	6.016e-023
*	o3	Gas	1.347e-022	3.558e-023
*	n2o3	Gas	5.283e-024	1.395e-024
*	c4	Gas	1.113e-024	2.940e-025
*	c5	Gas	6.054e-027	1.599e-027
*	n2o4	Gas	6.086e-030	1.607e-030
*	n2o5	Gas	2.975e-037	7.857e-038
*	*c	solid	7.278e+000	1.922e+000
*	*h2o	liquid	0.000e+000	0.000e+000
	Total	Gas	3.318e+001	8.761e+000
	Total	Cond.	7.278e+000	1.922e+000

The Products at room temperature and pressure

Reference state = reactants
H(R) = H- 9.68, E(R) = E- 9.66, 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)
1.)	1.0	813.2297	298.0	-1298.29	-1317.97	1.648	813.1933

Product concentrations

	Name		(mol/kg)	(mol gas/mol explosive)
*	n2	Gas	1.063e+001	2.808e+000
*	co2	Gas	7.948e+000	2.099e+000
*	h2o	Gas	7.152e+000	1.889e+000
*	co	Gas	3.688e+000	9.738e-001
*	h2	Gas	2.035e+000	5.373e-001
*	ch4	Gas	1.460e+000	3.854e-001
*	h3n	Gas	2.187e-001	5.775e-002
*	ch2o2	Gas	1.566e-002	4.135e-003
*	c2h6	Gas	1.382e-002	3.649e-003
*	ch2o	Gas	3.522e-003	9.301e-004
*	c2h4	Gas	2.553e-003	6.742e-004
*	chn	Gas	2.095e-003	5.531e-004
*	ch3oh	Gas	1.900e-003	5.018e-004
*	chno	Gas	1.285e-003	3.394e-004
*	ch3	Gas	2.156e-004	5.694e-005
*	c3h8	Gas	3.142e-005	8.297e-006
*	c2h2	Gas	2.361e-005	6.235e-006
*	c3h6	Gas	2.141e-005	5.653e-006
*	h	Gas	1.898e-005	5.011e-006
*	cho	Gas	1.421e-005	3.752e-006
*	h2n	Gas	3.795e-006	1.002e-006
*	ho	Gas	3.055e-006	8.068e-007
*	no	Gas	2.616e-007	6.907e-008
*	h4n2	Gas	5.222e-008	1.379e-008
*	c2n2	Gas	1.795e-008	4.739e-009
*	c3o2	Gas	1.535e-008	4.054e-009
*	h2n2	Gas	1.065e-008	2.812e-009
*	cno	Gas	7.554e-009	1.995e-009
*	ch2	Gas	2.696e-009	7.120e-010
*	c2h4o	Gas	2.267e-009	5.987e-010
*	hno	Gas	1.463e-009	3.864e-010
*	h2o2	Gas	1.385e-009	3.658e-010
*	cn	Gas	1.034e-009	2.730e-010
*	n2o	Gas	4.457e-010	1.177e-010
*	hn	Gas	3.089e-010	8.157e-011
*	c2h	Gas	2.025e-010	5.347e-011
*	o2	Gas	8.593e-011	2.269e-011
*	o	Gas	5.178e-011	1.367e-011
*	c2o	Gas	2.986e-011	7.885e-012
*	n	Gas	5.297e-012	1.399e-012
*	ho2	Gas	4.161e-012	1.099e-012
*	hno2	Gas	2.996e-012	7.911e-013
*	cn2	Gas	1.764e-012	4.658e-013
*	no2h	Gas	1.619e-012	4.274e-013
*	c2n	Gas	1.039e-012	2.744e-013
*	n3	Gas	3.015e-013	7.962e-014
*	no2	Gas	2.421e-013	6.393e-014
*	ch	Gas	5.396e-014	1.425e-014
*	cnn	Gas	3.087e-016	8.152e-017
*	c	Gas	1.507e-016	3.979e-017
*	c4n2	Gas	1.626e-017	4.294e-018
*	c3	Gas	2.827e-018	7.465e-019
*	hno3	Gas	1.687e-018	4.454e-019
*	c2	Gas	1.092e-018	2.884e-019
*	no3	Gas	2.278e-022	6.016e-023
*	o3	Gas	1.347e-022	3.558e-023
*	n2o3	Gas	5.283e-024	1.395e-024
*	c4	Gas	1.113e-024	2.940e-025
*	c5	Gas	6.054e-027	1.599e-027

```
*    n2o4  Gas   6.086e-030  1.607e-030
*    n2o5  Gas   2.975e-037  7.857e-038
*      *c  solid 7.278e+000  1.922e+000
*    *h2o liquid 0.000e+000  0.000e+000

     Total Gas   3.318e+001  8.761e+000
     Total Cond. 7.278e+000  1.922e+000
The mechanical energy of detonation =     -9.904 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.904 kJ/cc

JWL Tail Fit results:
Initial E0 =    -10.357, Final E0 =    -10.205
E0(V=infty) =    -10.205
C =      1.562,  omega =      0.377
Final fitting error = 0.002857

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

    10.000     -8.464     -8.466      0.070      0.066
    20.000     -8.872     -8.866      0.025      0.025
    40.000     -9.172     -9.174      0.010      0.010
    80.000     -9.408     -9.411      0.004      0.004
   160.000     -9.596     -9.594      0.002      0.001

JWL Fit results:
E0(V=infty) =    -10.205
R[1] =      4.927, R[2] =      1.110, omega =      0.377
A    =   1045.247, B    =     11.078, C     =      1.562
Final fitting error = 0.009668

     V/V0     Actual E     Fit E    Actual P      Fit P
              (kJ/cc)     (kJ/cc)    (GPa)        (GPa)
     0.765      3.555      3.555     30.211     31.159
     1.000     -1.123     -1.233     12.866     12.789
     2.200     -6.308     -6.254      1.386      1.512
     4.100     -7.591     -7.666      0.341      0.341
     6.500     -8.117     -8.152      0.144      0.127
    10.000     -8.464     -8.466      0.070      0.066
    20.000     -8.872     -8.866      0.025      0.025
    40.000     -9.172     -9.174      0.010      0.010
    80.000     -9.408     -9.411      0.004      0.004
   160.000     -9.596     -9.594      0.002      0.001
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
                                   The Composition
```

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
HMX	60.00	53.50	56.57	17866	155.47	0.000	296.17	$C_4H_8N_8O_8$
TNT	40.00	46.50	43.43	-15057	137.32	0.000	227.13	$C_7H_5N_3O_6$

```
Heat of formation =      9.677 cal/gm
Standard volume   =      0.557 cc/gm
Standard entropy  =      0.000 cal/k/gm
Standard energy   =      9.663 cal/gm

The elements and percent by mole
     c             21.803
     h             26.692
     n             22.933
     o             28.571
The average mol. wt. = 264.065 g/mol
```

A.2 Complete printout BKWC product library

```
Input>library file, bkwc.chl
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
Input>composition, hmx, 60, tnt, 40, weight
                                   The Composition
```

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
HMX	60.00	53.50	56.57	17866	155.47	0.000	296.17	$C_4H_8N_8O_8$
TNT	40.00	46.50	43.43	-15057	137.32	0.000	227.13	$C_7H_5N_3O_6$

```
Heat of formation =      9.677 cal/gm
Standard volume   =      0.557 cc/gm
Standard entropy  =      0.000 cal/k/gm
Standard energy   =      9.663 cal/gm

The elements and percent by mole
     c             21.803
     h             26.692
     n             22.933
     o             28.571
The average mol. wt. = 264.065 g/mol
Input>gas eos, bkw
Input>standard run, rho, 1.795982
The initial damping was too small
Undertaking a gradient line search instead
Too many iterations in the etanewt solver
Failed to find equilibrium.  Will try again.
The hugoniot reference state:
P0 = 1.000000 ATM, V0 = 0.556798 cc/gm, E0 = 9.663045 cal/gm
Using  130705 ATM as a lower bound for the C-J pressure
Using  326763 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    =   8.21407e+003 m/s
The particle velocity =   2.04465e+003 m/s
The speed of sound    =   6.16942e+003 m/s

P0 =       1 atm, V0 =  0.55680 cc/gm, E0 =   9.66304 cal/gm

                          Reference state = reactants
                H(R) = H- 9.68, E(R) = E- 9.66, S(R) = S- 0.00

          P           V         T       H(R)       E(R)       S(R)      VGS
       (ATM)       (CC/GM)     (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)  297690.1      0.4182   3997.6   3514.60     499.61     1.643     0.3807

Product concentrations
         Name    (mol/kg) (mol gas/mol explosive)
      h2o  Gas   1.249e+001  3.299e+000
       n2  Gas   1.074e+001  2.837e+000
      co2  Gas   6.453e+000  1.704e+000
       co  Gas   1.350e+000  3.566e-001
    ch2o2  Gas   9.005e-003  2.378e-003
       no  Gas   5.185e-003  1.369e-003
      ch4  Gas   1.050e-003  2.772e-004
       o2  Gas   7.915e-004  2.090e-004
     c2h4  Gas   6.696e-004  1.768e-004
       h2  Gas   3.205e-004  8.463e-005
    ch3oh  Gas   2.006e-004  5.298e-005
```

h3n	Gas	9.269e-005	2.448e-005
ch2o	Gas	5.190e-006	1.370e-006
ch3	Gas	3.401e-009	8.980e-010
c2h6	Gas	8.665e-011	2.288e-011
no2	Gas	3.001e-013	7.924e-014
*c	solid	1.262e+001	3.332e+000
Total	Gas	3.106e+001	8.201e+000
Total	Cond.	1.262e+001	3.332e+000

The C-J Adiabat

Reference state = reactants
H(R) = H- 9.68, E(R) = E- 9.66, 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)
1.)	121456.1	0.5568	3157.1	1489.24	-148.53	1.643	0.5116

Product concentrations

Name		(mol/kg)	(mol gas/mol explosive)
h2o	Gas	1.240e+001	3.273e+000
n2	Gas	1.074e+001	2.837e+000
co2	Gas	5.234e+000	1.382e+000
co	Gas	3.872e+000	1.023e+000
ch4	Gas	2.979e-002	7.866e-003
ch2o2	Gas	1.687e-002	4.456e-003
h2	Gas	1.510e-002	3.986e-003
c2h4	Gas	5.671e-003	1.498e-003
h3n	Gas	2.777e-003	7.332e-004
ch3oh	Gas	1.252e-003	3.305e-004
no	Gas	5.511e-004	1.455e-004
ch2o	Gas	1.848e-004	4.880e-005
o2	Gas	1.120e-005	2.958e-006
ch3	Gas	1.111e-006	2.933e-007
c2h6	Gas	2.506e-007	6.616e-008
no2	Gas	1.751e-012	4.623e-013
*c	solid	1.126e+001	2.975e+000
Total	Gas	3.232e+001	8.534e+000
Total	Cond.	1.126e+001	2.975e+000

Reference state = reactants
H(R) = H- 9.68, E(R) = E- 9.66, 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)
1.)	13117.4	1.2250	1815.0	-412.57	-801.70	1.643	1.1894

Product concentrations

Name		(mol/kg)	(mol gas/mol explosive)
n2	Gas	1.072e+001	2.830e+000
h2o	Gas	9.730e+000	2.569e+000
co	Gas	6.574e+000	1.736e+000
co2	Gas	5.227e+000	1.380e+000
ch4	Gas	9.249e-001	2.442e-001
h2	Gas	8.185e-001	2.161e-001
h3n	Gas	5.846e-002	1.544e-002
ch2o2	Gas	5.779e-003	1.526e-003
c2h4	Gas	4.429e-003	1.170e-003
ch2o	Gas	1.423e-003	3.758e-004
ch3oh	Gas	9.908e-004	2.616e-004
c2h6	Gas	5.863e-004	1.548e-004
ch3	Gas	2.655e-005	7.011e-006
no	Gas	1.859e-007	4.909e-008
o2	Gas	4.716e-011	1.245e-011
no2	Gas	3.850e-015	1.017e-015
*c	solid	7.686e+000	2.030e+000

```
     Total Gas   3.406e+001  8.995e+000
     Total Cond. 7.686e+000  2.030e+000


                          Reference state = reactants
                  H(R) = H- 9.68, E(R) = E- 9.66, S(R) = S- 0.00

          P           V         T       H(R)      E(R)      S(R)     VGS
       (ATM)      (CC/GM)     (K)    (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)  12604.4      1.2452   1800.0   -427.91   -808.00    1.643    1.2099

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
       n2  Gas   1.072e+001  2.830e+000
      h2o  Gas   9.663e+000  2.552e+000
       co  Gas   6.555e+000  1.731e+000
      co2  Gas   5.271e+000  1.392e+000
      ch4  Gas   9.465e-001  2.499e-001
       h2  Gas   8.419e-001  2.223e-001
      h3n  Gas   5.916e-002  1.562e-002
    ch2o2  Gas   5.586e-003  1.475e-003
     c2h4  Gas   4.237e-003  1.119e-003
     ch2o  Gas   1.406e-003  3.714e-004
    ch3oh  Gas   9.534e-004  2.518e-004
     c2h6  Gas   6.150e-004  1.624e-004
      ch3  Gas   2.587e-005  6.831e-006
       no  Gas   1.591e-007  4.202e-008
       o2  Gas   3.761e-011  9.932e-012
      no2  Gas   3.220e-015  8.503e-016
       *c  solid 7.641e+000  2.018e+000

     Total Gas   3.407e+001  8.995e+000
     Total Cond. 7.641e+000  2.018e+000

                          Reference state = reactants
                  H(R) = H- 9.68, E(R) = E- 9.66, S(R) = S- 0.00

          P           V         T       H(R)      E(R)      S(R)     VGS
       (ATM)      (CC/GM)     (K)    (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)   3290.4      2.2829   1390.9   -784.91   -966.81    1.643    2.2472

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*      n2  Gas   1.072e+001  2.830e+000
*     h2o  Gas   9.663e+000  2.552e+000
*      co  Gas   6.555e+000  1.731e+000
*     co2  Gas   5.271e+000  1.392e+000
*     ch4  Gas   9.465e-001  2.499e-001
*      h2  Gas   8.419e-001  2.223e-001
*     h3n  Gas   5.916e-002  1.562e-002
*   ch2o2  Gas   5.586e-003  1.475e-003
*    c2h4  Gas   4.237e-003  1.119e-003
*    ch2o  Gas   1.406e-003  3.714e-004
*   ch3oh  Gas   9.534e-004  2.518e-004
*    c2h6  Gas   6.150e-004  1.624e-004
*     ch3  Gas   2.587e-005  6.831e-006
*      no  Gas   1.591e-007  4.202e-008
*      o2  Gas   3.761e-011  9.932e-012
*     no2  Gas   3.220e-015  8.503e-016
*      *c  solid 7.641e+000  2.018e+000

     Total Gas   3.407e+001  8.995e+000
     Total Cond. 7.641e+000  2.018e+000

                          Reference state = reactants
                  H(R) = H- 9.68, E(R) = E- 9.66, S(R) = S- 0.00

          P           V         T       H(R)      E(R)      S(R)     VGS
       (ATM)      (CC/GM)     (K)    (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
```

```
 1.)    1409.6      3.6192   1189.4   -912.12  -1035.65    1.643    3.5835

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.072e+001  2.830e+000
*      h2o  Gas   9.663e+000  2.552e+000
*       co  Gas   6.555e+000  1.731e+000
*      co2  Gas   5.271e+000  1.392e+000
*      ch4  Gas   9.465e-001  2.499e-001
*       h2  Gas   8.419e-001  2.223e-001
*      h3n  Gas   5.916e-002  1.562e-002
*    ch2o2  Gas   5.586e-003  1.475e-003
*     c2h4  Gas   4.237e-003  1.119e-003
*     ch2o  Gas   1.406e-003  3.714e-004
*    ch3oh  Gas   9.534e-004  2.518e-004
*     c2h6  Gas   6.150e-004  1.624e-004
*      ch3  Gas   2.587e-005  6.831e-006
*       no  Gas   1.591e-007  4.202e-008
*       o2  Gas   3.761e-011  9.932e-012
*      no2  Gas   3.220e-015  8.503e-016
*       *c  solid 7.641e+000  2.018e+000

     Total Gas   3.407e+001  8.995e+000
     Total Cond. 7.641e+000  2.018e+000

                          Reference state = reactants
                H(R) = H- 9.68, E(R) = E- 9.66, S(R) = S- 0.00

          P          V         T       H(R)      E(R)      S(R)     VGS
       (ATM)      (CC/GM)     (K)    (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)     696.3      5.5680   1043.9   -988.05  -1081.94    1.643    5.5323

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.072e+001  2.830e+000
*      h2o  Gas   9.663e+000  2.552e+000
*       co  Gas   6.555e+000  1.731e+000
*      co2  Gas   5.271e+000  1.392e+000
*      ch4  Gas   9.465e-001  2.499e-001
*       h2  Gas   8.419e-001  2.223e-001
*      h3n  Gas   5.916e-002  1.562e-002
*    ch2o2  Gas   5.586e-003  1.475e-003
*     c2h4  Gas   4.237e-003  1.119e-003
*     ch2o  Gas   1.406e-003  3.714e-004
*    ch3oh  Gas   9.534e-004  2.518e-004
*     c2h6  Gas   6.150e-004  1.624e-004
*      ch3  Gas   2.587e-005  6.831e-006
*       no  Gas   1.591e-007  4.202e-008
*       o2  Gas   3.761e-011  9.932e-012
*      no2  Gas   3.220e-015  8.503e-016
*       *c  solid 7.641e+000  2.018e+000

     Total Gas   3.407e+001  8.995e+000
     Total Cond. 7.641e+000  2.018e+000

                          Reference state = reactants
                H(R) = H- 9.68, E(R) = E- 9.66, S(R) = S- 0.00

          P          V         T       H(R)      E(R)      S(R)     VGS
       (ATM)      (CC/GM)     (K)    (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)     249.4     11.1360    859.1  -1069.56  -1136.81    1.643   11.1003

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.072e+001  2.830e+000
*      h2o  Gas   9.663e+000  2.552e+000
*       co  Gas   6.555e+000  1.731e+000
*      co2  Gas   5.271e+000  1.392e+000
*      ch4  Gas   9.465e-001  2.499e-001
```

```
*      h2  Gas   8.419e-001  2.223e-001
*     h3n  Gas   5.916e-002  1.562e-002
*   ch2o2  Gas   5.586e-003  1.475e-003
*    c2h4  Gas   4.237e-003  1.119e-003
*    ch2o  Gas   1.406e-003  3.714e-004
*   ch3oh  Gas   9.534e-004  2.518e-004
*    c2h6  Gas   6.150e-004  1.624e-004
*     ch3  Gas   2.587e-005  6.831e-006
*      no  Gas   1.591e-007  4.202e-008
*      o2  Gas   3.761e-011  9.932e-012
*     no2  Gas   3.220e-015  8.503e-016
*      *c  solid 7.641e+000  2.018e+000

     Total Gas   3.407e+001  8.995e+000
     Total Cond. 7.641e+000  2.018e+000

                          Reference state = reactants
                H(R) = H- 9.68, E(R) = E- 9.66, S(R) = S- 0.00

          P           V         T       H(R)       E(R)       S(R)      VGS
       (ATM)       (CC/GM)     (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)    96.0      22.2719    710.7  -1125.89   -1177.69     1.643    22.2363

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*      n2  Gas   1.072e+001  2.830e+000
*     h2o  Gas   9.663e+000  2.552e+000
*      co  Gas   6.555e+000  1.731e+000
*     co2  Gas   5.271e+000  1.392e+000
*     ch4  Gas   9.465e-001  2.499e-001
*      h2  Gas   8.419e-001  2.223e-001
*     h3n  Gas   5.916e-002  1.562e-002
*   ch2o2  Gas   5.586e-003  1.475e-003
*    c2h4  Gas   4.237e-003  1.119e-003
*    ch2o  Gas   1.406e-003  3.714e-004
*   ch3oh  Gas   9.534e-004  2.518e-004
*    c2h6  Gas   6.150e-004  1.624e-004
*     ch3  Gas   2.587e-005  6.831e-006
*      no  Gas   1.591e-007  4.202e-008
*      o2  Gas   3.761e-011  9.932e-012
*     no2  Gas   3.220e-015  8.503e-016
*      *c  solid 7.641e+000  2.018e+000

     Total Gas   3.407e+001  8.995e+000
     Total Cond. 7.641e+000  2.018e+000

                          Reference state = reactants
                H(R) = H- 9.68, E(R) = E- 9.66, S(R) = S- 0.00

          P           V         T       H(R)       E(R)       S(R)      VGS
       (ATM)       (CC/GM)     (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)    38.2      44.5439    585.9  -1168.55   -1209.72     1.643    44.5083

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*      n2  Gas   1.072e+001  2.830e+000
*     h2o  Gas   9.663e+000  2.552e+000
*      co  Gas   6.555e+000  1.731e+000
*     co2  Gas   5.271e+000  1.392e+000
*     ch4  Gas   9.465e-001  2.499e-001
*      h2  Gas   8.419e-001  2.223e-001
*     h3n  Gas   5.916e-002  1.562e-002
*   ch2o2  Gas   5.586e-003  1.475e-003
*    c2h4  Gas   4.237e-003  1.119e-003
*    ch2o  Gas   1.406e-003  3.714e-004
*   ch3oh  Gas   9.534e-004  2.518e-004
*    c2h6  Gas   6.150e-004  1.624e-004
*     ch3  Gas   2.587e-005  6.831e-006
*      no  Gas   1.591e-007  4.202e-008
```

```
*      o2  Gas   3.761e-011  9.932e-012
*     no2  Gas   3.220e-015  8.503e-016
*      *c  solid 7.641e+000  2.018e+000

     Total Gas   3.407e+001  8.995e+000
     Total Cond. 7.641e+000  2.018e+000

                          Reference state = reactants
                H(R) = H- 9.68, E(R) = E- 9.66, S(R) = S- 0.00

          P          V         T       H(R)      E(R)      S(R)     VGS
       (ATM)      (CC/GM)     (K)    (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)    15.3     89.0878    479.4  -1202.28  -1235.35    1.643   89.0522

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*      n2  Gas   1.072e+001  2.830e+000
*     h2o  Gas   9.663e+000  2.552e+000
*      co  Gas   6.555e+000  1.731e+000
*     co2  Gas   5.271e+000  1.392e+000
*     ch4  Gas   9.465e-001  2.499e-001
*      h2  Gas   8.419e-001  2.223e-001
*     h3n  Gas   5.916e-002  1.562e-002
*   ch2o2  Gas   5.586e-003  1.475e-003
*    c2h4  Gas   4.237e-003  1.119e-003
*    ch2o  Gas   1.406e-003  3.714e-004
*   ch3oh  Gas   9.534e-004  2.518e-004
*    c2h6  Gas   6.150e-004  1.624e-004
*     ch3  Gas   2.587e-005  6.831e-006
*      no  Gas   1.591e-007  4.202e-008
*      o2  Gas   3.761e-011  9.932e-012
*     no2  Gas   3.220e-015  8.503e-016
*      *c  solid 7.641e+000  2.018e+000

     Total Gas   3.407e+001  8.995e+000
     Total Cond. 7.641e+000  2.018e+000

                          The End of the Adiabat

                          Reference state = reactants
                H(R) = H- 9.68, E(R) = E- 9.66, S(R) = S- 0.00

          P          V         T       H(R)      E(R)      S(R)     VGS
       (ATM)      (CC/GM)     (K)    (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)     2.0    411.0341    298.0  -1255.16  -1275.41    1.643  410.9986

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*      n2  Gas   1.072e+001  2.830e+000
*     h2o  Gas   9.663e+000  2.552e+000
*      co  Gas   6.555e+000  1.731e+000
*     co2  Gas   5.271e+000  1.392e+000
*     ch4  Gas   9.465e-001  2.499e-001
*      h2  Gas   8.419e-001  2.223e-001
*     h3n  Gas   5.916e-002  1.562e-002
*   ch2o2  Gas   5.586e-003  1.475e-003
*    c2h4  Gas   4.237e-003  1.119e-003
*    ch2o  Gas   1.406e-003  3.714e-004
*   ch3oh  Gas   9.534e-004  2.518e-004
*    c2h6  Gas   6.150e-004  1.624e-004
*     ch3  Gas   2.587e-005  6.831e-006
*      no  Gas   1.591e-007  4.202e-008
*      o2  Gas   3.761e-011  9.932e-012
*     no2  Gas   3.220e-015  8.503e-016
*      *c  solid 7.641e+000  2.018e+000

     Total Gas   3.407e+001  8.995e+000
     Total Cond. 7.641e+000  2.018e+000
```

The Products at room temperature and pressure

Reference state = reactants
H(R) = H- 9.68, E(R) = E- 9.66, 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)
1.)	1.0	834.7028	298.0	-1255.21	-1275.41	1.691	834.6673

Product concentrations

	Name		(mol/kg)	(mol gas/mol explosive)
*	n2	Gas	1.072e+001	2.830e+000
*	h2o	Gas	9.663e+000	2.552e+000
*	co	Gas	6.555e+000	1.731e+000
*	co2	Gas	5.271e+000	1.392e+000
*	ch4	Gas	9.465e-001	2.499e-001
*	h2	Gas	8.419e-001	2.223e-001
*	h3n	Gas	5.916e-002	1.562e-002
*	ch2o2	Gas	5.586e-003	1.475e-003
*	c2h4	Gas	4.237e-003	1.119e-003
*	ch2o	Gas	1.406e-003	3.714e-004
*	ch3oh	Gas	9.534e-004	2.518e-004
*	c2h6	Gas	6.150e-004	1.624e-004
*	ch3	Gas	2.587e-005	6.831e-006
*	no	Gas	1.591e-007	4.202e-008
*	o2	Gas	3.761e-011	9.932e-012
*	no2	Gas	3.220e-015	8.503e-016
*	*c	solid	7.641e+000	2.018e+000
	Total	Gas	3.407e+001	8.995e+000
	Total	Cond.	7.641e+000	2.018e+000

The mechanical energy of detonation = -9.584 kJ/cc
The thermal energy of detonation = -0.000 kJ/cc
The total energy of detonation = -9.584 kJ/cc

JWL Tail Fit results:
Initial E0 = -10.041, Final E0 = -9.915
E0(V=infty) = -9.915
C = 1.567, omega = 0.373
Final fitting error = 0.002440

V/V0	Actual E (kJ/cc)	Fit E (kJ/cc)	Actual P (GPa)	Fit P (GPa)
10.000	-8.130	-8.132	0.071	0.066
20.000	-8.542	-8.538	0.025	0.026
40.000	-8.850	-8.851	0.010	0.010
80.000	-9.090	-9.094	0.004	0.004
160.000	-9.283	-9.281	0.002	0.001

JWL Fit results:
E0(V=infty) = -9.915
R[1] = 4.657, R[2] = 1.092, omega = 0.373
A = 797.430, B = 9.434, C = 1.567
Final fitting error = 0.006421

V/V0	Actual E (kJ/cc)	Fit E (kJ/cc)	Actual P (GPa)	Fit P (GPa)
0.751	3.754	3.754	30.163	30.613
1.000	-1.116	-1.182	12.307	12.307
2.200	-6.024	-5.991	1.329	1.414
4.100	-7.265	-7.331	0.333	0.333
6.500	-7.782	-7.814	0.143	0.128
10.000	-8.130	-8.132	0.071	0.067
20.000	-8.542	-8.538	0.025	0.026
40.000	-8.850	-8.851	0.010	0.010

```
    80.000     -9.090     -9.094      0.004      0.004
   160.000     -9.283     -9.281      0.002      0.001
```

A.3 Summary printout

A.3.1 BKWS Product Library

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

The composition:
```

Name	% wt.	% mol	% vol	Heat of formation (cal/mol)	Mol. wt.	TMD (g/cc)	
HMX	60.00	53.50	56.57	17866	296.17	1.91	$C_4H_8N_8O_8$
TNT	40.00	46.50	43.43	-15057	227.13	1.65	$C_7H_5N_3O_6$


```
Product library title: bkws library

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


The composition:
```

Name	% wt.	% mol	% vol	Heat of formation (cal/mol)	Mol. wt.	TMD (g/cc)	
HMX	60.00	53.50	56.57	17866	296.17	1.91	$C_4H_8N_8O_8$
TNT	40.00	46.50	43.43	-15057	227.13	1.65	$C_7H_5N_3O_6$


```
Density  =  1.7960 g/cc   Mixture TMD =  1.7960 g/cc   % TMD = 100.0000


The C-J condition:
The pressure          =          30.21 GPa
The volume            =          0.426 cc/g
The density           =          2.349 g/cc
The energy            =           3.56 kJ/cc explosive
The temperature       =           3948 K
The shock velocity    =          8.454 mm/us
The particle velocity =          1.990 mm/us
The speed of sound    =          6.464 mm/us
Gamma                 =          3.249


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    -1.12
   2.20    -6.31     130       99        84       70       145
   4.10    -7.59     131       98        86       72       138
   6.50    -8.12     130       98        86       73       133
  10.00    -8.46     130       97        87       74       129
  20.00    -8.87     129       97        87       75       124
  40.00    -9.17     128       97        88       75       119
  80.00    -9.41     128       96        88       76       114
 160.00    -9.60

Freezing occurred at T =     1800.0 K and relative V =   2.225
The mechanical energy of detonation =     -9.904 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.904 kJ/cc

JWL Fit results:
E0   =   -10.205 kJ/cc
```

```
A    =  1045.25 GPa, B    =   11.08 GPa , C     =    1.56 GPa
R[1]       4.93,     R[2] =    1.11,      omega =    0.38
RMS fitting error =   0.97 %
```

A.3.2 BKWC Product Library

```
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)
hmx        60.00  53.50  56.57    17866   296.17     1.91 c4h8n8o8
tnt        40.00  46.50  43.43   -15057   227.13     1.65 c7h5n3o6
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)
hmx        60.00  53.50  56.57    17866   296.17     1.91 c4h8n8o8
tnt        40.00  46.50  43.43   -15057   227.13     1.65 c7h5n3o6

Density  =  1.7960 g/cc   Mixture TMD =  1.7960 g/cc   % TMD = 100.0000


The C-J condition:
The pressure          =          30.16 GPa
The volume            =          0.418 cc/g
The density           =          2.391 g/cc
The energy            =           3.75 kJ/cc explosive
The temperature       =           3998 K
The shock velocity    =          8.214 mm/us
The particle velocity =          2.045 mm/us
The speed of sound    =          6.169 mm/us
Gamma                 =          3.017


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    -1.12
   2.20    -6.02     124       95        81       67      138
   4.10    -7.26     125       94        82       69      132
   6.50    -7.78     125       94        83       70      127
  10.00    -8.13     125       94        83       71      124
  20.00    -8.54     124       93        84       72      119
  40.00    -8.85     124       93        84       73      114
  80.00    -9.09     123       93        85       74      110
 160.00    -9.28

Freezing occurred at T =     1800.0 K and relative V =   2.236
The mechanical energy of detonation =     -9.584 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.584 kJ/cc

JWL Fit results:
E0   =   -9.915 kJ/cc
A    =  797.43 GPa, B    =    9.43 GPa , C     =    1.57 GPa
R[1] =    4.66,     R[2] =    1.09,      omega =    0.37
RMS fitting error =   0.64 %
```

Appendix B Octol 70/30

B.1 Complete printout product library BKWC

```
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)
HMX       70.00  64.15  66.95    17866     155.47      0.000     296.17  C4H8N8O8
TNT       30.00  35.85  33.05   -15057     137.32      0.000     227.13  C7H5N3O6

Heat of formation =     22.338 cal/gm
Standard volume   =      0.549 cc/gm
Standard entropy  =      0.000 cal/k/gm
Standard energy   =     22.325 cal/gm

The elements and percent by mole
     c             19.911
     h             27.165
     n             24.352
     o             28.571
The average mol. wt. = 271.420 g/mol
Input>composition, hmx, 70, tnt, 30, weight
                                    The Composition

Name      % wt. % mol % vol. Heat of  Standard  Standard  Mol.    Formula
                             formation  volume   entropy     wt.
                             (cal/mol) (cc/mol) (cal/K/mol)
HMX       70.00 64.15 66.95  17866      155.47   0.000    296.17  C4H8N8O8
TNT       30.00 35.85 33.05 -15057      137.32   0.000    227.13  C7H5N3O6

Heat of formation =     22.338 cal/gm
Standard volume   =      0.549 cc/gm
Standard entropy  =      0.000 cal/k/gm
Standard energy   =     22.325 cal/gm

The elements and percent by mole
     c             19.911
     h             27.165
     n             24.352
     o             28.571
The average mol. wt. = 271.420 g/mol
Input>standard run, rho, 1.822049
The hugoniot reference state:
P0 = 1.000000 ATM, V0 = 0.548833 cc/gm, E0 = 22.324802 cal/gm
Using  139998 ATM as a lower bound for the C-J pressure
Using  349996 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    =   8.46337e+003 m/s
The particle velocity =   2.09385e+003 m/s
The speed of sound    =   6.36952e+003 m/s
```

P0 = 1 atm, V0 = 0.54883 cc/gm, E0 = 22.32480 cal/gm

Reference state = reactants
H(R) = H-22.34, E(R) = E-22.32, 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)
1.)	318664.9	0.4131	4033.0	3711.63	523.95	1.648	0.3815

Product concentrations

Name		(mol/kg)	(mol gas/mol explosive)
h2o	Gas	1.275e+001	3.459e+000
n2	Gas	1.143e+001	3.103e+000
co2	Gas	6.457e+000	1.753e+000
co	Gas	1.150e+000	3.123e-001
ch2o2	Gas	7.561e-003	2.052e-003
no	Gas	5.708e-003	1.549e-003
o2	Gas	9.946e-004	2.699e-004
ch4	Gas	7.083e-004	1.922e-004
c2h4	Gas	4.685e-004	1.272e-004
h2	Gas	2.061e-004	5.594e-005
ch3oh	Gas	1.470e-004	3.991e-005
h3n	Gas	6.286e-005	1.706e-005
ch2o	Gas	3.094e-006	8.397e-007
ch3	Gas	1.507e-009	4.090e-010
c2h6	Gas	3.110e-011	8.442e-012
no2	Gas	1.770e-013	4.805e-014
*c	solid	1.108e+001	3.008e+000
Total	Gas	3.180e+001	8.632e+000
Total	Cond.	1.108e+001	3.008e+000

The C-J Adiabat

Reference state = reactants
H(R) = H-22.34, E(R) = E-22.32, 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)
1.)	129967.2	0.5488	3177.5	1571.71	-155.76	1.648	0.5099

Product concentrations

Name		(mol/kg)	(mol gas/mol explosive)
h2o	Gas	1.267e+001	3.438e+000
n2	Gas	1.143e+001	3.103e+000
co2	Gas	5.309e+000	1.441e+000
co	Gas	3.516e+000	9.542e-001
ch4	Gas	2.372e-002	6.439e-003
ch2o2	Gas	1.560e-002	4.235e-003
h2	Gas	1.128e-002	3.063e-003
c2h4	Gas	4.738e-003	1.286e-003
h3n	Gas	2.212e-003	6.004e-004
ch3oh	Gas	1.069e-003	2.900e-004
no	Gas	6.052e-004	1.642e-004
ch2o	Gas	1.353e-004	3.674e-005
o2	Gas	1.338e-005	3.630e-006
ch3	Gas	6.720e-007	1.824e-007
c2h6	Gas	1.362e-007	3.695e-008
no2	Gas	1.296e-012	3.517e-013
*c	solid	9.825e+000	2.667e+000
Total	Gas	3.298e+001	8.953e+000
Total	Cond.	9.825e+000	2.667e+000

Reference state = reactants
H(R) = H-22.34, E(R) = E-22.32, S(R) = S- 0.00

P	V	T	H(R)	E(R)	S(R)	VGS

	P (ATM)	V (CC/GM)	T (K)	H(R) (CAL/GM)	E(R) (CAL/GM)	S(R) (CAL/K/GM)	VGS (CC/GM)
1.)	13688.5	1.2074	1800.6	-437.92	-838.18	1.648	1.1778

Product concentrations

Name		(mol/kg)	(mol gas/mol explosive)
n2	Gas	1.141e+001	3.096e+000
h2o	Gas	1.012e+001	2.748e+000
co	Gas	6.075e+000	1.649e+000
co2	Gas	5.310e+000	1.441e+000
ch4	Gas	8.914e-001	2.419e-001
h2	Gas	7.447e-001	2.021e-001
h3n	Gas	5.740e-002	1.558e-002
ch2o2	Gas	5.640e-003	1.531e-003
c2h4	Gas	3.963e-003	1.076e-003
ch2o	Gas	1.242e-003	3.371e-004
ch3oh	Gas	9.463e-004	2.569e-004
c2h6	Gas	5.050e-004	1.371e-004
ch3	Gas	2.078e-005	5.639e-006
no	Gas	1.661e-007	4.507e-008
o2	Gas	3.997e-011	1.085e-011
no2	Gas	2.885e-015	7.831e-016
*c	solid	6.406e+000	1.739e+000
Total	Gas	3.462e+001	9.397e+000
Total	Cond.	6.406e+000	1.739e+000

Reference state = reactants
H(R) = H-22.34, E(R) = E-22.32, 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)
1.)	13668.9	1.2081	1800.0	-438.50	-838.42	1.648	1.1786

Product concentrations

Name		(mol/kg)	(mol gas/mol explosive)
n2	Gas	1.141e+001	3.096e+000
h2o	Gas	1.012e+001	2.747e+000
co	Gas	6.074e+000	1.649e+000
co2	Gas	5.312e+000	1.442e+000
ch4	Gas	8.922e-001	2.422e-001
h2	Gas	7.455e-001	2.024e-001
h3n	Gas	5.743e-002	1.559e-002
ch2o2	Gas	5.633e-003	1.529e-003
c2h4	Gas	3.956e-003	1.074e-003
ch2o	Gas	1.242e-003	3.370e-004
ch3oh	Gas	9.451e-004	2.565e-004
c2h6	Gas	5.059e-004	1.373e-004
ch3	Gas	2.076e-005	5.634e-006
no	Gas	1.651e-007	4.481e-008
o2	Gas	3.963e-011	1.076e-011
no2	Gas	2.866e-015	7.780e-016
*c	solid	6.405e+000	1.738e+000
Total	Gas	3.462e+001	9.397e+000
Total	Cond.	6.405e+000	1.738e+000

Reference state = reactants
H(R) = H-22.34, E(R) = E-22.32, 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)
1.)	3374.4	2.2502	1365.2	-822.73	-1006.61	1.648	2.2203

Product concentrations

	Name		(mol/kg)	(mol gas/mol explosive)
*	n2	Gas	1.141e+001	3.096e+000
*	h2o	Gas	1.012e+001	2.747e+000
*	co	Gas	6.074e+000	1.649e+000
*	co2	Gas	5.312e+000	1.442e+000

```
*      ch4  Gas    8.922e-001  2.422e-001
*       h2  Gas    7.455e-001  2.024e-001
*      h3n  Gas    5.743e-002  1.559e-002
*    ch2o2  Gas    5.633e-003  1.529e-003
*     c2h4  Gas    3.956e-003  1.074e-003
*     ch2o  Gas    1.242e-003  3.370e-004
*    ch3oh  Gas    9.451e-004  2.565e-004
*     c2h6  Gas    5.059e-004  1.373e-004
*      ch3  Gas    2.076e-005  5.634e-006
*       no  Gas    1.651e-007  4.481e-008
*       o2  Gas    3.963e-011  1.076e-011
*      no2  Gas    2.866e-015  7.780e-016
*       *c  solid  6.405e+000  1.738e+000

      Total Gas    3.462e+001  9.397e+000
      Total Cond.  6.405e+000  1.738e+000

                          Reference state = reactants
                 H(R) = H-22.34, E(R) = E-22.32, S(R) = S- 0.00

          P           V         T       H(R)       E(R)       S(R)      VGS
       (ATM)       (CC/GM)     (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)    1430.8      3.5674   1159.9   -952.26  -1075.86    1.648    3.5375

Product concentrations
          Name    (mol/kg) (mol gas/mol explosive)
*       n2  Gas    1.141e+001  3.096e+000
*      h2o  Gas    1.012e+001  2.747e+000
*       co  Gas    6.074e+000  1.649e+000
*      co2  Gas    5.312e+000  1.442e+000
*      ch4  Gas    8.922e-001  2.422e-001
*       h2  Gas    7.455e-001  2.024e-001
*      h3n  Gas    5.743e-002  1.559e-002
*    ch2o2  Gas    5.633e-003  1.529e-003
*     c2h4  Gas    3.956e-003  1.074e-003
*     ch2o  Gas    1.242e-003  3.370e-004
*    ch3oh  Gas    9.451e-004  2.565e-004
*     c2h6  Gas    5.059e-004  1.373e-004
*      ch3  Gas    2.076e-005  5.634e-006
*       no  Gas    1.651e-007  4.481e-008
*       o2  Gas    3.963e-011  1.076e-011
*      no2  Gas    2.866e-015  7.780e-016
*       *c  solid  6.405e+000  1.738e+000

      Total Gas    3.462e+001  9.397e+000
      Total Cond.  6.405e+000  1.738e+000

                          Reference state = reactants
                 H(R) = H-22.34, E(R) = E-22.32, S(R) = S- 0.00

          P           V         T       H(R)       E(R)       S(R)      VGS
       (ATM)       (CC/GM)     (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)     701.0      5.4883   1012.6  -1028.81  -1121.98    1.648    5.4584

Product concentrations
          Name    (mol/kg) (mol gas/mol explosive)
*       n2  Gas    1.141e+001  3.096e+000
*      h2o  Gas    1.012e+001  2.747e+000
*       co  Gas    6.074e+000  1.649e+000
*      co2  Gas    5.312e+000  1.442e+000
*      ch4  Gas    8.922e-001  2.422e-001
*       h2  Gas    7.455e-001  2.024e-001
*      h3n  Gas    5.743e-002  1.559e-002
*    ch2o2  Gas    5.633e-003  1.529e-003
*     c2h4  Gas    3.956e-003  1.074e-003
*     ch2o  Gas    1.242e-003  3.370e-004
*    ch3oh  Gas    9.451e-004  2.565e-004
*     c2h6  Gas    5.059e-004  1.373e-004
*      ch3  Gas    2.076e-005  5.634e-006
```

```
*       no  Gas    1.651e-007  4.481e-008
*       o2  Gas    3.963e-011  1.076e-011
*      no2  Gas    2.866e-015  7.780e-016
*       *c  solid  6.405e+000  1.738e+000

     Total Gas    3.462e+001  9.397e+000
     Total Cond.  6.405e+000  1.738e+000

                          Reference state = reactants
                H(R) = H-22.34, E(R) = E-22.32, S(R) = S- 0.00

          P          V         T       H(R)      E(R)      S(R)     VGS
       (ATM)      (CC/GM)     (K)    (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)    248.4     10.9767    826.7  -1110.14  -1176.14    1.648   10.9468

Product concentrations
         Name    (mol/kg) (mol gas/mol explosive)
*       n2  Gas    1.141e+001  3.096e+000
*      h2o  Gas    1.012e+001  2.747e+000
*       co  Gas    6.074e+000  1.649e+000
*      co2  Gas    5.312e+000  1.442e+000
*      ch4  Gas    8.922e-001  2.422e-001
*       h2  Gas    7.455e-001  2.024e-001
*      h3n  Gas    5.743e-002  1.559e-002
*    ch2o2  Gas    5.633e-003  1.529e-003
*     c2h4  Gas    3.956e-003  1.074e-003
*     ch2o  Gas    1.242e-003  3.370e-004
*    ch3oh  Gas    9.451e-004  2.565e-004
*     c2h6  Gas    5.059e-004  1.373e-004
*      ch3  Gas    2.076e-005  5.634e-006
*       no  Gas    1.651e-007  4.481e-008
*       o2  Gas    3.963e-011  1.076e-011
*      no2  Gas    2.866e-015  7.780e-016
*       *c  solid  6.405e+000  1.738e+000

     Total Gas    3.462e+001  9.397e+000
     Total Cond.  6.405e+000  1.738e+000

                          Reference state = reactants
                H(R) = H-22.34, E(R) = E-22.32, S(R) = S- 0.00

          P          V         T       H(R)      E(R)      S(R)     VGS
       (ATM)      (CC/GM)     (K)    (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)     94.7     21.9533    678.5  -1165.73  -1216.07    1.648   21.9235

Product concentrations
         Name    (mol/kg) (mol gas/mol explosive)
*       n2  Gas    1.141e+001  3.096e+000
*      h2o  Gas    1.012e+001  2.747e+000
*       co  Gas    6.074e+000  1.649e+000
*      co2  Gas    5.312e+000  1.442e+000
*      ch4  Gas    8.922e-001  2.422e-001
*       h2  Gas    7.455e-001  2.024e-001
*      h3n  Gas    5.743e-002  1.559e-002
*    ch2o2  Gas    5.633e-003  1.529e-003
*     c2h4  Gas    3.956e-003  1.074e-003
*     ch2o  Gas    1.242e-003  3.370e-004
*    ch3oh  Gas    9.451e-004  2.565e-004
*     c2h6  Gas    5.059e-004  1.373e-004
*      ch3  Gas    2.076e-005  5.634e-006
*       no  Gas    1.651e-007  4.481e-008
*       o2  Gas    3.963e-011  1.076e-011
*      no2  Gas    2.866e-015  7.780e-016
*       *c  solid  6.405e+000  1.738e+000

     Total Gas    3.462e+001  9.397e+000
     Total Cond.  6.405e+000  1.738e+000

                          Reference state = reactants
```

H(R) = H-22.34, E(R) = E-22.32, 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)
1.)	37.3	43.9066	554.9	-1207.42	-1247.08	1.648	43.8768

Product concentrations

	Name		(mol/kg)	(mol gas/mol explosive)
*	n2	Gas	1.141e+001	3.096e+000
*	h2o	Gas	1.012e+001	2.747e+000
*	co	Gas	6.074e+000	1.649e+000
*	co2	Gas	5.312e+000	1.442e+000
*	ch4	Gas	8.922e-001	2.422e-001
*	h2	Gas	7.455e-001	2.024e-001
*	h3n	Gas	5.743e-002	1.559e-002
*	ch2o2	Gas	5.633e-003	1.529e-003
*	c2h4	Gas	3.956e-003	1.074e-003
*	ch2o	Gas	1.242e-003	3.370e-004
*	ch3oh	Gas	9.451e-004	2.565e-004
*	c2h6	Gas	5.059e-004	1.373e-004
*	ch3	Gas	2.076e-005	5.634e-006
*	no	Gas	1.651e-007	4.481e-008
*	o2	Gas	3.963e-011	1.076e-011
*	no2	Gas	2.866e-015	7.780e-016
*	*c	solid	6.405e+000	1.738e+000
	Total	Gas	3.462e+001	9.397e+000
	Total	Cond.	6.405e+000	1.738e+000

Reference state = reactants

H(R) = H-22.34, E(R) = E-22.32, 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)
1.)	14.9	87.8132	450.5	-1240.08	-1271.67	1.648	87.7834

Product concentrations

	Name		(mol/kg)	(mol gas/mol explosive)
*	n2	Gas	1.141e+001	3.096e+000
*	h2o	Gas	1.012e+001	2.747e+000
*	co	Gas	6.074e+000	1.649e+000
*	co2	Gas	5.312e+000	1.442e+000
*	ch4	Gas	8.922e-001	2.422e-001
*	h2	Gas	7.455e-001	2.024e-001
*	h3n	Gas	5.743e-002	1.559e-002
*	ch2o2	Gas	5.633e-003	1.529e-003
*	c2h4	Gas	3.956e-003	1.074e-003
*	ch2o	Gas	1.242e-003	3.370e-004
*	ch3oh	Gas	9.451e-004	2.565e-004
*	c2h6	Gas	5.059e-004	1.373e-004
*	ch3	Gas	2.076e-005	5.634e-006
*	no	Gas	1.651e-007	4.481e-008
*	o2	Gas	3.963e-011	1.076e-011
*	no2	Gas	2.866e-015	7.780e-016
*	*c	solid	6.405e+000	1.738e+000
	Total	Gas	3.462e+001	9.397e+000
	Total	Cond.	6.405e+000	1.738e+000

The End of the Adiabat

Reference state = reactants

H(R) = H-22.34, E(R) = E-22.32, 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)
1.)	2.6	321.2276	298.0	-1284.46	-1305.06	1.648	321.1978

Product concentrations

```
         Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.141e+001  3.096e+000
*      h2o  Gas   1.012e+001  2.747e+000
*       co  Gas   6.074e+000  1.649e+000
*      co2  Gas   5.312e+000  1.442e+000
*      ch4  Gas   8.922e-001  2.422e-001
*       h2  Gas   7.455e-001  2.024e-001
*      h3n  Gas   5.743e-002  1.559e-002
*    ch2o2  Gas   5.633e-003  1.529e-003
*     c2h4  Gas   3.956e-003  1.074e-003
*     ch2o  Gas   1.242e-003  3.370e-004
*    ch3oh  Gas   9.451e-004  2.565e-004
*     c2h6  Gas   5.059e-004  1.373e-004
*      ch3  Gas   2.076e-005  5.634e-006
*       no  Gas   1.651e-007  4.481e-008
*       o2  Gas   3.963e-011  1.076e-011
*      no2  Gas   2.866e-015  7.780e-016
*       *c  solid 6.405e+000  1.738e+000

      Total Gas   3.462e+001  9.397e+000
      Total Cond. 6.405e+000  1.738e+000

                The Products at room temperature and pressure

                              Reference state = reactants
                H(R) = H-22.34, E(R) = E-22.32, S(R) = S- 0.00

          P           V         T       H(R)      E(R)      S(R)     VGS
       (ATM)      (CC/GM)     (K)    (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)     1.0    848.3321    298.0  -1284.53  -1305.06    1.715  848.3023

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.141e+001  3.096e+000
*      h2o  Gas   1.012e+001  2.747e+000
*       co  Gas   6.074e+000  1.649e+000
*      co2  Gas   5.312e+000  1.442e+000
*      ch4  Gas   8.922e-001  2.422e-001
*       h2  Gas   7.455e-001  2.024e-001
*      h3n  Gas   5.743e-002  1.559e-002
*    ch2o2  Gas   5.633e-003  1.529e-003
*     c2h4  Gas   3.956e-003  1.074e-003
*     ch2o  Gas   1.242e-003  3.370e-004
*    ch3oh  Gas   9.451e-004  2.565e-004
*     c2h6  Gas   5.059e-004  1.373e-004
*      ch3  Gas   2.076e-005  5.634e-006
*       no  Gas   1.651e-007  4.481e-008
*       o2  Gas   3.963e-011  1.076e-011
*      no2  Gas   2.866e-015  7.780e-016
*       *c  solid 6.405e+000  1.738e+000

      Total Gas   3.462e+001  9.397e+000
      Total Cond. 6.405e+000  1.738e+000
The mechanical energy of detonation =     -9.949 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.949 kJ/cc

JWL Tail Fit results:
Initial E0 =    -10.413, Final E0 =    -10.284
E0(V=infty) =    -10.284
C =      1.629,  omega =      0.387
Final fitting error = 0.002569

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

    10.000     -8.553     -8.555      0.071      0.067
    20.000     -8.966     -8.962      0.025      0.026
    40.000     -9.271     -9.273      0.010      0.010
```

```
    80.000     -9.507     -9.510      0.004      0.004
   160.000     -9.694     -9.692      0.002      0.001

JWL Fit results:
E0(V=infty) =    -10.284
R[1] =      4.669, R[2] =      1.098, omega =      0.387
A    =    871.734, B    =     10.080, C     =      1.629
Final fitting error = 0.006604

     V/V0     Actual E     Fit E    Actual P      Fit P
              (kJ/cc)     (kJ/cc)    (GPa)        (GPa)
     0.753      3.994      3.994     32.289     32.789
     1.000     -1.187     -1.259     13.169     13.169
     2.200     -6.390     -6.353      1.387      1.476
     4.100     -7.674     -7.742      0.342      0.342
     6.500     -8.202     -8.234      0.145      0.130
    10.000     -8.553     -8.555      0.071      0.067
    20.000     -8.966     -8.962      0.025      0.026
    40.000     -9.271     -9.273      0.010      0.010
    80.000     -9.507     -9.510      0.004      0.004
   160.000     -9.694     -9.692      0.002      0.001
```

B.2 Complete printout with bkws product library

```
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 formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
HMX	70.00	64.15	66.95	17866	155.47	0.000	296.17	$C_4H_8N_8O_8$
TNT	30.00	35.85	33.05	-15057	137.32	0.000	227.13	$C_7H_5N_3O_6$

```
Heat of formation =     22.338 cal/gm
Standard volume   =      0.549 cc/gm
Standard entropy  =      0.000 cal/k/gm
Standard energy   =     22.325 cal/gm

The elements and percent by mole
     c             19.911
     h             27.165
     n             24.352
     o             28.571
The average mol. wt. = 271.420 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, hmx, 70, tnt, 30, weight
                                The Composition
```

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
HMX	70.00	64.15	66.95	17866	155.47	0.000	296.17	$C_4H_8N_8O_8$
TNT	30.00	35.85	33.05	-15057	137.32	0.000	227.13	$C_7H_5N_3O_6$

```
Heat of formation =     22.338 cal/gm
Standard volume   =      0.549 cc/gm
Standard entropy  =      0.000 cal/k/gm
Standard energy   =     22.325 cal/gm
```

```
The elements and percent by mole
     c             19.911
     h             27.165
     n             24.352
     o             28.571
The average mol. wt. = 271.420 g/mol
Input>gas eos, bkw
Input>standard run, rho, 1.822049

P0 = 1.000000 ATM, V0 = 0.548833 cc/gm, E0 = 22.324802 cal/gm
Using  144187 ATM as a lower bound for the C-J pressure
Using  360467 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    =   8.67661e+003 m/s
The particle velocity =   2.02735e+003 m/s
The speed of sound    =   6.64926e+003 m/s

P0 =       1 atm, V0 =  0.54883 cc/gm, E0 =  22.32480 cal/gm

                          Reference state = reactants
                H(R) = H-22.34, E(R) = E-22.32, S(R) = S- 0.00

         P           V         T       H(R)      E(R)      S(R)      VGS
       (ATM)      (CC/GM)     (K)    (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)  316318.3      0.4206   3978.8   3713.19    491.19    1.614    0.4027

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
       n2  Gas   1.078e+001  2.926e+000
      co2  Gas   9.020e+000  2.448e+000
      h2o  Gas   4.318e+000  1.172e+000
    ch2o2  Gas   2.103e+000  5.709e-001
      h3n  Gas   1.237e+000  3.357e-001
     c2h6  Gas   8.138e-001  2.209e-001
      ch4  Gas   7.149e-001  1.940e-001
       h2  Gas   1.755e-001  4.764e-002
    ch3oh  Gas   1.717e-001  4.661e-002
       co  Gas   5.185e-002  1.407e-002
     h4n2  Gas   2.273e-002  6.170e-003
       no  Gas   1.809e-002  4.910e-003
     c2h4  Gas   9.092e-003  2.468e-003
      ch3  Gas   6.634e-003  1.801e-003
     h2o2  Gas   5.922e-003  1.607e-003
       o2  Gas   3.359e-003  9.116e-004
      h2n  Gas   3.157e-003  8.569e-004
     ch2o  Gas   2.999e-003  8.141e-004
     h2n2  Gas   1.678e-003  4.555e-004
       ho  Gas   1.577e-003  4.280e-004
      cno  Gas   1.143e-003  3.101e-004
     chno  Gas   1.008e-003  2.735e-004
        h  Gas   7.078e-004  1.921e-004
        o  Gas   2.499e-004  6.783e-005
      no2  Gas   1.255e-004  3.407e-005
     c3h8  Gas   6.968e-005  1.891e-005
      ch2  Gas   4.852e-005  1.317e-005
      ho2  Gas   3.924e-005  1.065e-005
      cho  Gas   3.696e-005  1.003e-005
      hno  Gas   3.020e-005  8.198e-006
      chn  Gas   2.355e-005  6.391e-006
      n2o  Gas   1.695e-005  4.600e-006
        n  Gas   1.405e-005  3.814e-006
       hn  Gas   6.523e-006  1.770e-006
     c2h2  Gas   5.646e-006  1.533e-006
       cn  Gas   2.682e-006  7.280e-007
       n3  Gas   1.011e-006  2.743e-007
```

no3	Gas	9.832e-007	2.668e-007
c3h6	Gas	7.428e-007	2.016e-007
hno2	Gas	7.030e-007	1.908e-007
cn2	Gas	4.737e-007	1.286e-007
hno3	Gas	5.570e-008	1.512e-008
ch	Gas	4.134e-008	1.122e-008
c2h	Gas	2.280e-008	6.190e-009
no2h	Gas	1.758e-008	4.772e-009
c	Gas	8.547e-009	2.320e-009
o3	Gas	2.977e-009	8.081e-010
n2o4	Gas	2.323e-009	6.306e-010
c2n2	Gas	8.741e-010	2.372e-010
c2h4o	Gas	5.074e-010	1.377e-010
c2n	Gas	2.812e-010	7.633e-011
c2	Gas	2.200e-010	5.971e-011
c2o	Gas	6.660e-011	1.808e-011
n2o3	Gas	1.752e-011	4.756e-012
cnn	Gas	8.479e-012	2.301e-012
c3o2	Gas	2.547e-013	6.914e-014
c3	Gas	4.148e-014	1.126e-014
n2o5	Gas	2.382e-014	6.464e-015
c4	Gas	1.394e-023	3.784e-024
c4n2	Gas	1.032e-031	2.801e-032
c5	Gas	1.913e-034	5.191e-035
*c	solid	4.980e+000	1.352e+000
*h2o	liquid	0.000e+000	0.000e+000
Total	Gas	2.947e+001	7.998e+000
Total	Cond.	4.980e+000	1.352e+000

The C-J Adiabat
Reference state = reactants
H(R) = H-22.34, E(R) = E-22.32, 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)
1.)	134931.8	0.5488	3221.6	1637.86	-155.60	1.614	0.5195

Product concentrations

Name		(mol/kg)	(mol gas/mol explosive)
n2	Gas	1.096e+001	2.975e+000
co2	Gas	9.086e+000	2.466e+000
h2o	Gas	6.748e+000	1.832e+000
ch4	Gas	1.121e+000	3.044e-001
h3n	Gas	9.370e-001	2.543e-001
h2	Gas	7.392e-001	2.006e-001
ch2o2	Gas	6.625e-001	1.798e-001
co	Gas	4.997e-001	1.356e-001
c2h6	Gas	2.514e-001	6.822e-002
ch3oh	Gas	7.244e-002	1.966e-002
c2h4	Gas	1.494e-002	4.056e-003
ch2o	Gas	9.478e-003	2.572e-003
ch3	Gas	8.446e-003	2.292e-003
chno	Gas	3.276e-003	8.890e-004
no	Gas	2.083e-003	5.653e-004
h2n	Gas	1.500e-003	4.071e-004
ho	Gas	1.112e-003	3.019e-004
h	Gas	1.069e-003	2.902e-004
h4n2	Gas	8.770e-004	2.380e-004
chn	Gas	4.866e-004	1.321e-004
h2o2	Gas	2.059e-004	5.589e-005
cho	Gas	2.000e-004	5.428e-005
cno	Gas	1.409e-004	3.823e-005
h2n2	Gas	1.268e-004	3.441e-005
c3h8	Gas	1.230e-004	3.337e-005
o2	Gas	7.260e-005	1.971e-005
c2h2	Gas	6.743e-005	1.830e-005
ch2	Gas	2.264e-005	6.145e-006
o	Gas	1.600e-005	4.344e-006

c3h6	Gas	1.102e-005	2.991e-006
hno	Gas	8.745e-006	2.374e-006
n2o	Gas	2.899e-006	7.867e-007
hn	Gas	2.792e-006	7.579e-007
cn	Gas	2.520e-006	6.841e-007
ho2	Gas	2.173e-006	5.899e-007
no2	Gas	1.424e-006	3.865e-007
n	Gas	1.292e-006	3.508e-007
hno2	Gas	1.202e-007	3.263e-008
c2h	Gas	1.122e-007	3.045e-008
cn2	Gas	1.112e-007	3.017e-008
n3	Gas	7.361e-008	1.998e-008
c2n2	Gas	3.026e-008	8.213e-009
ch	Gas	1.636e-008	4.441e-009
no2h	Gas	1.087e-008	2.950e-009
c2h4o	Gas	7.988e-009	2.168e-009
c2o	Gas	1.812e-009	4.919e-010
c2n	Gas	1.693e-009	4.595e-010
c	Gas	1.110e-009	3.013e-010
hno3	Gas	2.799e-010	7.596e-011
c3o2	Gas	2.496e-010	6.773e-011
no3	Gas	1.350e-010	3.665e-011
c2	Gas	3.627e-011	9.845e-012
cnn	Gas	1.288e-011	3.496e-012
o3	Gas	5.605e-012	1.521e-012
c3	Gas	2.356e-013	6.394e-014
n2o3	Gas	6.637e-014	1.801e-014
n2o4	Gas	1.392e-014	3.777e-015
n2o5	Gas	1.121e-019	3.043e-020
c4	Gas	5.266e-021	1.429e-021
c4n2	Gas	4.725e-024	1.283e-024
c5	Gas	2.820e-028	7.653e-029
*c	solid	6.703e+000	1.819e+000
*h2o	liquid	0.000e+000	0.000e+000
Total	Gas	3.112e+001	8.448e+000
Total	Cond.	6.703e+000	1.819e+000

Reference state = reactants
H(R) = H-22.34, E(R) = E-22.32, 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)
1.)	14345.5	1.2046	1800.0	-453.86	-872.37	1.614	1.1757

Product concentrations

Name		(mol/kg)	(mol gas/mol explosive)
n2	Gas	1.132e+001	3.071e+000
co2	Gas	8.040e+000	2.182e+000
h2o	Gas	7.404e+000	2.010e+000
co	Gas	3.309e+000	8.980e-001
h2	Gas	1.962e+000	5.326e-001
ch4	Gas	1.480e+000	4.016e-001
h3n	Gas	2.370e-001	6.432e-002
ch2o2	Gas	1.671e-002	4.536e-003
c2h6	Gas	1.473e-002	3.997e-003
ch2o	Gas	3.354e-003	9.102e-004
c2h4	Gas	2.434e-003	6.607e-004
ch3oh	Gas	2.019e-003	5.479e-004
chn	Gas	1.840e-003	4.993e-004
chno	Gas	1.245e-003	3.378e-004
ch3	Gas	2.063e-004	5.600e-005
c3h8	Gas	3.143e-005	8.531e-006
c2h2	Gas	1.964e-005	5.330e-006
c3h6	Gas	1.895e-005	5.143e-006
h	Gas	1.773e-005	4.813e-006
cho	Gas	1.263e-005	3.429e-006
h2n	Gas	3.901e-006	1.059e-006
ho	Gas	2.996e-006	8.131e-007

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        no  Gas    2.763e-007  7.500e-008
      h4n2  Gas    6.297e-008  1.709e-008
      c2n2  Gas    1.473e-008  3.997e-009
      h2n2  Gas    1.200e-008  3.256e-009
      c3o2  Gas    1.065e-008  2.892e-009
       cno  Gas    7.611e-009  2.066e-009
       ch2  Gas    2.492e-009  6.763e-010
     c2h4o  Gas    1.983e-009  5.381e-010
      h2o2  Gas    1.552e-009  4.211e-010
       hno  Gas    1.507e-009  4.091e-010
        cn  Gas    9.317e-010  2.529e-010
       n2o  Gas    4.791e-010  1.300e-010
        hn  Gas    3.008e-010  8.163e-011
       c2h  Gas    1.620e-010  4.397e-011
        o2  Gas    9.260e-011  2.513e-011
         o  Gas    5.177e-011  1.405e-011
       c2o  Gas    2.265e-011  6.147e-012
         n  Gas    5.253e-012  1.426e-012
       ho2  Gas    4.378e-012  1.188e-012
      hno2  Gas    3.184e-012  8.641e-013
       cn2  Gas    1.705e-012  4.627e-013
      no2h  Gas    1.644e-012  4.462e-013
       c2n  Gas    8.265e-013  2.243e-013
        n3  Gas    3.264e-013  8.860e-014
       no2  Gas    2.738e-013  7.431e-014
        ch  Gas    4.701e-014  1.276e-014
       cnn  Gas    2.716e-016  7.372e-017
         c  Gas    1.311e-016  3.558e-017
      c4n2  Gas    7.204e-018  1.955e-018
        c3  Gas    2.010e-018  5.456e-019
      hno3  Gas    1.998e-018  5.423e-019
        c2  Gas    8.925e-019  2.422e-019
       no3  Gas    2.889e-022  7.841e-023
        o3  Gas    1.483e-022  4.025e-023
      n2o3  Gas    6.125e-024  1.662e-024
        c4  Gas    6.333e-025  1.719e-025
        c5  Gas    2.488e-027  6.752e-028
      n2o4  Gas    8.736e-030  2.371e-030
      n2o5  Gas    4.178e-037  1.134e-037
        *c  solid  5.811e+000  1.577e+000
     *h2o liquid   0.000e+000  0.000e+000

     Total Gas    3.379e+001  9.171e+000
     Total Cond.  5.811e+000  1.577e+000

                          Reference state = reactants
                H(R) = H-22.34, E(R) = E-22.32, S(R) = S- 0.00

          P           V         T       H(R)       E(R)       S(R)      VGS
       (ATM)       (CC/GM)     (K)     (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)   14260.5      1.2074   1797.7   -456.35    -873.34     1.614     1.1785

Product concentrations
         Name    (mol/kg) (mol gas/mol explosive)
*       n2  Gas    1.132e+001  3.071e+000
*      co2  Gas    8.040e+000  2.182e+000
*      h2o  Gas    7.404e+000  2.010e+000
*       co  Gas    3.309e+000  8.980e-001
*       h2  Gas    1.962e+000  5.326e-001
*      ch4  Gas    1.480e+000  4.016e-001
*      h3n  Gas    2.370e-001  6.432e-002
*    ch2o2  Gas    1.671e-002  4.536e-003
*     c2h6  Gas    1.473e-002  3.997e-003
*     ch2o  Gas    3.354e-003  9.102e-004
*     c2h4  Gas    2.434e-003  6.607e-004
*    ch3oh  Gas    2.019e-003  5.479e-004
*      chn  Gas    1.840e-003  4.993e-004
*     chno  Gas    1.245e-003  3.378e-004
*      ch3  Gas    2.063e-004  5.600e-005
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*     c3h8  Gas   3.143e-005  8.531e-006
*     c2h2  Gas   1.964e-005  5.330e-006
*     c3h6  Gas   1.895e-005  5.143e-006
*        h  Gas   1.773e-005  4.813e-006
*      cho  Gas   1.263e-005  3.429e-006
*      h2n  Gas   3.901e-006  1.059e-006
*       ho  Gas   2.996e-006  8.131e-007
*       no  Gas   2.763e-007  7.500e-008
*     h4n2  Gas   6.297e-008  1.709e-008
*     c2n2  Gas   1.473e-008  3.997e-009
*     h2n2  Gas   1.200e-008  3.256e-009
*     c3o2  Gas   1.065e-008  2.892e-009
*      cno  Gas   7.611e-009  2.066e-009
*      ch2  Gas   2.492e-009  6.763e-010
*    c2h4o  Gas   1.983e-009  5.381e-010
*     h2o2  Gas   1.552e-009  4.211e-010
*      hno  Gas   1.507e-009  4.091e-010
*       cn  Gas   9.317e-010  2.529e-010
*      n2o  Gas   4.791e-010  1.300e-010
*       hn  Gas   3.008e-010  8.163e-011
*      c2h  Gas   1.620e-010  4.397e-011
*       o2  Gas   9.260e-011  2.513e-011
*        o  Gas   5.177e-011  1.405e-011
*      c2o  Gas   2.265e-011  6.147e-012
*        n  Gas   5.253e-012  1.426e-012
*      ho2  Gas   4.378e-012  1.188e-012
*     hno2  Gas   3.184e-012  8.641e-013
*      cn2  Gas   1.705e-012  4.627e-013
*     no2h  Gas   1.644e-012  4.462e-013
*      c2n  Gas   8.265e-013  2.243e-013
*       n3  Gas   3.264e-013  8.860e-014
*      no2  Gas   2.738e-013  7.431e-014
*       ch  Gas   4.701e-014  1.276e-014
*      cnn  Gas   2.716e-016  7.372e-017
*        c  Gas   1.311e-016  3.558e-017
*     c4n2  Gas   7.204e-018  1.955e-018
*       c3  Gas   2.010e-018  5.456e-019
*     hno3  Gas   1.998e-018  5.423e-019
*       c2  Gas   8.925e-019  2.422e-019
*      no3  Gas   2.889e-022  7.841e-023
*       o3  Gas   1.483e-022  4.025e-023
*     n2o3  Gas   6.125e-024  1.662e-024
*       c4  Gas   6.333e-025  1.719e-025
*       c5  Gas   2.488e-027  6.752e-028
*     n2o4  Gas   8.736e-030  2.371e-030
*     n2o5  Gas   4.178e-037  1.134e-037
*       *c  solid 5.811e+000  1.577e+000
*     *h2o liquid 0.000e+000  0.000e+000

      Total Gas   3.379e+001  9.171e+000
      Total Cond. 5.811e+000  1.577e+000

                          Reference state = reactants
                H(R) = H-22.34, E(R) = E-22.32, S(R) = S- 0.00

         P          V         T       H(R)      E(R)      S(R)      VGS
       (ATM)      (CC/GM)     (K)    (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)   3455.7      2.2502   1347.7   -859.33  -1047.64    1.614    2.2210

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.132e+001  3.071e+000
*      co2  Gas   8.040e+000  2.182e+000
*      h2o  Gas   7.404e+000  2.010e+000
*       co  Gas   3.309e+000  8.980e-001
*       h2  Gas   1.962e+000  5.326e-001
*      ch4  Gas   1.480e+000  4.016e-001
*      h3n  Gas   2.370e-001  6.432e-002
*    ch2o2  Gas   1.671e-002  4.536e-003
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*     c2h6  Gas   1.473e-002  3.997e-003
*     ch2o  Gas   3.354e-003  9.102e-004
*     c2h4  Gas   2.434e-003  6.607e-004
*    ch3oh  Gas   2.019e-003  5.479e-004
*      chn  Gas   1.840e-003  4.993e-004
*     chno  Gas   1.245e-003  3.378e-004
*      ch3  Gas   2.063e-004  5.600e-005
*     c3h8  Gas   3.143e-005  8.531e-006
*     c2h2  Gas   1.964e-005  5.330e-006
*     c3h6  Gas   1.895e-005  5.143e-006
*        h  Gas   1.773e-005  4.813e-006
*      cho  Gas   1.263e-005  3.429e-006
*      h2n  Gas   3.901e-006  1.059e-006
*       ho  Gas   2.996e-006  8.131e-007
*       no  Gas   2.763e-007  7.500e-008
*     h4n2  Gas   6.297e-008  1.709e-008
*     c2n2  Gas   1.473e-008  3.997e-009
*     h2n2  Gas   1.200e-008  3.256e-009
*     c3o2  Gas   1.065e-008  2.892e-009
*      cno  Gas   7.611e-009  2.066e-009
*      ch2  Gas   2.492e-009  6.763e-010
*    c2h4o  Gas   1.983e-009  5.381e-010
*     h2o2  Gas   1.552e-009  4.211e-010
*      hno  Gas   1.507e-009  4.091e-010
*       cn  Gas   9.317e-010  2.529e-010
*      n2o  Gas   4.791e-010  1.300e-010
*       hn  Gas   3.008e-010  8.163e-011
*      c2h  Gas   1.620e-010  4.397e-011
*       o2  Gas   9.260e-011  2.513e-011
*        o  Gas   5.177e-011  1.405e-011
*      c2o  Gas   2.265e-011  6.147e-012
*        n  Gas   5.253e-012  1.426e-012
*      ho2  Gas   4.378e-012  1.188e-012
*     hno2  Gas   3.184e-012  8.641e-013
*      cn2  Gas   1.705e-012  4.627e-013
*     no2h  Gas   1.644e-012  4.462e-013
*      c2n  Gas   8.265e-013  2.243e-013
*       n3  Gas   3.264e-013  8.860e-014
*      no2  Gas   2.738e-013  7.431e-014
*       ch  Gas   4.701e-014  1.276e-014
*      cnn  Gas   2.716e-016  7.372e-017
*        c  Gas   1.311e-016  3.558e-017
*     c4n2  Gas   7.204e-018  1.955e-018
*       c3  Gas   2.010e-018  5.456e-019
*     hno3  Gas   1.998e-018  5.423e-019
*       c2  Gas   8.925e-019  2.422e-019
*      no3  Gas   2.889e-022  7.841e-023
*       o3  Gas   1.483e-022  4.025e-023
*     n2o3  Gas   6.125e-024  1.662e-024
*       c4  Gas   6.333e-025  1.719e-025
*       c5  Gas   2.488e-027  6.752e-028
*     n2o4  Gas   8.736e-030  2.371e-030
*     n2o5  Gas   4.178e-037  1.134e-037
*       *c  solid 5.811e+000  1.577e+000
*     *h2o liquid 0.000e+000  0.000e+000

      Total Gas   3.379e+001  9.171e+000
      Total Cond. 5.811e+000  1.577e+000

                          Reference state = reactants
                 H(R) = H-22.34, E(R) = E-22.32, S(R) = S- 0.00

          P           V         T       H(R)       E(R)       S(R)      VGS
        (ATM)       (CC/GM)     (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)    1442.5       3.5674   1141.2   -993.43  -1118.04    1.614     3.5382

Product concentrations
          Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.132e+001  3.071e+000
```

```
*      co2  Gas   8.040e+000  2.182e+000
*      h2o  Gas   7.404e+000  2.010e+000
*       co  Gas   3.309e+000  8.980e-001
*       h2  Gas   1.962e+000  5.326e-001
*      ch4  Gas   1.480e+000  4.016e-001
*      h3n  Gas   2.370e-001  6.432e-002
*    ch2o2  Gas   1.671e-002  4.536e-003
*     c2h6  Gas   1.473e-002  3.997e-003
*     ch2o  Gas   3.354e-003  9.102e-004
*     c2h4  Gas   2.434e-003  6.607e-004
*    ch3oh  Gas   2.019e-003  5.479e-004
*      chn  Gas   1.840e-003  4.993e-004
*     chno  Gas   1.245e-003  3.378e-004
*      ch3  Gas   2.063e-004  5.600e-005
*     c3h8  Gas   3.143e-005  8.531e-006
*     c2h2  Gas   1.964e-005  5.330e-006
*     c3h6  Gas   1.895e-005  5.143e-006
*        h  Gas   1.773e-005  4.813e-006
*      cho  Gas   1.263e-005  3.429e-006
*      h2n  Gas   3.901e-006  1.059e-006
*       ho  Gas   2.996e-006  8.131e-007
*       no  Gas   2.763e-007  7.500e-008
*     h4n2  Gas   6.297e-008  1.709e-008
*     c2n2  Gas   1.473e-008  3.997e-009
*     h2n2  Gas   1.200e-008  3.256e-009
*     c3o2  Gas   1.065e-008  2.892e-009
*      cno  Gas   7.611e-009  2.066e-009
*      ch2  Gas   2.492e-009  6.763e-010
*    c2h4o  Gas   1.983e-009  5.381e-010
*     h2o2  Gas   1.552e-009  4.211e-010
*      hno  Gas   1.507e-009  4.091e-010
*       cn  Gas   9.317e-010  2.529e-010
*      n2o  Gas   4.791e-010  1.300e-010
*       hn  Gas   3.008e-010  8.163e-011
*      c2h  Gas   1.620e-010  4.397e-011
*       o2  Gas   9.260e-011  2.513e-011
*        o  Gas   5.177e-011  1.405e-011
*      c2o  Gas   2.265e-011  6.147e-012
*        n  Gas   5.253e-012  1.426e-012
*      ho2  Gas   4.378e-012  1.188e-012
*     hno2  Gas   3.184e-012  8.641e-013
*      cn2  Gas   1.705e-012  4.627e-013
*     no2h  Gas   1.644e-012  4.462e-013
*      c2n  Gas   8.265e-013  2.243e-013
*       n3  Gas   3.264e-013  8.860e-014
*      no2  Gas   2.738e-013  7.431e-014
*       ch  Gas   4.701e-014  1.276e-014
*      cnn  Gas   2.716e-016  7.372e-017
*        c  Gas   1.311e-016  3.558e-017
*     c4n2  Gas   7.204e-018  1.955e-018
*       c3  Gas   2.010e-018  5.456e-019
*     hno3  Gas   1.998e-018  5.423e-019
*       c2  Gas   8.925e-019  2.422e-019
*      no3  Gas   2.889e-022  7.841e-023
*       o3  Gas   1.483e-022  4.025e-023
*     n2o3  Gas   6.125e-024  1.662e-024
*       c4  Gas   6.333e-025  1.719e-025
*       c5  Gas   2.488e-027  6.752e-028
*     n2o4  Gas   8.736e-030  2.371e-030
*     n2o5  Gas   4.178e-037  1.134e-037
*       *c  solid 5.811e+000  1.577e+000
*     *h2o liquid 0.000e+000  0.000e+000

      Total Gas   3.379e+001  9.171e+000
      Total Cond. 5.811e+000  1.577e+000

                          Reference state = reactants
                H(R) = H-22.34, E(R) = E-22.32, 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)
1.)	697.8	5.4883	995.6	-1071.51	-1164.24	1.614	5.4591

Product concentrations

	Name		(mol/kg)	(mol gas/mol explosive)
*	n2	Gas	1.132e+001	3.071e+000
*	co2	Gas	8.040e+000	2.182e+000
*	h2o	Gas	7.404e+000	2.010e+000
*	co	Gas	3.309e+000	8.980e-001
*	h2	Gas	1.962e+000	5.326e-001
*	ch4	Gas	1.480e+000	4.016e-001
*	h3n	Gas	2.370e-001	6.432e-002
*	ch2o2	Gas	1.671e-002	4.536e-003
*	c2h6	Gas	1.473e-002	3.997e-003
*	ch2o	Gas	3.354e-003	9.102e-004
*	c2h4	Gas	2.434e-003	6.607e-004
*	ch3oh	Gas	2.019e-003	5.479e-004
*	chn	Gas	1.840e-003	4.993e-004
*	chno	Gas	1.245e-003	3.378e-004
*	ch3	Gas	2.063e-004	5.600e-005
*	c3h8	Gas	3.143e-005	8.531e-006
*	c2h2	Gas	1.964e-005	5.330e-006
*	c3h6	Gas	1.895e-005	5.143e-006
*	h	Gas	1.773e-005	4.813e-006
*	cho	Gas	1.263e-005	3.429e-006
*	h2n	Gas	3.901e-006	1.059e-006
*	ho	Gas	2.996e-006	8.131e-007
*	no	Gas	2.763e-007	7.500e-008
*	h4n2	Gas	6.297e-008	1.709e-008
*	c2n2	Gas	1.473e-008	3.997e-009
*	h2n2	Gas	1.200e-008	3.256e-009
*	c3o2	Gas	1.065e-008	2.892e-009
*	cno	Gas	7.611e-009	2.066e-009
*	ch2	Gas	2.492e-009	6.763e-010
*	c2h4o	Gas	1.983e-009	5.381e-010
*	h2o2	Gas	1.552e-009	4.211e-010
*	hno	Gas	1.507e-009	4.091e-010
*	cn	Gas	9.317e-010	2.529e-010
*	n2o	Gas	4.791e-010	1.300e-010
*	hn	Gas	3.008e-010	8.163e-011
*	c2h	Gas	1.620e-010	4.397e-011
*	o2	Gas	9.260e-011	2.513e-011
*	o	Gas	5.177e-011	1.405e-011
*	c2o	Gas	2.265e-011	6.147e-012
*	n	Gas	5.253e-012	1.426e-012
*	ho2	Gas	4.378e-012	1.188e-012
*	hno2	Gas	3.184e-012	8.641e-013
*	cn2	Gas	1.705e-012	4.627e-013
*	no2h	Gas	1.644e-012	4.462e-013
*	c2n	Gas	8.265e-013	2.243e-013
*	n3	Gas	3.264e-013	8.860e-014
*	no2	Gas	2.738e-013	7.431e-014
*	ch	Gas	4.701e-014	1.276e-014
*	cnn	Gas	2.716e-016	7.372e-017
*	c	Gas	1.311e-016	3.558e-017
*	c4n2	Gas	7.204e-018	1.955e-018
*	c3	Gas	2.010e-018	5.456e-019
*	hno3	Gas	1.998e-018	5.423e-019
*	c2	Gas	8.925e-019	2.422e-019
*	no3	Gas	2.889e-022	7.841e-023
*	o3	Gas	1.483e-022	4.025e-023
*	n2o3	Gas	6.125e-024	1.662e-024
*	c4	Gas	6.333e-025	1.719e-025
*	c5	Gas	2.488e-027	6.752e-028
*	n2o4	Gas	8.736e-030	2.371e-030
*	n2o5	Gas	4.178e-037	1.134e-037
*	*c	solid	5.811e+000	1.577e+000
*	*h2o	liquid	0.000e+000	0.000e+000

```
     Total Gas   3.379e+001  9.171e+000
     Total Cond. 5.811e+000  1.577e+000


                          Reference state = reactants
                  H(R) = H-22.34, E(R) = E-22.32, S(R) = S- 0.00

         P          V         T       H(R)      E(R)      S(R)     VGS
       (ATM)      (CC/GM)     (K)    (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)    243.9     10.9767    814.6  -1152.95  -1217.78    1.614   10.9475

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*      n2  Gas   1.132e+001  3.071e+000
*     co2  Gas   8.040e+000  2.182e+000
*     h2o  Gas   7.404e+000  2.010e+000
*      co  Gas   3.309e+000  8.980e-001
*      h2  Gas   1.962e+000  5.326e-001
*     ch4  Gas   1.480e+000  4.016e-001
*     h3n  Gas   2.370e-001  6.432e-002
*   ch2o2  Gas   1.671e-002  4.536e-003
*    c2h6  Gas   1.473e-002  3.997e-003
*    ch2o  Gas   3.354e-003  9.102e-004
*    c2h4  Gas   2.434e-003  6.607e-004
*   ch3oh  Gas   2.019e-003  5.479e-004
*     chn  Gas   1.840e-003  4.993e-004
*    chno  Gas   1.245e-003  3.378e-004
*     ch3  Gas   2.063e-004  5.600e-005
*    c3h8  Gas   3.143e-005  8.531e-006
*    c2h2  Gas   1.964e-005  5.330e-006
*    c3h6  Gas   1.895e-005  5.143e-006
*       h  Gas   1.773e-005  4.813e-006
*     cho  Gas   1.263e-005  3.429e-006
*     h2n  Gas   3.901e-006  1.059e-006
*      ho  Gas   2.996e-006  8.131e-007
*      no  Gas   2.763e-007  7.500e-008
*    h4n2  Gas   6.297e-008  1.709e-008
*    c2n2  Gas   1.473e-008  3.997e-009
*    h2n2  Gas   1.200e-008  3.256e-009
*    c3o2  Gas   1.065e-008  2.892e-009
*     cno  Gas   7.611e-009  2.066e-009
*     ch2  Gas   2.492e-009  6.763e-010
*   c2h4o  Gas   1.983e-009  5.381e-010
*    h2o2  Gas   1.552e-009  4.211e-010
*     hno  Gas   1.507e-009  4.091e-010
*      cn  Gas   9.317e-010  2.529e-010
*     n2o  Gas   4.791e-010  1.300e-010
*      hn  Gas   3.008e-010  8.163e-011
*     c2h  Gas   1.620e-010  4.397e-011
*      o2  Gas   9.260e-011  2.513e-011
*       o  Gas   5.177e-011  1.405e-011
*     c2o  Gas   2.265e-011  6.147e-012
*       n  Gas   5.253e-012  1.426e-012
*     ho2  Gas   4.378e-012  1.188e-012
*    hno2  Gas   3.184e-012  8.641e-013
*     cn2  Gas   1.705e-012  4.627e-013
*    no2h  Gas   1.644e-012  4.462e-013
*     c2n  Gas   8.265e-013  2.243e-013
*      n3  Gas   3.264e-013  8.860e-014
*     no2  Gas   2.738e-013  7.431e-014
*      ch  Gas   4.701e-014  1.276e-014
*     cnn  Gas   2.716e-016  7.372e-017
*       c  Gas   1.311e-016  3.558e-017
*    c4n2  Gas   7.204e-018  1.955e-018
*      c3  Gas   2.010e-018  5.456e-019
*    hno3  Gas   1.998e-018  5.423e-019
*      c2  Gas   8.925e-019  2.422e-019
*     no3  Gas   2.889e-022  7.841e-023
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*       o3  Gas   1.483e-022  4.025e-023
*     n2o3  Gas   6.125e-024  1.662e-024
*       c4  Gas   6.333e-025  1.719e-025
*       c5  Gas   2.488e-027  6.752e-028
*     n2o4  Gas   8.736e-030  2.371e-030
*     n2o5  Gas   4.178e-037  1.134e-037
*       *c  solid 5.811e+000  1.577e+000
*     *h2o liquid 0.000e+000  0.000e+000

      Total Gas   3.379e+001  9.171e+000
      Total Cond. 5.811e+000  1.577e+000

                          Reference state = reactants
                 H(R) = H-22.34, E(R) = E-22.32, S(R) = S- 0.00

          P           V         T       H(R)       E(R)      S(R)     VGS
        (ATM)       (CC/GM)     (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)     92.6      21.9533    671.7  -1207.68  -1256.87    1.614   21.9241

Product concentrations
          Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.132e+001  3.071e+000
*      co2  Gas   8.040e+000  2.182e+000
*      h2o  Gas   7.404e+000  2.010e+000
*       co  Gas   3.309e+000  8.980e-001
*       h2  Gas   1.962e+000  5.326e-001
*      ch4  Gas   1.480e+000  4.016e-001
*      h3n  Gas   2.370e-001  6.432e-002
*    ch2o2  Gas   1.671e-002  4.536e-003
*     c2h6  Gas   1.473e-002  3.997e-003
*     ch2o  Gas   3.354e-003  9.102e-004
*     c2h4  Gas   2.434e-003  6.607e-004
*    ch3oh  Gas   2.019e-003  5.479e-004
*      chn  Gas   1.840e-003  4.993e-004
*     chno  Gas   1.245e-003  3.378e-004
*      ch3  Gas   2.063e-004  5.600e-005
*     c3h8  Gas   3.143e-005  8.531e-006
*     c2h2  Gas   1.964e-005  5.330e-006
*     c3h6  Gas   1.895e-005  5.143e-006
*        h  Gas   1.773e-005  4.813e-006
*      cho  Gas   1.263e-005  3.429e-006
*      h2n  Gas   3.901e-006  1.059e-006
*       ho  Gas   2.996e-006  8.131e-007
*       no  Gas   2.763e-007  7.500e-008
*     h4n2  Gas   6.297e-008  1.709e-008
*     c2n2  Gas   1.473e-008  3.997e-009
*     h2n2  Gas   1.200e-008  3.256e-009
*     c3o2  Gas   1.065e-008  2.892e-009
*      cno  Gas   7.611e-009  2.066e-009
*      ch2  Gas   2.492e-009  6.763e-010
*    c2h4o  Gas   1.983e-009  5.381e-010
*     h2o2  Gas   1.552e-009  4.211e-010
*      hno  Gas   1.507e-009  4.091e-010
*       cn  Gas   9.317e-010  2.529e-010
*      n2o  Gas   4.791e-010  1.300e-010
*       hn  Gas   3.008e-010  8.163e-011
*      c2h  Gas   1.620e-010  4.397e-011
*       o2  Gas   9.260e-011  2.513e-011
*        o  Gas   5.177e-011  1.405e-011
*      c2o  Gas   2.265e-011  6.147e-012
*        n  Gas   5.253e-012  1.426e-012
*      ho2  Gas   4.378e-012  1.188e-012
*     hno2  Gas   3.184e-012  8.641e-013
*      cn2  Gas   1.705e-012  4.627e-013
*     no2h  Gas   1.644e-012  4.462e-013
*      c2n  Gas   8.265e-013  2.243e-013
*       n3  Gas   3.264e-013  8.860e-014
*      no2  Gas   2.738e-013  7.431e-014
*       ch  Gas   4.701e-014  1.276e-014
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*      cnn  Gas    2.716e-016  7.372e-017
*        c  Gas    1.311e-016  3.558e-017
*     c4n2  Gas    7.204e-018  1.955e-018
*       c3  Gas    2.010e-018  5.456e-019
*     hno3  Gas    1.998e-018  5.423e-019
*       c2  Gas    8.925e-019  2.422e-019
*      no3  Gas    2.889e-022  7.841e-023
*       o3  Gas    1.483e-022  4.025e-023
*     n2o3  Gas    6.125e-024  1.662e-024
*       c4  Gas    6.333e-025  1.719e-025
*       c5  Gas    2.488e-027  6.752e-028
*     n2o4  Gas    8.736e-030  2.371e-030
*     n2o5  Gas    4.178e-037  1.134e-037
*       *c  solid  5.811e+000  1.577e+000
*     *h2o liquid  0.000e+000  0.000e+000

      Total Gas    3.379e+001  9.171e+000
      Total Cond.  5.811e+000  1.577e+000

                          Reference state = reactants
                 H(R) = H-22.34, E(R) = E-22.32, S(R) = S- 0.00

          P          V          T       H(R)       E(R)       S(R)      VGS
        (ATM)      (CC/GM)      (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)     36.5     43.9066     552.7  -1248.39   -1287.17     1.614    43.8775

Product concentrations
          Name    (mol/kg)  (mol gas/mol explosive)
*       n2  Gas    1.132e+001  3.071e+000
*      co2  Gas    8.040e+000  2.182e+000
*      h2o  Gas    7.404e+000  2.010e+000
*       co  Gas    3.309e+000  8.980e-001
*       h2  Gas    1.962e+000  5.326e-001
*      ch4  Gas    1.480e+000  4.016e-001
*      h3n  Gas    2.370e-001  6.432e-002
*    ch2o2  Gas    1.671e-002  4.536e-003
*     c2h6  Gas    1.473e-002  3.997e-003
*     ch2o  Gas    3.354e-003  9.102e-004
*     c2h4  Gas    2.434e-003  6.607e-004
*    ch3oh  Gas    2.019e-003  5.479e-004
*      chn  Gas    1.840e-003  4.993e-004
*     chno  Gas    1.245e-003  3.378e-004
*      ch3  Gas    2.063e-004  5.600e-005
*     c3h8  Gas    3.143e-005  8.531e-006
*     c2h2  Gas    1.964e-005  5.330e-006
*     c3h6  Gas    1.895e-005  5.143e-006
*        h  Gas    1.773e-005  4.813e-006
*      cho  Gas    1.263e-005  3.429e-006
*      h2n  Gas    3.901e-006  1.059e-006
*       ho  Gas    2.996e-006  8.131e-007
*       no  Gas    2.763e-007  7.500e-008
*     h4n2  Gas    6.297e-008  1.709e-008
*     c2n2  Gas    1.473e-008  3.997e-009
*     h2n2  Gas    1.200e-008  3.256e-009
*     c3o2  Gas    1.065e-008  2.892e-009
*      cno  Gas    7.611e-009  2.066e-009
*      ch2  Gas    2.492e-009  6.763e-010
*    c2h4o  Gas    1.983e-009  5.381e-010
*     h2o2  Gas    1.552e-009  4.211e-010
*      hno  Gas    1.507e-009  4.091e-010
*       cn  Gas    9.317e-010  2.529e-010
*      n2o  Gas    4.791e-010  1.300e-010
*       hn  Gas    3.008e-010  8.163e-011
*      c2h  Gas    1.620e-010  4.397e-011
*       o2  Gas    9.260e-011  2.513e-011
*        o  Gas    5.177e-011  1.405e-011
*      c2o  Gas    2.265e-011  6.147e-012
*        n  Gas    5.253e-012  1.426e-012
*      ho2  Gas    4.378e-012  1.188e-012
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*     hno2  Gas    3.184e-012  8.641e-013
*      cn2  Gas    1.705e-012  4.627e-013
*     no2h  Gas    1.644e-012  4.462e-013
*      c2n  Gas    8.265e-013  2.243e-013
*       n3  Gas    3.264e-013  8.860e-014
*      no2  Gas    2.738e-013  7.431e-014
*       ch  Gas    4.701e-014  1.276e-014
*      cnn  Gas    2.716e-016  7.372e-017
*        c  Gas    1.311e-016  3.558e-017
*     c4n2  Gas    7.204e-018  1.955e-018
*       c3  Gas    2.010e-018  5.456e-019
*     hno3  Gas    1.998e-018  5.423e-019
*       c2  Gas    8.925e-019  2.422e-019
*      no3  Gas    2.889e-022  7.841e-023
*       o3  Gas    1.483e-022  4.025e-023
*     n2o3  Gas    6.125e-024  1.662e-024
*       c4  Gas    6.333e-025  1.719e-025
*       c5  Gas    2.488e-027  6.752e-028
*     n2o4  Gas    8.736e-030  2.371e-030
*     n2o5  Gas    4.178e-037  1.134e-037
*       *c  solid  5.811e+000  1.577e+000
*     *h2o liquid  0.000e+000  0.000e+000

      Total Gas    3.379e+001  9.171e+000
      Total Cond.  5.811e+000  1.577e+000

                          Reference state = reactants
                 H(R) = H-22.34, E(R) = E-22.32, S(R) = S- 0.00

          P           V         T       H(R)       E(R)       S(R)      VGS
        (ATM)      (CC/GM)     (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)     14.6     87.8132    451.6  -1280.25   -1311.25    1.614    87.7841

Product concentrations
          Name    (mol/kg) (mol gas/mol explosive)
*       n2  Gas    1.132e+001  3.071e+000
*      co2  Gas    8.040e+000  2.182e+000
*      h2o  Gas    7.404e+000  2.010e+000
*       co  Gas    3.309e+000  8.980e-001
*       h2  Gas    1.962e+000  5.326e-001
*      ch4  Gas    1.480e+000  4.016e-001
*      h3n  Gas    2.370e-001  6.432e-002
*    ch2o2  Gas    1.671e-002  4.536e-003
*     c2h6  Gas    1.473e-002  3.997e-003
*     ch2o  Gas    3.354e-003  9.102e-004
*     c2h4  Gas    2.434e-003  6.607e-004
*    ch3oh  Gas    2.019e-003  5.479e-004
*      chn  Gas    1.840e-003  4.993e-004
*     chno  Gas    1.245e-003  3.378e-004
*      ch3  Gas    2.063e-004  5.600e-005
*     c3h8  Gas    3.143e-005  8.531e-006
*     c2h2  Gas    1.964e-005  5.330e-006
*     c3h6  Gas    1.895e-005  5.143e-006
*        h  Gas    1.773e-005  4.813e-006
*      cho  Gas    1.263e-005  3.429e-006
*      h2n  Gas    3.901e-006  1.059e-006
*       ho  Gas    2.996e-006  8.131e-007
*       no  Gas    2.763e-007  7.500e-008
*     h4n2  Gas    6.297e-008  1.709e-008
*     c2n2  Gas    1.473e-008  3.997e-009
*     h2n2  Gas    1.200e-008  3.256e-009
*     c3o2  Gas    1.065e-008  2.892e-009
*      cno  Gas    7.611e-009  2.066e-009
*      ch2  Gas    2.492e-009  6.763e-010
*    c2h4o  Gas    1.983e-009  5.381e-010
*     h2o2  Gas    1.552e-009  4.211e-010
*      hno  Gas    1.507e-009  4.091e-010
*       cn  Gas    9.317e-010  2.529e-010
*      n2o  Gas    4.791e-010  1.300e-010
```

```
*       hn  Gas   3.008e-010  8.163e-011
*      c2h  Gas   1.620e-010  4.397e-011
*       o2  Gas   9.260e-011  2.513e-011
*        o  Gas   5.177e-011  1.405e-011
*      c2o  Gas   2.265e-011  6.147e-012
*        n  Gas   5.253e-012  1.426e-012
*      ho2  Gas   4.378e-012  1.188e-012
*     hno2  Gas   3.184e-012  8.641e-013
*      cn2  Gas   1.705e-012  4.627e-013
*     no2h  Gas   1.644e-012  4.462e-013
*      c2n  Gas   8.265e-013  2.243e-013
*       n3  Gas   3.264e-013  8.860e-014
*      no2  Gas   2.738e-013  7.431e-014
*       ch  Gas   4.701e-014  1.276e-014
*      cnn  Gas   2.716e-016  7.372e-017
*        c  Gas   1.311e-016  3.558e-017
*     c4n2  Gas   7.204e-018  1.955e-018
*       c3  Gas   2.010e-018  5.456e-019
*     hno3  Gas   1.998e-018  5.423e-019
*       c2  Gas   8.925e-019  2.422e-019
*      no3  Gas   2.889e-022  7.841e-023
*       o3  Gas   1.483e-022  4.025e-023
*     n2o3  Gas   6.125e-024  1.662e-024
*       c4  Gas   6.333e-025  1.719e-025
*       c5  Gas   2.488e-027  6.752e-028
*     n2o4  Gas   8.736e-030  2.371e-030
*     n2o5  Gas   4.178e-037  1.134e-037
*       *c  solid 5.811e+000  1.577e+000
*     *h2o liquid 0.000e+000  0.000e+000

      Total Gas   3.379e+001  9.171e+000
      Total Cond. 5.811e+000  1.577e+000

                          The End of the Adiabat

                          Reference state = reactants
                  H(R) = H-22.34, E(R) = E-22.32, S(R) = S- 0.00

          P          V         T       H(R)      E(R)      S(R)     VGS
        (ATM)      (CC/GM)     (K)    (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)      2.5    333.7113    298.0  -1324.79  -1344.91    1.614  333.6822

Product concentrations
          Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.132e+001  3.071e+000
*      co2  Gas   8.040e+000  2.182e+000
*      h2o  Gas   7.404e+000  2.010e+000
*       co  Gas   3.309e+000  8.980e-001
*       h2  Gas   1.962e+000  5.326e-001
*      ch4  Gas   1.480e+000  4.016e-001
*      h3n  Gas   2.370e-001  6.432e-002
*    ch2o2  Gas   1.671e-002  4.536e-003
*     c2h6  Gas   1.473e-002  3.997e-003
*     ch2o  Gas   3.354e-003  9.102e-004
*     c2h4  Gas   2.434e-003  6.607e-004
*    ch3oh  Gas   2.019e-003  5.479e-004
*      chn  Gas   1.840e-003  4.993e-004
*     chno  Gas   1.245e-003  3.378e-004
*      ch3  Gas   2.063e-004  5.600e-005
*     c3h8  Gas   3.143e-005  8.531e-006
*     c2h2  Gas   1.964e-005  5.330e-006
*     c3h6  Gas   1.895e-005  5.143e-006
*        h  Gas   1.773e-005  4.813e-006
*      cho  Gas   1.263e-005  3.429e-006
*      h2n  Gas   3.901e-006  1.059e-006
*       ho  Gas   2.996e-006  8.131e-007
*       no  Gas   2.763e-007  7.500e-008
*     h4n2  Gas   6.297e-008  1.709e-008
*     c2n2  Gas   1.473e-008  3.997e-009
```

```
*    h2n2  Gas   1.200e-008  3.256e-009
*    c3o2  Gas   1.065e-008  2.892e-009
*     cno  Gas   7.611e-009  2.066e-009
*     ch2  Gas   2.492e-009  6.763e-010
*   c2h4o  Gas   1.983e-009  5.381e-010
*    h2o2  Gas   1.552e-009  4.211e-010
*     hno  Gas   1.507e-009  4.091e-010
*      cn  Gas   9.317e-010  2.529e-010
*     n2o  Gas   4.791e-010  1.300e-010
*      hn  Gas   3.008e-010  8.163e-011
*     c2h  Gas   1.620e-010  4.397e-011
*      o2  Gas   9.260e-011  2.513e-011
*       o  Gas   5.177e-011  1.405e-011
*     c2o  Gas   2.265e-011  6.147e-012
*       n  Gas   5.253e-012  1.426e-012
*     ho2  Gas   4.378e-012  1.188e-012
*    hno2  Gas   3.184e-012  8.641e-013
*     cn2  Gas   1.705e-012  4.627e-013
*    no2h  Gas   1.644e-012  4.462e-013
*     c2n  Gas   8.265e-013  2.243e-013
*      n3  Gas   3.264e-013  8.860e-014
*     no2  Gas   2.738e-013  7.431e-014
*      ch  Gas   4.701e-014  1.276e-014
*     cnn  Gas   2.716e-016  7.372e-017
*       c  Gas   1.311e-016  3.558e-017
*    c4n2  Gas   7.204e-018  1.955e-018
*      c3  Gas   2.010e-018  5.456e-019
*    hno3  Gas   1.998e-018  5.423e-019
*      c2  Gas   8.925e-019  2.422e-019
*     no3  Gas   2.889e-022  7.841e-023
*      o3  Gas   1.483e-022  4.025e-023
*    n2o3  Gas   6.125e-024  1.662e-024
*      c4  Gas   6.333e-025  1.719e-025
*      c5  Gas   2.488e-027  6.752e-028
*    n2o4  Gas   8.736e-030  2.371e-030
*    n2o5  Gas   4.178e-037  1.134e-037
*      *c  solid 5.811e+000  1.577e+000
*    *h2o liquid 0.000e+000  0.000e+000

     Total Gas   3.379e+001  9.171e+000
     Total Cond. 5.811e+000  1.577e+000
```

The Products at room temperature and pressure

Reference state = reactants
H(R) = H-22.34, E(R) = E-22.32, 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)
1.)	1.0	828.2455	298.0	-1324.87	-1344.91	1.675	828.2165

Product concentrations

```
         Name   (mol/kg) (mol gas/mol explosive)
*      n2  Gas   1.132e+001  3.071e+000
*     co2  Gas   8.040e+000  2.182e+000
*     h2o  Gas   7.404e+000  2.010e+000
*      co  Gas   3.309e+000  8.980e-001
*      h2  Gas   1.962e+000  5.326e-001
*     ch4  Gas   1.480e+000  4.016e-001
*     h3n  Gas   2.370e-001  6.432e-002
*   ch2o2  Gas   1.671e-002  4.536e-003
*    c2h6  Gas   1.473e-002  3.997e-003
*    ch2o  Gas   3.354e-003  9.102e-004
*    c2h4  Gas   2.434e-003  6.607e-004
*   ch3oh  Gas   2.019e-003  5.479e-004
*     chn  Gas   1.840e-003  4.993e-004
*    chno  Gas   1.245e-003  3.378e-004
*     ch3  Gas   2.063e-004  5.600e-005
*    c3h8  Gas   3.143e-005  8.531e-006
```

```
*    c2h2  Gas   1.964e-005  5.330e-006
*    c3h6  Gas   1.895e-005  5.143e-006
*       h  Gas   1.773e-005  4.813e-006
*     cho  Gas   1.263e-005  3.429e-006
*     h2n  Gas   3.901e-006  1.059e-006
*      ho  Gas   2.996e-006  8.131e-007
*      no  Gas   2.763e-007  7.500e-008
*    h4n2  Gas   6.297e-008  1.709e-008
*    c2n2  Gas   1.473e-008  3.997e-009
*    h2n2  Gas   1.200e-008  3.256e-009
*    c3o2  Gas   1.065e-008  2.892e-009
*     cno  Gas   7.611e-009  2.066e-009
*     ch2  Gas   2.492e-009  6.763e-010
*   c2h4o  Gas   1.983e-009  5.381e-010
*    h2o2  Gas   1.552e-009  4.211e-010
*     hno  Gas   1.507e-009  4.091e-010
*      cn  Gas   9.317e-010  2.529e-010
*     n2o  Gas   4.791e-010  1.300e-010
*      hn  Gas   3.008e-010  8.163e-011
*     c2h  Gas   1.620e-010  4.397e-011
*      o2  Gas   9.260e-011  2.513e-011
*       o  Gas   5.177e-011  1.405e-011
*     c2o  Gas   2.265e-011  6.147e-012
*       n  Gas   5.253e-012  1.426e-012
*     ho2  Gas   4.378e-012  1.188e-012
*    hno2  Gas   3.184e-012  8.641e-013
*     cn2  Gas   1.705e-012  4.627e-013
*    no2h  Gas   1.644e-012  4.462e-013
*     c2n  Gas   8.265e-013  2.243e-013
*      n3  Gas   3.264e-013  8.860e-014
*     no2  Gas   2.738e-013  7.431e-014
*      ch  Gas   4.701e-014  1.276e-014
*     cnn  Gas   2.716e-016  7.372e-017
*       c  Gas   1.311e-016  3.558e-017
*    c4n2  Gas   7.204e-018  1.955e-018
*      c3  Gas   2.010e-018  5.456e-019
*    hno3  Gas   1.998e-018  5.423e-019
*      c2  Gas   8.925e-019  2.422e-019
*     no3  Gas   2.889e-022  7.841e-023
*      o3  Gas   1.483e-022  4.025e-023
*    n2o3  Gas   6.125e-024  1.662e-024
*      c4  Gas   6.333e-025  1.719e-025
*      c5  Gas   2.488e-027  6.752e-028
*    n2o4  Gas   8.736e-030  2.371e-030
*    n2o5  Gas   4.178e-037  1.134e-037
*      *c  solid 5.811e+000  1.577e+000
*    *h2o liquid 0.000e+000  0.000e+000

     Total Gas   3.379e+001  9.171e+000
     Total Cond. 5.811e+000  1.577e+000
The mechanical energy of detonation =    -10.253 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.253 kJ/cc

JWL Tail Fit results:
Initial E0 =    -10.712, Final E0 =    -10.561
E0(V=infty) =    -10.561
C =      1.630,  omega =      0.392
Final fitting error = 0.002999

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

    10.000     -8.876     -8.878      0.071      0.066
    20.000     -9.284     -9.278      0.025      0.025
    40.000     -9.582     -9.584      0.009      0.010
    80.000     -9.813     -9.816      0.004      0.004
   160.000     -9.996     -9.994      0.001      0.001
```

```
JWL Fit results:
E0(V=infty) =    -10.561
R[1] =      4.952, R[2] =      1.117, omega =      0.392
A    =   1143.269, B    =     11.838, C     =      1.630
Final fitting error = 0.010014
```

V/V0	Actual E (kJ/cc)	Fit E (kJ/cc)	Actual P (GPa)	Fit P (GPa)
0.766	3.745	3.745	32.051	33.089
1.000	-1.186	-1.305	13.672	13.584
2.200	-6.658	-6.599	1.445	1.580
4.100	-7.987	-8.064	0.350	0.350
6.500	-8.523	-8.560	0.146	0.129
10.000	-8.876	-8.877	0.071	0.066
20.000	-9.284	-9.278	0.025	0.025
40.000	-9.582	-9.584	0.009	0.010
80.000	-9.813	-9.816	0.004	0.004
160.000	-9.996	-9.994	0.001	0.001

B.3 Summary printout

B.3.1 BKWC Product Library

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

The composition:

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
HMX	70.00	64.15	66.95	17866	155.47	0.000	296.17	$C_4H_8N_8O_8$
TNT	30.00	35.85	33.05	-15057	137.32	0.000	227.13	$C_7H_5N_3O_6$

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

The composition:

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
HMX	70.00	64.15	66.95	17866	155.47	0.000	296.17	$C_4H_8N_8O_8$
TNT	30.00	35.85	33.05	-15057	137.32	0.000	227.13	$C_7H_5N_3O_6$

```
Density = 1.8220 g/cc  Mixture TMD =1.8220 g/cc  % TMD = 100.0000


The C-J condition:
The pressure          =          32.29 GPa
The volume            =          0.413 cc/g
The density           =          2.421 g/cc
The energy            =           3.99 kJ/cc explosive
The temperature       =           4033 K
The shock velocity    =          8.463 mm/us
The particle velocity =          2.094 mm/us
The speed of sound    =          6.370 mm/us
Gamma                 =          3.042
```

Cylinder runs:

V/V0 (rel.)	Energy (kJ/cc)	% of standards TATB 1.83g/cc	PETN 1.76g/cc	HMX 1.89g/cc	CL-20 2.04g/cc	TRITON 1.70g/cc
1.00	-1.19					
2.20	-6.39	132	101	86	71	147
4.10	-7.67	132	99	87	73	139
6.50	-8.20	132	99	87	74	134
10.00	-8.55	131	98	87	75	130
20.00	-8.97	131	98	88	75	125

```
  40.00    -9.27     130       98       88       76       120
  80.00    -9.51     129       97       89       77       115
 160.00    -9.69

Freezing occurred at T =     1800.0 K and relative V =   2.201
The mechanical energy of detonation =     -9.949 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.949 kJ/cc

JWL Fit results:
E0   =   -10.284 kJ/cc
A    =   871.73 GPa, B = 10.08 GPa , C  =  1.63 GPa
R[1] =     4.67,  R[2] =  1.10,   omega =  0.39
RMS fitting error =   0.66 %
```

B.3.2 BKWS Product Library

```
Product library title: bkws library
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)
HMX      70.00 64.15 66.95  17866      155.47   0.000   296.17  C4H8N8O8
TNT      30.00 35.85 33.05 -15057      137.32   0.000   227.13  C7H5N3O6

Product library title: bkws library
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)
HMX      70.00 64.15 66.95  17866      155.47   0.000   296.17  C4H8N8O8
TNT      30.00 35.85 33.05 -15057      137.32   0.000   227.13  C7H5N3O6

Density = 1.8220 g/cc Mixture TMD = 1.8220 g/cc  % TMD = 100.0000


The C-J condition:
The pressure          =          32.05 GPa
The volume            =          0.421 cc/g
The density           =          2.378 g/cc
The energy            =           3.74 kJ/cc explosive
The temperature       =           3979 K
The shock velocity    =          8.677 mm/us
The particle velocity =          2.027 mm/us
The speed of sound    =          6.649 mm/us
Gamma                 =          3.280


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    -1.19
   2.20    -6.66     137       105       89       74       153
   4.10    -7.99     137       103       90       76       145
   6.50    -8.52     137       103       90       77       139
  10.00    -8.88     136       102       91       77       135
  20.00    -9.28     135       101       91       78       129
  40.00    -9.58     134       101       91       79       124
  80.00    -9.81     133       100       92       79       119
 160.00   -10.00

Freezing occurred at T =     1800.0 K and relative V =   2.195
The mechanical energy of detonation =    -10.253 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.253 kJ/cc
```

```
JWL Fit results:
E0   =  -10.561 kJ/cc
A    = 1143.27 GPa, B  = 11.84 GPa , C  =  1.63 GPa
R[1] =    4.95,   R[2] =  1.12,   omega =  0.39
RMS fitting error =   1.00 %
```

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(3) Laurence E. Fried, W. Michael Howard, P. Clark Souers (August 20, 1998): Cheetah 2.0 User's Manual, UCRL-MA-117541 Rev.5, Lawrence Livermore National Laboratory.