Card GAP test of Comp A-5

Gunnar Ove Nevstad

Forsvarets forskningsinstitutt/Norwegian Defence Research Establishment (FFI)

21 February 2008

FFI-rapport 2008/00469

87301

ISBN 978-82-464-1338-9

Keywords

Comp A-5

Sjokkfølsomhet

Card GAP test

Approved by

Jan Ivar Botnan Director

English summary

Comp A-5 pressed to 95.4 %TMD (1.702 g/cm^3) has been tested in NOL Card Gap test. The transition between no go and go was found to be 222-3 cards or 56.5 mm. This result indicates that Comp A-5 is relatively shock sensitive compared to more modern PBX compositions.

Sammendrag

Comp A-5 presset til 95.4% av TMD (1.702 g/cm^3) er blitt testet i NOL Card GAP test. Overgangen mellom ingen reaksjon og detonasjon ble funnet å være 222-3 kort eller 56.5 mm. Dette resultatet tilsier at Comp A-5 har en relativ høy sjokkfølsomhet sammenlignet med mer moderne PBX komposisjoner.

Contents

1 Introduction

STANAG 4488 (1) gives and overview of recommended tests for characterization of the shock sensitivity of energetic materials. For booster explosives there are two alternatives, a test using 20 mm and one using 40 mm charges. Normally we perform the 40 mm Intermediate Scale Gap test. However, since our object to be tested only can be filled into the test tubes by pressing we need a press tool. Since we at the moment do not have a pressing tool for charges with 40 mm diameter, but only a tool for 36 mm charges, we decided to use the NOL Card Gap test for testing the shock sensitivity of Comp A-5. This test uses the same barrier material in form of cellulose acetate cards as the intermediate scale gap test but a different booster material. The NOL Card Gap test uses two 80 g Tetryl Charges as booster (2).

2 Experimentally

2.1 The explosive

The tested explosive was produced by Dyno Nobel. Appendix A gives the control report of the tested explosive composition. Nammo Raufoss AS did perform the pressing of the pellets. Due to problems with releasing the pellets from the tool after pressing, some graphite had to be added.

2.2 Card GAP test

For testing the shock sensitivity of Comp A-5 we did use the standard NOL Card Gap test with two 80 g Tetryl pellets as boosters. The barrier was cellulose acetate cards with thickness 0.01

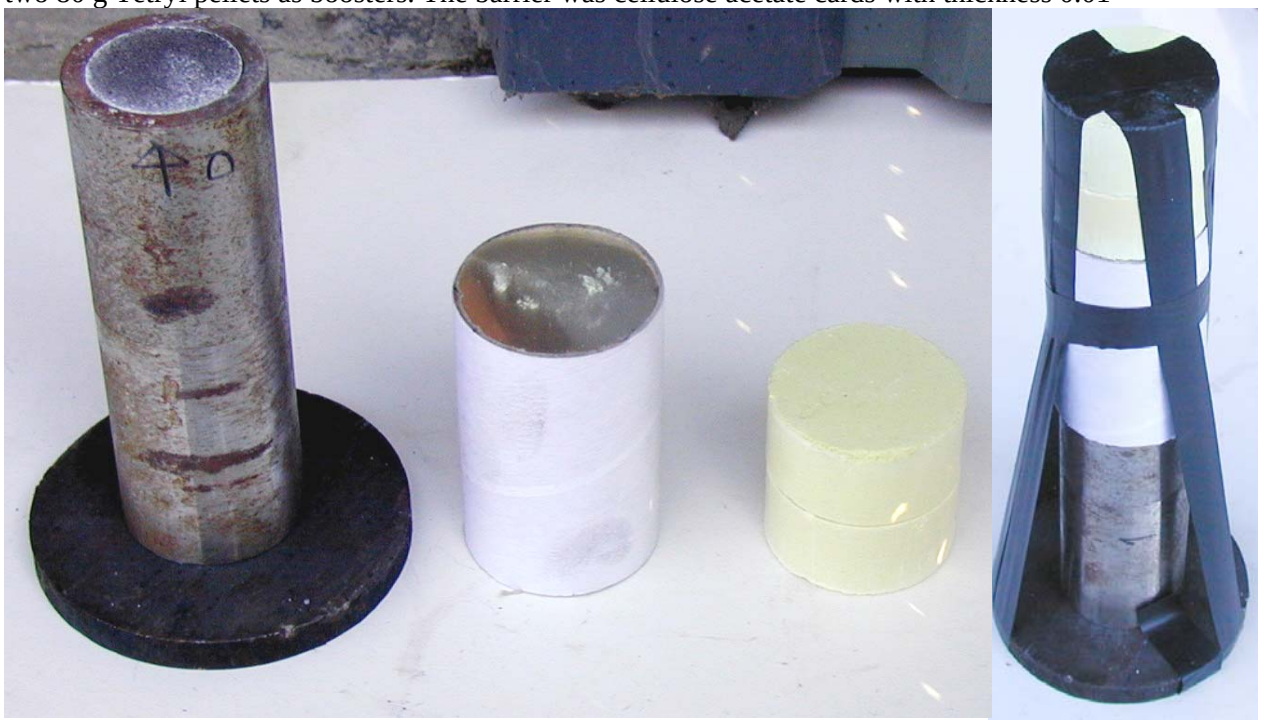

Figure 2.1 Pictures of shot No 1 before and after it was assembled.

inch or 2.54 mm. The test tubes were made from a seamless steel tube, length 140 mm, inner diameter 36.4 mm and wall thickness 6 mm. Figure 2.1 gives pictures of the tube, the cards and the boosters before and after assembling. To initiate the booster we used a detonator No. 8. The witness plate was a circular steel plate with diameter 110 mm.

2.3 Theoretical calculations

Theoretical calculations have been performed with Cheetah 2.0 code (3) for both TMD and the actual density we had for the pellets tested in NOL Card Gap test. Calculations have been performed with both the BKWC and the BKWS product databases. Complete printouts of these calculations are given in Appendix B.

3 Results

3.1 Density of tested Comp A-5 pellets

Table 3.1 gives the density of each tested pellet. To fill one tube we used 4 pellets which were glued together and to the steel tube. Figure 2.1 give a picture of tube No 1 after it was filled.

Tube No	Pellet No	Weight (g)	Diameter (mm)	Height (mm)	Volume (cm^3)	Density (g/cm^3)
1	1	60.34	36.03	34.68	35.359	1.707
	2	60.36	36.03	34.65	35.328	1.709
	3	60.35	36.03	34.63	35.308	1.709
	4	60.31	36.02	35.18	35.849	1.682
2	5	60.33	36.02	34.63	35.288	1.710
	6	60.34	36.02	34.58	35.237	1.712
	7	60.36	36.02	34.62	35.278	1.711
	8	60.36	36.02	34.62	35.278	1.711
3	9	60.37	36.02	34.68	35.339	1.708
	10	60.38	36.02	35.06	35.726	1.690
	11	60.38	36.03	34.64	35.318	1.710
	12	60.35	36.02	34.71	35.370	1.706
4	13	60.32	36.02	34.83	35.492	1.700
	14	60.37	36.01	34.96	35.605	1.696
	15	60.36	36.01	34.94	35.584	1.696
	16	60.33	36.01	34.97	35.615	1.694
7	17	60.32	36.02	34.70	35.360	1.706
	18	60.37	36.00	34.80	35.422	1.704
	19	60.36	36.01	35.08	35.727	1.689
	20	60.36	36.00	35.19	35.819	1.685
5	21	61.35	36.00	35.36	35.992	1.705
	22	61.00	35.99	35.41	36.023	1.693
	23	61.04	36.00	35.32	35.951	1.698
	24	61.04	36.00	35.23	35.860	1.702
6	25	60.37	36.00	34.96	35.585	1.697
	26	61.33	36.00	35.34	35.972	1.705
	27	61.22	35.99	35.68	36.298	1.687
	28	60.81	35.99	35.33	35.942	1.692
8	29	59.82	36.01	34.33	34.963	1.711
	30	61.33	35.99	35.41	36.023	1.703
	31	61.37	36.00	35.31	35.941	1.708
	32	61.27	35.99	35.22	35.830	1.710
9	33	61.33	35.99	35.19	35.799	1.713
	34	61.35	36.00	35.23	35.860	1.711
	35	61.38	36.01	35.11	35.757	1.717
	36	61.36	36.00	35.07	35.697	1.719
10	37	60.34	36.00	35.06	35.687	1.691
	38	61.29	36.00	35.18	35.809	1.712
	39	60.25	36.01	34.63	35.269	1.708
	40	60.82	36.00	35.70	36.338	1.674
	Average					1.702±0.010

Table 3.1 Density of Comp A-5 pellets used in Card GAP Test.

Obtained density of the Comp A-5 pellets was 1.702 g/cm^3. TMD for this charge of Comp A-5 is 1.7847 g/cm^3. The obtained pellet density is therefore only 95.37 % of TMD.

3.2 Card Gap Test

Ten tubes were filled and tested in the NOL Card Gap test. For the first shot we started with a barrier thickness of 200 cards or 51 mm. The first shot went to full detonation as the picture of the witness plate in Figure 3.1 shows. For the second shot we increased the barrier thickness to 230 cards. This time we obtained no reaction as the picture of the witness plate in Figure 3.2 shows. The witness plate is intact without any hole and only a moderate dent. After getting conformation of that a barrier of 230 cards was a safe distance by firing additional two shots with a barrier thickness of 230 cards, we reduced the barrier thickness for the following shots. First we reduced the barrier thickness to 220 cards than to 225 cards before the last shot was fired with a barrier thickness of 220 cards. In Figures 3.3 to 3.10 are pictures of all witness plates in addition to other rests from each of these 8 shots given.

Figure 3.1 Shot No 1, tube No 1, barrier thickness 200 cards, detonation.

Figure 3.2 Shot No 2, tube No 2, barrier thickness 230 cards, no reaction.

Figure 3.3 Shot No 3, tube No 3, barrier 230 cards, no reaction.

Figure 3.4 Shot No 4, tube No 4, barrier 230 cards, no reaction.

Figure 3.5 Shot No 5, tube No 5, barrier 220 cards, detonation.

Figure 3.6 Shot No 6, tube No 6, barrier 220 cards, detonation.

Figure 3.7 Shot No 7, tube No 7, barrier 225 cards, no reaction.

Figure 3.8 Shot No 8, tube No 8, barrier 225 cards, no reaction.

Figure 3.9 Shot No 9, tube No 9, barrier 225 cards, no reaction.

Figure 3.10 Shot No 10, tube No10, barrier 220 cards, detonation.

Shot No.	Tube No.	Barrier Thickness (Cards)	Barrier Thickness (mm)	Reaction
1	1	200	50.8	Detonation
2	2	230	58.2	No Reaction
3	3	230	58.2	No Reaction
4	4	230	58.2	No Reaction
5	5	220	55.88	Detonation
6	6	220	55.88	Detonation
7	7	225	57.15	No Reaction
8	8	225	57.15	No Reaction
9	9	225	57.15	No Reaction
10	10	220	55.88	Detonation

Table 3.2 Summary of the results of the firings in Card GAP-test of Comp A-5.

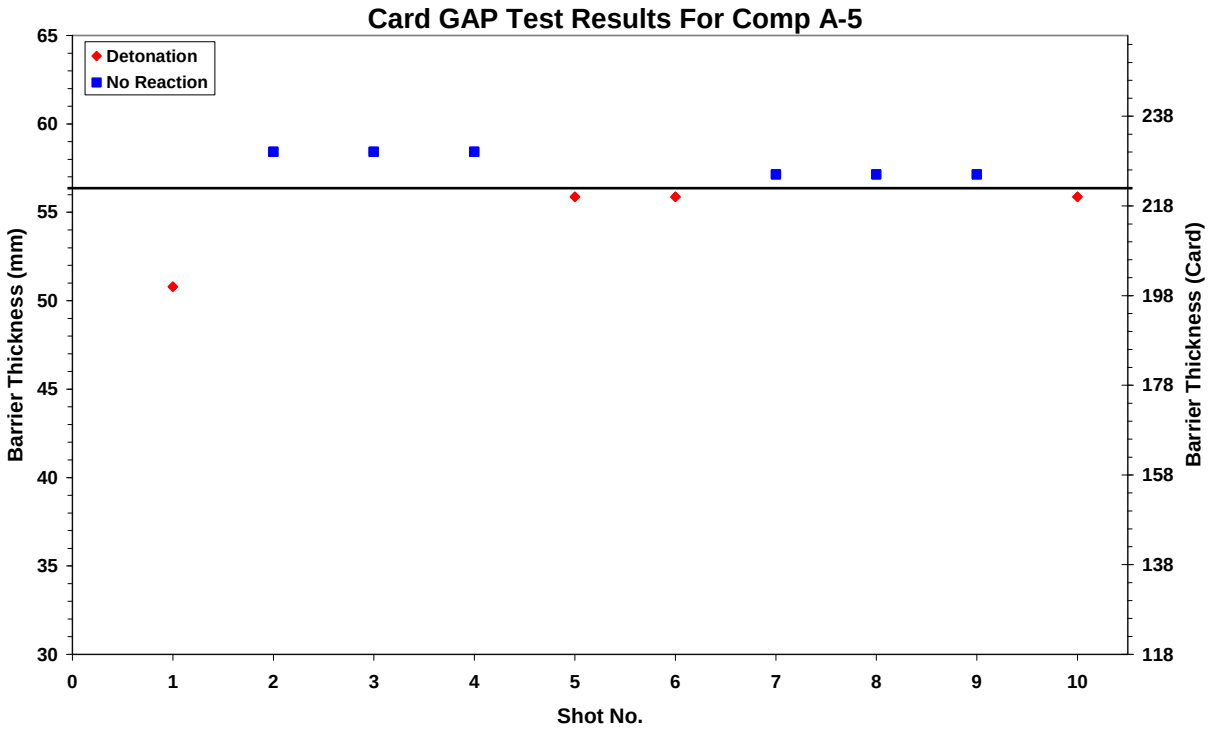

Figure 3.11 Plot of the results in Card Gap test for Comp A-5.

Table 3.2 summarizes the results for all ten tested tubes. Figure 3.11 gives a plot of the Comp A-5 test series. From Table 3.2 and Figure 3.11 we can see that the transition between full detonation and no reaction is narrow. All shots with barrier thickness of 225 cards or more gave no reaction while shots with barrier thickness of 220 cards or lower went all to full detonation. The obtained result of 222-3 cards or 56.5 mm in barrier thickness for the transition between a no go/go reactions indicates that Comp A-5 is a relative shock sensitive composition.

3.3 Theoretical calculations

Performance of Comp A-5 at TMD (Theoretical Maximum Density) is higher with respect to both detonation velocity and pressure compared with Octol 70/30 (HMX/TNT). However compared with press filled HMX/Binder (95/5) compositions as for example PBXN-5 has Comp A-5 approximately 10% lower detonation pressure and 200 m/s lower detonation velocity. For fillings of Comp A-5 with density equal to those tested in the NOL Card Gap test, the actually product density will give a reduction in detonation pressure of 10% and in the velocity of 300 m/s, Table 3.3, compares with a filling of TMD.

Properties at C-J condition	**Comp A-5**				**PBXN-5***	**Octol 70/30**
Density g/cm^3	**1.78467**		**1.7020**		**1.9031**	**1.8220**
Product library	***BKWC***	***BKWS***	***BKWC***	***BKWS***	***BKWC***	***BKWC***
Pressure (GPa)	33.27	32.88	29.74	29.57	36.64	32.29
Volume (cc/g)	0.425	0.430	0.444	0.448	0.400	0.413
Density (g/cc)	2.355	2.327	2.250	2.233	2.502	2.421
Energy (kJ/cc)	4.03	3.83	3.62	3.52	4.39	3.99
Temperature (K)	4148	4085	4191	4140	3987	4033
Shock velocity (m/s)	8776	8891	8471	8549	8966	8463
Particle velocity (m/s)	2125	2072	2063	2032	2147	2094
Speed of sound (m/s)	6651	6818	6408	6517	6819	6370
Gamma	3.131	3.290	3.107	3.206	3.176	3.042
Freezing at 1800 K gives						
Total energy of detonation (kJ/cc)	**-10.179**	**-10.444**	**-9.554**	**-9.825**	**-10.702**	**-9.949**

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

Table 3.3 Cheetah 2.0 Code calculated properties for Comp A-5, PBXN-5 and Octol 70/30.

Appendix A

A.1 Control report for tested composition

DYNO
High Energy Materials

KONTROLLRAPPORT
i henhold til EN 10204 - 3.1

Kjøper/ Mottaker Nammo Raufoss AS Postboks 162 2831 Raufoss	Bestillingsnummer 58159-0/ROFST/3 Bestillingsdato 16.02.07	Rapport nummer 088 Kontroll dato 22.02.07
Produsent Dyno Nobel ASA N-3476 Sætre NORGE	Produksjonsdato 13.11.06	Offentlig oppdragsnummer
Lot nummer DDP07B0056-0001	Mengde 20 kg	Art.nr. 0166819
Sprengstofftype **Composition A-5, Klasse 2**	Leveringsbetingelser/ Teknisk underlag MIL-DTL-14970D	

Analyseresultater

	Sammensetning		Tetthet	Volumvekt	Ubrente partikler på	
	RDX	Stearinsyre			USSS nr. 40	USSS nr. 60
Spesifikasjon	98,5 - 99,0 %	1,0 - 1,5 %	≤ 0,10 %	≥ 0,95 g/ml	0	Max. 5
Charge nr. 03/06	98,7	1,3	0,02	1,07	0	0

	Kornfordeling, % gjennom USSS nr.		Gap Test		Cyklotoksanon, %
	12	200	Regular detonation	Regular not detonation	
Spesifikasjon	> 99,0	≤ 2,4	mm H_2O	≤ 28 mm H_2O	≤ 0,30
Charge nr. 03/06	100	0,7	-	-	0,19

DYNO
High Energy Materials
Manager QA

Kvalitetssjef

Figure A.1 Control report for Comp A-5 class 2.

Appendix B Complete printout for standard Cheetah run

B.1 Product library BKWS

```
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, steacid, 1.3, rdx, 98.7, weight

                              The Composition
Name      % wt.  % mol  % vol.   Heat of  Standard   Standard     Mol.  Formula
                                  formation volume     entropy     wt.
                                  (cal/mol) (cc/mol)  (cal/K/mol)
RDX      98.70  98.98  97.53      16496    122.99     0.000      222.13  C3H6N6O6
Stearacid 1.30   1.02   2.47     -228967    302.30     0.000      284.47  C18H36O2

Heat of formation =      62.836 cal/gm
Standard volume   =       0.560 cc/gm
Standard entropy  =       0.000 cal/k/gm
Standard energy   =      62.822 cal/gm

The elements and percent by mole
     c              14.762
     h              29.525
     o              27.904
     n              27.809
The average mol. wt. = 222.761 g/mol
Input>gas eos, bkw
Input>standard run, rho, 1.784673
The hugoniot reference state:
P0 = 1.000000 ATM, V0 = 0.560327 cc/gm, E0 = 62.822270 cal/gm
Using  149504 ATM as a lower bound for the C-J pressure
Using  373760 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    =   8.89067e+003 m/s
The particle velocity =   2.07219e+003 m/s
The speed of sound    =   6.81848e+003 m/s

P0 =       1 atm, V0 =  0.56033 cc/gm, E0 =  62.82227 cal/gm

                              Reference state = reactants
                    H(R) = H-62.84, E(R) = E-62.82, 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.)  324494.5     0.4297   4084.9   3890.22    513.16    1.676    0.4288

Product concentrations
         Name    (mol/kg) (mol gas/mol explosive)
       n2  Gas   1.255e+001  2.795e+000
      co2  Gas   8.742e+000  1.947e+000
      h2o  Gas   4.604e+000  1.026e+000
    ch2o2  Gas   2.178e+000  4.851e-001
      h3n  Gas   1.467e+000  3.269e-001
     c2h6  Gas   9.434e-001  2.102e-001
      ch4  Gas   8.112e-001  1.807e-001
       h2  Gas   2.094e-001  4.665e-002
    ch3oh  Gas   1.943e-001  4.329e-002
       co  Gas   5.659e-002  1.261e-002
     h4n2  Gas   3.181e-002  7.086e-003
       no  Gas   2.441e-002  5.439e-003
```

c2h4	Gas	1.109e-002	2.471e-003
ch3	Gas	8.717e-003	1.942e-003
h2o2	Gas	7.503e-003	1.671e-003
o2	Gas	4.584e-003	1.021e-003
h2n	Gas	4.402e-003	9.805e-004
ch2o	Gas	3.417e-003	7.611e-004
h2n2	Gas	2.420e-003	5.391e-004
ho	Gas	2.059e-003	4.587e-004
cno	Gas	1.585e-003	3.530e-004
chno	Gas	1.152e-003	2.566e-004
h	Gas	9.913e-004	2.208e-004
o	Gas	3.824e-004	8.519e-005
no2	Gas	1.767e-004	3.936e-005
c3h8	Gas	7.961e-005	1.773e-005
ch2	Gas	7.525e-005	1.676e-005
ho2	Gas	5.443e-005	1.213e-005
cho	Gas	4.639e-005	1.033e-005
hno	Gas	4.169e-005	9.288e-006
chn	Gas	2.971e-005	6.618e-006
n	Gas	2.374e-005	5.288e-006
n2o	Gas	2.312e-005	5.151e-006
hn	Gas	1.031e-005	2.297e-006
c2h2	Gas	7.572e-006	1.687e-006
cn	Gas	4.199e-006	9.353e-007
n3	Gas	1.664e-006	3.707e-007
no3	Gas	1.586e-006	3.533e-007
hno2	Gas	9.297e-007	2.071e-007
c3h6	Gas	8.751e-007	1.949e-007
cn2	Gas	7.782e-007	1.733e-007
hno3	Gas	7.792e-008	1.736e-008
ch	Gas	7.435e-008	1.656e-008
c2h	Gas	3.605e-008	8.031e-009
no2h	Gas	2.313e-008	5.153e-009
c	Gas	1.663e-008	3.705e-009
o3	Gas	4.950e-009	1.103e-009
n2o4	Gas	4.033e-009	8.984e-010
c2n2	Gas	1.215e-009	2.707e-010
c2h4o	Gas	6.213e-010	1.384e-010
c2n	Gas	4.678e-010	1.042e-010
c2	Gas	4.514e-010	1.006e-010
c2o	Gas	9.663e-011	2.153e-011
n2o3	Gas	2.853e-011	6.356e-012
cnn	Gas	1.503e-011	3.347e-012
c3o2	Gas	2.898e-013	6.456e-014
c3	Gas	7.832e-014	1.745e-014
n2o5	Gas	4.496e-014	1.001e-014
c4	Gas	2.919e-023	6.501e-024
c4n2	Gas	1.562e-031	3.479e-032
c5	Gas	3.842e-034	8.557e-035
*c	solid	2.471e-001	5.503e-002
*h2o	liquid	0.000e+000	0.000e+000
Total	Gas	3.186e+001	7.097e+000
Total	Cond.	2.471e-001	5.503e-002

The C-J Adiabat

Reference state = reactants
H(R) = H-62.84, E(R) = E-62.82, 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.)	139677.1	0.5603	3290.5	1730.88	-164.53	1.676	0.5512

Product concentrations

Name		(mol/kg)	(mol gas/mol explosive)
n2	Gas	1.276e+001	2.842e+000
co2	Gas	8.786e+000	1.957e+000
h2o	Gas	7.159e+000	1.595e+000

ch4	Gas	1.289e+000	2.872e-001
h3n	Gas	1.130e+000	2.517e-001
h2	Gas	8.504e-001	1.894e-001
ch2o2	Gas	7.018e-001	1.563e-001
co	Gas	5.138e-001	1.145e-001
c2h6	Gas	3.091e-001	6.885e-002
ch3oh	Gas	8.411e-002	1.874e-002
c2h4	Gas	1.823e-002	4.062e-003
ch3	Gas	1.090e-002	2.429e-003
ch2o	Gas	1.047e-002	2.333e-003
chno	Gas	3.625e-003	8.074e-004
no	Gas	2.802e-003	6.241e-004
h2n	Gas	2.062e-003	4.593e-004
h	Gas	1.417e-003	3.156e-004
ho	Gas	1.401e-003	3.120e-004
h4n2	Gas	1.301e-003	2.899e-004
chn	Gas	5.667e-004	1.262e-004
h2o2	Gas	2.693e-004	6.000e-005
cho	Gas	2.345e-004	5.223e-005
cno	Gas	1.939e-004	4.320e-005
h2n2	Gas	1.878e-004	4.184e-005
c3h8	Gas	1.470e-004	3.274e-005
o2	Gas	9.995e-005	2.226e-005
c2h2	Gas	8.359e-005	1.862e-005
ch2	Gas	3.388e-005	7.547e-006
o	Gas	2.389e-005	5.321e-006
c3h6	Gas	1.277e-005	2.845e-006
hno	Gas	1.183e-005	2.634e-006
hn	Gas	4.224e-006	9.409e-007
n2o	Gas	3.918e-006	8.728e-007
cn	Gas	3.700e-006	8.243e-007
ho2	Gas	2.991e-006	6.664e-007
n	Gas	2.114e-006	4.709e-007
no2	Gas	2.056e-006	4.580e-007
cn2	Gas	1.763e-007	3.928e-008
c2h	Gas	1.607e-007	3.581e-008
hno2	Gas	1.564e-007	3.483e-008
n3	Gas	1.202e-007	2.679e-008
c2n2	Gas	3.774e-008	8.407e-009
ch	Gas	2.738e-008	6.099e-009
no2h	Gas	1.368e-008	3.048e-009
c2h4o	Gas	9.142e-009	2.037e-009
c2n	Gas	2.519e-009	5.611e-010
c2o	Gas	2.287e-009	5.094e-010
c	Gas	2.012e-009	4.482e-010
hno3	Gas	4.048e-010	9.018e-011
c3o2	Gas	2.369e-010	5.276e-011
no3	Gas	2.356e-010	5.248e-011
c2	Gas	6.859e-011	1.528e-011
cnn	Gas	2.082e-011	4.639e-012
o3	Gas	9.400e-012	2.094e-012
c3	Gas	3.890e-013	8.665e-014
n2o3	Gas	1.091e-013	2.431e-014
n2o4	Gas	2.726e-014	6.073e-015
n2o5	Gas	2.331e-019	5.192e-020
c4	Gas	8.594e-021	1.914e-021
c4n2	Gas	4.638e-024	1.033e-024
c5	Gas	3.717e-028	8.281e-029
*c	solid	2.097e+000	4.671e-001
*h2o	liquid	0.000e+000	0.000e+000
Total	Gas	3.364e+001	7.493e+000
Total	Cond.	2.097e+000	4.671e-001

Reference state = reactants
H(R) = H-62.84, E(R) = E-62.82, 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.)   15005.7      1.2307   1800.0   -481.68   -928.91    1.676    1.2235

Product concentrations
         Name    (mol/kg) (mol gas/mol explosive)
       n2  Gas   1.318e+001  2.937e+000
      h2o  Gas   8.023e+000  1.787e+000
      co2  Gas   7.781e+000  1.733e+000
       co  Gas   3.126e+000  6.963e-001
       h2  Gas   2.150e+000  4.789e-001
      ch4  Gas   1.729e+000  3.850e-001
      h3n  Gas   2.901e-001  6.462e-002
     c2h6  Gas   1.835e-002  4.088e-003
    ch2o2  Gas   1.735e-002  3.865e-003
     ch2o  Gas   3.414e-003  7.605e-004
     c2h4  Gas   2.713e-003  6.044e-004
    ch3oh  Gas   2.294e-003  5.110e-004
      chn  Gas   1.872e-003  4.171e-004
     chno  Gas   1.277e-003  2.845e-004
      ch3  Gas   2.276e-004  5.071e-005
     c3h8  Gas   3.856e-005  8.590e-006
     c3h6  Gas   2.064e-005  4.598e-006
     c2h2  Gas   1.924e-005  4.286e-006
        h  Gas   1.869e-005  4.163e-006
      cho  Gas   1.205e-005  2.685e-006
      h2n  Gas   4.527e-006  1.008e-006
       ho  Gas   3.073e-006  6.846e-007
       no  Gas   2.976e-007  6.630e-008
     h4n2  Gas   8.554e-008  1.905e-008
     h2n2  Gas   1.503e-008  3.349e-009
     c2n2  Gas   1.418e-008  3.160e-009
      cno  Gas   7.903e-009  1.760e-009
     c3o2  Gas   7.845e-009  1.747e-009
      ch2  Gas   2.639e-009  5.879e-010
    c2h4o  Gas   1.957e-009  4.359e-010
     h2o2  Gas   1.673e-009  3.726e-010
      hno  Gas   1.621e-009  3.612e-010
       cn  Gas   9.501e-010  2.117e-010
      n2o  Gas   5.291e-010  1.179e-010
       hn  Gas   3.304e-010  7.360e-011
      c2h  Gas   1.520e-010  3.385e-011
       o2  Gas   9.402e-011  2.094e-011
        o  Gas   5.298e-011  1.180e-011
      c2o  Gas   1.894e-011  4.219e-012
        n  Gas   5.752e-012  1.281e-012
      ho2  Gas   4.443e-012  9.898e-013
     hno2  Gas   3.294e-012  7.338e-013
      cn2  Gas   1.849e-012  4.119e-013
     no2h  Gas   1.647e-012  3.669e-013
      c2n  Gas   7.691e-013  1.713e-013
       n3  Gas   3.898e-013  8.684e-014
      no2  Gas   2.912e-013  6.487e-014
       ch  Gas   4.700e-014  1.047e-014
      cnn  Gas   2.758e-016  6.143e-017
        c  Gas   1.288e-016  2.869e-017
     c4n2  Gas   4.458e-018  9.931e-019
     hno3  Gas   2.100e-018  4.678e-019
       c3  Gas   1.701e-018  3.788e-019
       c2  Gas   8.361e-019  1.863e-019
      no3  Gas   3.135e-022  6.983e-023
       o3  Gas   1.438e-022  3.203e-023
     n2o3  Gas   6.317e-024  1.407e-024
       c4  Gas   4.561e-025  1.016e-025
       c5  Gas   1.419e-027  3.161e-028
     n2o4  Gas   9.859e-030  2.196e-030
     n2o5  Gas   4.367e-037  9.729e-038
       *c  solid 1.449e+000  3.228e-001
     *h2o liquid 0.000e+000  0.000e+000

     Total Gas   3.633e+001  8.093e+000
```

Total Cond. 1.449e+000 3.228e-001

Reference state = reactants
H(R) = H-62.84, E(R) = E-62.82, 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.)	14942.0	1.2327	1798.2	-483.58	-929.65	1.676	1.2255

Product concentrations

	Name		(mol/kg)	(mol gas/mol explosive)
*	n2	Gas	1.318e+001	2.937e+000
*	h2o	Gas	8.023e+000	1.787e+000
*	co2	Gas	7.781e+000	1.733e+000
*	co	Gas	3.126e+000	6.963e-001
*	h2	Gas	2.150e+000	4.789e-001
*	ch4	Gas	1.729e+000	3.850e-001
*	h3n	Gas	2.901e-001	6.462e-002
*	c2h6	Gas	1.835e-002	4.088e-003
*	ch2o2	Gas	1.735e-002	3.865e-003
*	ch2o	Gas	3.414e-003	7.605e-004
*	c2h4	Gas	2.713e-003	6.044e-004
*	ch3oh	Gas	2.294e-003	5.110e-004
*	chn	Gas	1.872e-003	4.171e-004
*	chno	Gas	1.277e-003	2.845e-004
*	ch3	Gas	2.276e-004	5.071e-005
*	c3h8	Gas	3.856e-005	8.590e-006
*	c3h6	Gas	2.064e-005	4.598e-006
*	c2h2	Gas	1.924e-005	4.286e-006
*	h	Gas	1.869e-005	4.163e-006
*	cho	Gas	1.205e-005	2.685e-006
*	h2n	Gas	4.527e-006	1.008e-006
*	ho	Gas	3.073e-006	6.846e-007
*	no	Gas	2.976e-007	6.630e-008
*	h4n2	Gas	8.554e-008	1.905e-008
*	h2n2	Gas	1.503e-008	3.349e-009
*	c2n2	Gas	1.418e-008	3.160e-009
*	cno	Gas	7.903e-009	1.760e-009
*	c3o2	Gas	7.845e-009	1.747e-009
*	ch2	Gas	2.639e-009	5.879e-010
*	c2h4o	Gas	1.957e-009	4.359e-010
*	h2o2	Gas	1.673e-009	3.726e-010
*	hno	Gas	1.621e-009	3.612e-010
*	cn	Gas	9.501e-010	2.117e-010
*	n2o	Gas	5.291e-010	1.179e-010
*	hn	Gas	3.304e-010	7.360e-011
*	c2h	Gas	1.520e-010	3.385e-011
*	o2	Gas	9.402e-011	2.094e-011
*	o	Gas	5.298e-011	1.180e-011
*	c2o	Gas	1.894e-011	4.219e-012
*	n	Gas	5.752e-012	1.281e-012
*	ho2	Gas	4.443e-012	9.898e-013
*	hno2	Gas	3.294e-012	7.338e-013
*	cn2	Gas	1.849e-012	4.119e-013
*	no2h	Gas	1.647e-012	3.669e-013
*	c2n	Gas	7.691e-013	1.713e-013
*	n3	Gas	3.898e-013	8.684e-014
*	no2	Gas	2.912e-013	6.487e-014
*	ch	Gas	4.700e-014	1.047e-014
*	cnn	Gas	2.758e-016	6.143e-017
*	c	Gas	1.288e-016	2.869e-017
*	c4n2	Gas	4.458e-018	9.931e-019
*	hno3	Gas	2.100e-018	4.678e-019
*	c3	Gas	1.701e-018	3.788e-019
*	c2	Gas	8.361e-019	1.863e-019
*	no3	Gas	3.135e-022	6.983e-023
*	o3	Gas	1.438e-022	3.203e-023
*	n2o3	Gas	6.317e-024	1.407e-024
*	c4	Gas	4.561e-025	1.016e-025

```
*       c5  Gas   1.419e-027  3.161e-028
*     n2o4  Gas   9.859e-030  2.196e-030
*     n2o5  Gas   4.367e-037  9.729e-038
*       *c  solid 1.449e+000  3.228e-001
*     *h2o liquid 0.000e+000  0.000e+000

      Total Gas   3.633e+001  8.093e+000
      Total Cond. 1.449e+000  3.228e-001

                              Reference state = reactants
                  H(R) = H-62.84, E(R) = E-62.82, 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.)   3566.9       2.2973   1314.1   -916.69  -1115.13    1.676    2.2901

Product concentrations
          Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.318e+001  2.937e+000
*      h2o  Gas   8.023e+000  1.787e+000
*      co2  Gas   7.781e+000  1.733e+000
*       co  Gas   3.126e+000  6.963e-001
*       h2  Gas   2.150e+000  4.789e-001
*      ch4  Gas   1.729e+000  3.850e-001
*      h3n  Gas   2.901e-001  6.462e-002
*     c2h6  Gas   1.835e-002  4.088e-003
*    ch2o2  Gas   1.735e-002  3.865e-003
*     ch2o  Gas   3.414e-003  7.605e-004
*     c2h4  Gas   2.713e-003  6.044e-004
*    ch3oh  Gas   2.294e-003  5.110e-004
*      chn  Gas   1.872e-003  4.171e-004
*     chno  Gas   1.277e-003  2.845e-004
*      ch3  Gas   2.276e-004  5.071e-005
*     c3h8  Gas   3.856e-005  8.590e-006
*     c3h6  Gas   2.064e-005  4.598e-006
*     c2h2  Gas   1.924e-005  4.286e-006
*        h  Gas   1.869e-005  4.163e-006
*      cho  Gas   1.205e-005  2.685e-006
*      h2n  Gas   4.527e-006  1.008e-006
*       ho  Gas   3.073e-006  6.846e-007
*       no  Gas   2.976e-007  6.630e-008
*     h4n2  Gas   8.554e-008  1.905e-008
*     h2n2  Gas   1.503e-008  3.349e-009
*     c2n2  Gas   1.418e-008  3.160e-009
*      cno  Gas   7.903e-009  1.760e-009
*     c3o2  Gas   7.845e-009  1.747e-009
*      ch2  Gas   2.639e-009  5.879e-010
*    c2h4o  Gas   1.957e-009  4.359e-010
*     h2o2  Gas   1.673e-009  3.726e-010
*      hno  Gas   1.621e-009  3.612e-010
*       cn  Gas   9.501e-010  2.117e-010
*      n2o  Gas   5.291e-010  1.179e-010
*       hn  Gas   3.304e-010  7.360e-011
*      c2h  Gas   1.520e-010  3.385e-011
*       o2  Gas   9.402e-011  2.094e-011
*        o  Gas   5.298e-011  1.180e-011
*      c2o  Gas   1.894e-011  4.219e-012
*        n  Gas   5.752e-012  1.281e-012
*      ho2  Gas   4.443e-012  9.898e-013
*     hno2  Gas   3.294e-012  7.338e-013
*      cn2  Gas   1.849e-012  4.119e-013
*     no2h  Gas   1.647e-012  3.669e-013
*      c2n  Gas   7.691e-013  1.713e-013
*       n3  Gas   3.898e-013  8.684e-014
*      no2  Gas   2.912e-013  6.487e-014
*       ch  Gas   4.700e-014  1.047e-014
*      cnn  Gas   2.758e-016  6.143e-017
*        c  Gas   1.288e-016  2.869e-017
*     c4n2  Gas   4.458e-018  9.931e-019
```

```
*     hno3  Gas    2.100e-018  4.678e-019
*       c3  Gas    1.701e-018  3.788e-019
*       c2  Gas    8.361e-019  1.863e-019
*      no3  Gas    3.135e-022  6.983e-023
*       o3  Gas    1.438e-022  3.203e-023
*     n2o3  Gas    6.317e-024  1.407e-024
*       c4  Gas    4.561e-025  1.016e-025
*       c5  Gas    1.419e-027  3.161e-028
*     n2o4  Gas    9.859e-030  2.196e-030
*     n2o5  Gas    4.367e-037  9.729e-038
*       *c  solid  1.449e+000  3.228e-001
*     *h2o liquid  0.000e+000  0.000e+000

      Total Gas    3.633e+001  8.093e+000
      Total Cond.  1.449e+000  3.228e-001

                              Reference state = reactants
                    H(R) = H-62.84, E(R) = E-62.82, 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.)    1464.1      3.6421   1093.1  -1059.62  -1188.75    1.676    3.6348

Product concentrations
          Name    (mol/kg) (mol gas/mol explosive)
*       n2  Gas    1.318e+001  2.937e+000
*      h2o  Gas    8.023e+000  1.787e+000
*      co2  Gas    7.781e+000  1.733e+000
*       co  Gas    3.126e+000  6.963e-001
*       h2  Gas    2.150e+000  4.789e-001
*      ch4  Gas    1.729e+000  3.850e-001
*      h3n  Gas    2.901e-001  6.462e-002
*     c2h6  Gas    1.835e-002  4.088e-003
*    ch2o2  Gas    1.735e-002  3.865e-003
*     ch2o  Gas    3.414e-003  7.605e-004
*     c2h4  Gas    2.713e-003  6.044e-004
*    ch3oh  Gas    2.294e-003  5.110e-004
*      chn  Gas    1.872e-003  4.171e-004
*     chno  Gas    1.277e-003  2.845e-004
*      ch3  Gas    2.276e-004  5.071e-005
*     c3h8  Gas    3.856e-005  8.590e-006
*     c3h6  Gas    2.064e-005  4.598e-006
*     c2h2  Gas    1.924e-005  4.286e-006
*        h  Gas    1.869e-005  4.163e-006
*      cho  Gas    1.205e-005  2.685e-006
*      h2n  Gas    4.527e-006  1.008e-006
*       ho  Gas    3.073e-006  6.846e-007
*       no  Gas    2.976e-007  6.630e-008
*     h4n2  Gas    8.554e-008  1.905e-008
*     h2n2  Gas    1.503e-008  3.349e-009
*     c2n2  Gas    1.418e-008  3.160e-009
*      cno  Gas    7.903e-009  1.760e-009
*     c3o2  Gas    7.845e-009  1.747e-009
*      ch2  Gas    2.639e-009  5.879e-010
*    c2h4o  Gas    1.957e-009  4.359e-010
*     h2o2  Gas    1.673e-009  3.726e-010
*      hno  Gas    1.621e-009  3.612e-010
*       cn  Gas    9.501e-010  2.117e-010
*      n2o  Gas    5.291e-010  1.179e-010
*       hn  Gas    3.304e-010  7.360e-011
*      c2h  Gas    1.520e-010  3.385e-011
*       o2  Gas    9.402e-011  2.094e-011
*        o  Gas    5.298e-011  1.180e-011
*      c2o  Gas    1.894e-011  4.219e-012
*        n  Gas    5.752e-012  1.281e-012
*      ho2  Gas    4.443e-012  9.898e-013
*     hno2  Gas    3.294e-012  7.338e-013
*      cn2  Gas    1.849e-012  4.119e-013
*     no2h  Gas    1.647e-012  3.669e-013
```

```
*      c2n  Gas   7.691e-013  1.713e-013
*       n3  Gas   3.898e-013  8.684e-014
*      no2  Gas   2.912e-013  6.487e-014
*       ch  Gas   4.700e-014  1.047e-014
*      cnn  Gas   2.758e-016  6.143e-017
*        c  Gas   1.288e-016  2.869e-017
*     c4n2  Gas   4.458e-018  9.931e-019
*     hno3  Gas   2.100e-018  4.678e-019
*       c3  Gas   1.701e-018  3.788e-019
*       c2  Gas   8.361e-019  1.863e-019
*      no3  Gas   3.135e-022  6.983e-023
*       o3  Gas   1.438e-022  3.203e-023
*     n2o3  Gas   6.317e-024  1.407e-024
*       c4  Gas   4.561e-025  1.016e-025
*       c5  Gas   1.419e-027  3.161e-028
*     n2o4  Gas   9.859e-030  2.196e-030
*     n2o5  Gas   4.367e-037  9.729e-038
*       *c  solid 1.449e+000  3.228e-001
*     *h2o liquid 0.000e+000  0.000e+000

      Total Gas   3.633e+001  8.093e+000
      Total Cond. 1.449e+000  3.228e-001

                              Reference state = reactants
                  H(R) = H-62.84, E(R) = E-62.82, 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.)    696.6       5.6033    938.6   -1141.75   -1236.26     1.676    5.5960

Product concentrations
          Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.318e+001  2.937e+000
*      h2o  Gas   8.023e+000  1.787e+000
*      co2  Gas   7.781e+000  1.733e+000
*       co  Gas   3.126e+000  6.963e-001
*       h2  Gas   2.150e+000  4.789e-001
*      ch4  Gas   1.729e+000  3.850e-001
*      h3n  Gas   2.901e-001  6.462e-002
*     c2h6  Gas   1.835e-002  4.088e-003
*    ch2o2  Gas   1.735e-002  3.865e-003
*     ch2o  Gas   3.414e-003  7.605e-004
*     c2h4  Gas   2.713e-003  6.044e-004
*    ch3oh  Gas   2.294e-003  5.110e-004
*      chn  Gas   1.872e-003  4.171e-004
*     chno  Gas   1.277e-003  2.845e-004
*      ch3  Gas   2.276e-004  5.071e-005
*     c3h8  Gas   3.856e-005  8.590e-006
*     c3h6  Gas   2.064e-005  4.598e-006
*     c2h2  Gas   1.924e-005  4.286e-006
*        h  Gas   1.869e-005  4.163e-006
*      cho  Gas   1.205e-005  2.685e-006
*      h2n  Gas   4.527e-006  1.008e-006
*       ho  Gas   3.073e-006  6.846e-007
*       no  Gas   2.976e-007  6.630e-008
*     h4n2  Gas   8.554e-008  1.905e-008
*     h2n2  Gas   1.503e-008  3.349e-009
*     c2n2  Gas   1.418e-008  3.160e-009
*      cno  Gas   7.903e-009  1.760e-009
*     c3o2  Gas   7.845e-009  1.747e-009
*      ch2  Gas   2.639e-009  5.879e-010
*    c2h4o  Gas   1.957e-009  4.359e-010
*     h2o2  Gas   1.673e-009  3.726e-010
*      hno  Gas   1.621e-009  3.612e-010
*       cn  Gas   9.501e-010  2.117e-010
*      n2o  Gas   5.291e-010  1.179e-010
*       hn  Gas   3.304e-010  7.360e-011
*      c2h  Gas   1.520e-010  3.385e-011
*       o2  Gas   9.402e-011  2.094e-011
```

```
*       o  Gas   5.298e-011  1.180e-011
*     c2o  Gas   1.894e-011  4.219e-012
*       n  Gas   5.752e-012  1.281e-012
*     ho2  Gas   4.443e-012  9.898e-013
*    hno2  Gas   3.294e-012  7.338e-013
*     cn2  Gas   1.849e-012  4.119e-013
*    no2h  Gas   1.647e-012  3.669e-013
*     c2n  Gas   7.691e-013  1.713e-013
*      n3  Gas   3.898e-013  8.684e-014
*     no2  Gas   2.912e-013  6.487e-014
*      ch  Gas   4.700e-014  1.047e-014
*     cnn  Gas   2.758e-016  6.143e-017
*       c  Gas   1.288e-016  2.869e-017
*    c4n2  Gas   4.458e-018  9.931e-019
*    hno3  Gas   2.100e-018  4.678e-019
*      c3  Gas   1.701e-018  3.788e-019
*      c2  Gas   8.361e-019  1.863e-019
*     no3  Gas   3.135e-022  6.983e-023
*      o3  Gas   1.438e-022  3.203e-023
*    n2o3  Gas   6.317e-024  1.407e-024
*      c4  Gas   4.561e-025  1.016e-025
*      c5  Gas   1.419e-027  3.161e-028
*    n2o4  Gas   9.859e-030  2.196e-030
*    n2o5  Gas   4.367e-037  9.729e-038
*      *c  solid 1.449e+000  3.228e-001
*    *h2o liquid 0.000e+000  0.000e+000

     Total Gas   3.633e+001  8.093e+000
     Total Cond. 1.449e+000  3.228e-001

                              Reference state = reactants
                   H(R) = H-62.84, E(R) = E-62.82, 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.)    237.0     11.2065    749.0  -1225.82  -1290.13    1.676   11.1993

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
*      n2  Gas   1.318e+001  2.937e+000
*     h2o  Gas   8.023e+000  1.787e+000
*     co2  Gas   7.781e+000  1.733e+000
*      co  Gas   3.126e+000  6.963e-001
*      h2  Gas   2.150e+000  4.789e-001
*     ch4  Gas   1.729e+000  3.850e-001
*     h3n  Gas   2.901e-001  6.462e-002
*    c2h6  Gas   1.835e-002  4.088e-003
*   ch2o2  Gas   1.735e-002  3.865e-003
*    ch2o  Gas   3.414e-003  7.605e-004
*    c2h4  Gas   2.713e-003  6.044e-004
*   ch3oh  Gas   2.294e-003  5.110e-004
*     chn  Gas   1.872e-003  4.171e-004
*    chno  Gas   1.277e-003  2.845e-004
*     ch3  Gas   2.276e-004  5.071e-005
*    c3h8  Gas   3.856e-005  8.590e-006
*    c3h6  Gas   2.064e-005  4.598e-006
*    c2h2  Gas   1.924e-005  4.286e-006
*       h  Gas   1.869e-005  4.163e-006
*     cho  Gas   1.205e-005  2.685e-006
*     h2n  Gas   4.527e-006  1.008e-006
*      ho  Gas   3.073e-006  6.846e-007
*      no  Gas   2.976e-007  6.630e-008
*    h4n2  Gas   8.554e-008  1.905e-008
*    h2n2  Gas   1.503e-008  3.349e-009
*    c2n2  Gas   1.418e-008  3.160e-009
*     cno  Gas   7.903e-009  1.760e-009
*    c3o2  Gas   7.845e-009  1.747e-009
*     ch2  Gas   2.639e-009  5.879e-010
*   c2h4o  Gas   1.957e-009  4.359e-010
```

```
*     h2o2  Gas    1.673e-009  3.726e-010
*      hno  Gas    1.621e-009  3.612e-010
*       cn  Gas    9.501e-010  2.117e-010
*      n2o  Gas    5.291e-010  1.179e-010
*       hn  Gas    3.304e-010  7.360e-011
*      c2h  Gas    1.520e-010  3.385e-011
*       o2  Gas    9.402e-011  2.094e-011
*        o  Gas    5.298e-011  1.180e-011
*      c2o  Gas    1.894e-011  4.219e-012
*        n  Gas    5.752e-012  1.281e-012
*      ho2  Gas    4.443e-012  9.898e-013
*     hno2  Gas    3.294e-012  7.338e-013
*      cn2  Gas    1.849e-012  4.119e-013
*     no2h  Gas    1.647e-012  3.669e-013
*      c2n  Gas    7.691e-013  1.713e-013
*       n3  Gas    3.898e-013  8.684e-014
*      no2  Gas    2.912e-013  6.487e-014
*       ch  Gas    4.700e-014  1.047e-014
*      cnn  Gas    2.758e-016  6.143e-017
*        c  Gas    1.288e-016  2.869e-017
*     c4n2  Gas    4.458e-018  9.931e-019
*     hno3  Gas    2.100e-018  4.678e-019
*       c3  Gas    1.701e-018  3.788e-019
*       c2  Gas    8.361e-019  1.863e-019
*      no3  Gas    3.135e-022  6.983e-023
*       o3  Gas    1.438e-022  3.203e-023
*     n2o3  Gas    6.317e-024  1.407e-024
*       c4  Gas    4.561e-025  1.016e-025
*       c5  Gas    1.419e-027  3.161e-028
*     n2o4  Gas    9.859e-030  2.196e-030
*     n2o5  Gas    4.367e-037  9.729e-038
*       *c  solid  1.449e+000  3.228e-001
*     *h2o liquid  0.000e+000  0.000e+000

      Total Gas    3.633e+001  8.093e+000
      Total Cond.  1.449e+000  3.228e-001

                              Reference state = reactants
                    H(R) = H-62.84, E(R) = E-62.82, 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.)     87.6      22.4131    602.1   -1280.91   -1328.42     1.676    22.4058

Product concentrations
          Name    (mol/kg)  (mol gas/mol explosive)
*       n2  Gas    1.318e+001  2.937e+000
*      h2o  Gas    8.023e+000  1.787e+000
*      co2  Gas    7.781e+000  1.733e+000
*       co  Gas    3.126e+000  6.963e-001
*       h2  Gas    2.150e+000  4.789e-001
*      ch4  Gas    1.729e+000  3.850e-001
*      h3n  Gas    2.901e-001  6.462e-002
*     c2h6  Gas    1.835e-002  4.088e-003
*    ch2o2  Gas    1.735e-002  3.865e-003
*     ch2o  Gas    3.414e-003  7.605e-004
*     c2h4  Gas    2.713e-003  6.044e-004
*    ch3oh  Gas    2.294e-003  5.110e-004
*      chn  Gas    1.872e-003  4.171e-004
*     chno  Gas    1.277e-003  2.845e-004
*      ch3  Gas    2.276e-004  5.071e-005
*     c3h8  Gas    3.856e-005  8.590e-006
*     c3h6  Gas    2.064e-005  4.598e-006
*     c2h2  Gas    1.924e-005  4.286e-006
*        h  Gas    1.869e-005  4.163e-006
*      cho  Gas    1.205e-005  2.685e-006
*      h2n  Gas    4.527e-006  1.008e-006
*       ho  Gas    3.073e-006  6.846e-007
*       no  Gas    2.976e-007  6.630e-008
```

```
*     h4n2  Gas    8.554e-008  1.905e-008
*     h2n2  Gas    1.503e-008  3.349e-009
*     c2n2  Gas    1.418e-008  3.160e-009
*      cno  Gas    7.903e-009  1.760e-009
*     c3o2  Gas    7.845e-009  1.747e-009
*      ch2  Gas    2.639e-009  5.879e-010
*    c2h4o  Gas    1.957e-009  4.359e-010
*     h2o2  Gas    1.673e-009  3.726e-010
*      hno  Gas    1.621e-009  3.612e-010
*       cn  Gas    9.501e-010  2.117e-010
*      n2o  Gas    5.291e-010  1.179e-010
*       hn  Gas    3.304e-010  7.360e-011
*      c2h  Gas    1.520e-010  3.385e-011
*       o2  Gas    9.402e-011  2.094e-011
*        o  Gas    5.298e-011  1.180e-011
*      c2o  Gas    1.894e-011  4.219e-012
*        n  Gas    5.752e-012  1.281e-012
*      ho2  Gas    4.443e-012  9.898e-013
*     hno2  Gas    3.294e-012  7.338e-013
*      cn2  Gas    1.849e-012  4.119e-013
*     no2h  Gas    1.647e-012  3.669e-013
*      c2n  Gas    7.691e-013  1.713e-013
*       n3  Gas    3.898e-013  8.684e-014
*      no2  Gas    2.912e-013  6.487e-014
*       ch  Gas    4.700e-014  1.047e-014
*      cnn  Gas    2.758e-016  6.143e-017
*        c  Gas    1.288e-016  2.869e-017
*     c4n2  Gas    4.458e-018  9.931e-019
*     hno3  Gas    2.100e-018  4.678e-019
*       c3  Gas    1.701e-018  3.788e-019
*       c2  Gas    8.361e-019  1.863e-019
*      no3  Gas    3.135e-022  6.983e-023
*       o3  Gas    1.438e-022  3.203e-023
*     n2o3  Gas    6.317e-024  1.407e-024
*       c4  Gas    4.561e-025  1.016e-025
*       c5  Gas    1.419e-027  3.161e-028
*     n2o4  Gas    9.859e-030  2.196e-030
*     n2o5  Gas    4.367e-037  9.729e-038
*       *c  solid  1.449e+000  3.228e-001
*     *h2o liquid  0.000e+000  0.000e+000

      Total Gas    3.633e+001  8.093e+000
      Total Cond.  1.449e+000  3.228e-001

                              Reference state = reactants
                   H(R) = H-62.84, E(R) = E-62.82, 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.)    33.6      44.8261     483.0   -1320.84   -1357.31     1.676    44.8189

Product concentrations
         Name    (mol/kg)  (mol gas/mol explosive)
*       n2  Gas   1.318e+001  2.937e+000
*      h2o  Gas   8.023e+000  1.787e+000
*      co2  Gas   7.781e+000  1.733e+000
*       co  Gas   3.126e+000  6.963e-001
*       h2  Gas   2.150e+000  4.789e-001
*      ch4  Gas   1.729e+000  3.850e-001
*      h3n  Gas   2.901e-001  6.462e-002
*     c2h6  Gas   1.835e-002  4.088e-003
*    ch2o2  Gas   1.735e-002  3.865e-003
*     ch2o  Gas   3.414e-003  7.605e-004
*     c2h4  Gas   2.713e-003  6.044e-004
*    ch3oh  Gas   2.294e-003  5.110e-004
*      chn  Gas   1.872e-003  4.171e-004
*     chno  Gas   1.277e-003  2.845e-004
*      ch3  Gas   2.276e-004  5.071e-005
*     c3h8  Gas   3.856e-005  8.590e-006
```

```
*     c3h6  Gas   2.064e-005  4.598e-006
*     c2h2  Gas   1.924e-005  4.286e-006
*        h  Gas   1.869e-005  4.163e-006
*      cho  Gas   1.205e-005  2.685e-006
*      h2n  Gas   4.527e-006  1.008e-006
*       ho  Gas   3.073e-006  6.846e-007
*       no  Gas   2.976e-007  6.630e-008
*     h4n2  Gas   8.554e-008  1.905e-008
*     h2n2  Gas   1.503e-008  3.349e-009
*     c2n2  Gas   1.418e-008  3.160e-009
*      cno  Gas   7.903e-009  1.760e-009
*     c3o2  Gas   7.845e-009  1.747e-009
*      ch2  Gas   2.639e-009  5.879e-010
*    c2h4o  Gas   1.957e-009  4.359e-010
*     h2o2  Gas   1.673e-009  3.726e-010
*      hno  Gas   1.621e-009  3.612e-010
*       cn  Gas   9.501e-010  2.117e-010
*      n2o  Gas   5.291e-010  1.179e-010
*       hn  Gas   3.304e-010  7.360e-011
*      c2h  Gas   1.520e-010  3.385e-011
*       o2  Gas   9.402e-011  2.094e-011
*        o  Gas   5.298e-011  1.180e-011
*      c2o  Gas   1.894e-011  4.219e-012
*        n  Gas   5.752e-012  1.281e-012
*      ho2  Gas   4.443e-012  9.898e-013
*     hno2  Gas   3.294e-012  7.338e-013
*      cn2  Gas   1.849e-012  4.119e-013
*     no2h  Gas   1.647e-012  3.669e-013
*      c2n  Gas   7.691e-013  1.713e-013
*       n3  Gas   3.898e-013  8.684e-014
*      no2  Gas   2.912e-013  6.487e-014
*       ch  Gas   4.700e-014  1.047e-014
*      cnn  Gas   2.758e-016  6.143e-017
*        c  Gas   1.288e-016  2.869e-017
*     c4n2  Gas   4.458e-018  9.931e-019
*     hno3  Gas   2.100e-018  4.678e-019
*       c3  Gas   1.701e-018  3.788e-019
*       c2  Gas   8.361e-019  1.863e-019
*      no3  Gas   3.135e-022  6.983e-023
*       o3  Gas   1.438e-022  3.203e-023
*     n2o3  Gas   6.317e-024  1.407e-024
*       c4  Gas   4.561e-025  1.016e-025
*       c5  Gas   1.419e-027  3.161e-028
*     n2o4  Gas   9.859e-030  2.196e-030
*     n2o5  Gas   4.367e-037  9.729e-038
*       *c  solid 1.449e+000  3.228e-001
*     *h2o liquid 0.000e+000  0.000e+000

      Total Gas   3.633e+001  8.093e+000
      Total Cond. 1.449e+000  3.228e-001

                              Reference state = reactants
                    H(R) = H-62.84, E(R) = E-62.82, 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.)    13.1      89.6523     385.1  -1351.25   -1379.69     1.676    89.6450

Product concentrations
          Name    (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.318e+001  2.937e+000
*      h2o  Gas   8.023e+000  1.787e+000
*      co2  Gas   7.781e+000  1.733e+000
*       co  Gas   3.126e+000  6.963e-001
*       h2  Gas   2.150e+000  4.789e-001
*      ch4  Gas   1.729e+000  3.850e-001
*      h3n  Gas   2.901e-001  6.462e-002
*     c2h6  Gas   1.835e-002  4.088e-003
*    ch2o2  Gas   1.735e-002  3.865e-003
```

```
*     ch2o  Gas    3.414e-003  7.605e-004
*     c2h4  Gas    2.713e-003  6.044e-004
*    ch3oh  Gas    2.294e-003  5.110e-004
*      chn  Gas    1.872e-003  4.171e-004
*     chno  Gas    1.277e-003  2.845e-004
*      ch3  Gas    2.276e-004  5.071e-005
*     c3h8  Gas    3.856e-005  8.590e-006
*     c3h6  Gas    2.064e-005  4.598e-006
*     c2h2  Gas    1.924e-005  4.286e-006
*        h  Gas    1.869e-005  4.163e-006
*      cho  Gas    1.205e-005  2.685e-006
*      h2n  Gas    4.527e-006  1.008e-006
*       ho  Gas    3.073e-006  6.846e-007
*       no  Gas    2.976e-007  6.630e-008
*     h4n2  Gas    8.554e-008  1.905e-008
*     h2n2  Gas    1.503e-008  3.349e-009
*     c2n2  Gas    1.418e-008  3.160e-009
*      cno  Gas    7.903e-009  1.760e-009
*     c3o2  Gas    7.845e-009  1.747e-009
*      ch2  Gas    2.639e-009  5.879e-010
*    c2h4o  Gas    1.957e-009  4.359e-010
*     h2o2  Gas    1.673e-009  3.726e-010
*      hno  Gas    1.621e-009  3.612e-010
*       cn  Gas    9.501e-010  2.117e-010
*      n2o  Gas    5.291e-010  1.179e-010
*       hn  Gas    3.304e-010  7.360e-011
*      c2h  Gas    1.520e-010  3.385e-011
*       o2  Gas    9.402e-011  2.094e-011
*        o  Gas    5.298e-011  1.180e-011
*      c2o  Gas    1.894e-011  4.219e-012
*        n  Gas    5.752e-012  1.281e-012
*      ho2  Gas    4.443e-012  9.898e-013
*     hno2  Gas    3.294e-012  7.338e-013
*      cn2  Gas    1.849e-012  4.119e-013
*     no2h  Gas    1.647e-012  3.669e-013
*      c2n  Gas    7.691e-013  1.713e-013
*       n3  Gas    3.898e-013  8.684e-014
*      no2  Gas    2.912e-013  6.487e-014
*       ch  Gas    4.700e-014  1.047e-014
*      cnn  Gas    2.758e-016  6.143e-017
*        c  Gas    1.288e-016  2.869e-017
*     c4n2  Gas    4.458e-018  9.931e-019
*     hno3  Gas    2.100e-018  4.678e-019
*       c3  Gas    1.701e-018  3.788e-019
*       c2  Gas    8.361e-019  1.863e-019
*      no3  Gas    3.135e-022  6.983e-023
*       o3  Gas    1.438e-022  3.203e-023
*     n2o3  Gas    6.317e-024  1.407e-024
*       c4  Gas    4.561e-025  1.016e-025
*       c5  Gas    1.419e-027  3.161e-028
*     n2o4  Gas    9.859e-030  2.196e-030
*     n2o5  Gas    4.367e-037  9.729e-038
*       *c  solid  1.449e+000  3.228e-001
*     *h2o liquid  0.000e+000  0.000e+000

      Total Gas    3.633e+001  8.093e+000
      Total Cond.  1.449e+000  3.228e-001

                                The End of the Adiabat

                             Reference state = reactants
                   H(R) = H-62.84, E(R) = E-62.82, 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.)      4.7     191.5523     298.0   -1376.90   -1398.63     1.676   191.5451

Product concentrations
          Name    (mol/kg)  (mol gas/mol explosive)
```

```
*      n2  Gas   1.318e+001  2.937e+000
*     h2o  Gas   8.023e+000  1.787e+000
*     co2  Gas   7.781e+000  1.733e+000
*      co  Gas   3.126e+000  6.963e-001
*      h2  Gas   2.150e+000  4.789e-001
*     ch4  Gas   1.729e+000  3.850e-001
*     h3n  Gas   2.901e-001  6.462e-002
*    c2h6  Gas   1.835e-002  4.088e-003
*   ch2o2  Gas   1.735e-002  3.865e-003
*    ch2o  Gas   3.414e-003  7.605e-004
*    c2h4  Gas   2.713e-003  6.044e-004
*   ch3oh  Gas   2.294e-003  5.110e-004
*     chn  Gas   1.872e-003  4.171e-004
*    chno  Gas   1.277e-003  2.845e-004
*     ch3  Gas   2.276e-004  5.071e-005
*    c3h8  Gas   3.856e-005  8.590e-006
*    c3h6  Gas   2.064e-005  4.598e-006
*    c2h2  Gas   1.924e-005  4.286e-006
*       h  Gas   1.869e-005  4.163e-006
*     cho  Gas   1.205e-005  2.685e-006
*     h2n  Gas   4.527e-006  1.008e-006
*      ho  Gas   3.073e-006  6.846e-007
*      no  Gas   2.976e-007  6.630e-008
*    h4n2  Gas   8.554e-008  1.905e-008
*    h2n2  Gas   1.503e-008  3.349e-009
*    c2n2  Gas   1.418e-008  3.160e-009
*     cno  Gas   7.903e-009  1.760e-009
*    c3o2  Gas   7.845e-009  1.747e-009
*     ch2  Gas   2.639e-009  5.879e-010
*   c2h4o  Gas   1.957e-009  4.359e-010
*    h2o2  Gas   1.673e-009  3.726e-010
*     hno  Gas   1.621e-009  3.612e-010
*      cn  Gas   9.501e-010  2.117e-010
*     n2o  Gas   5.291e-010  1.179e-010
*      hn  Gas   3.304e-010  7.360e-011
*     c2h  Gas   1.520e-010  3.385e-011
*      o2  Gas   9.402e-011  2.094e-011
*       o  Gas   5.298e-011  1.180e-011
*     c2o  Gas   1.894e-011  4.219e-012
*       n  Gas   5.752e-012  1.281e-012
*     ho2  Gas   4.443e-012  9.898e-013
*    hno2  Gas   3.294e-012  7.338e-013
*     cn2  Gas   1.849e-012  4.119e-013
*    no2h  Gas   1.647e-012  3.669e-013
*     c2n  Gas   7.691e-013  1.713e-013
*      n3  Gas   3.898e-013  8.684e-014
*     no2  Gas   2.912e-013  6.487e-014
*      ch  Gas   4.700e-014  1.047e-014
*     cnn  Gas   2.758e-016  6.143e-017
*       c  Gas   1.288e-016  2.869e-017
*    c4n2  Gas   4.458e-018  9.931e-019
*    hno3  Gas   2.100e-018  4.678e-019
*      c3  Gas   1.701e-018  3.788e-019
*      c2  Gas   8.361e-019  1.863e-019
*     no3  Gas   3.135e-022  6.983e-023
*      o3  Gas   1.438e-022  3.203e-023
*    n2o3  Gas   6.317e-024  1.407e-024
*      c4  Gas   4.561e-025  1.016e-025
*      c5  Gas   1.419e-027  3.161e-028
*    n2o4  Gas   9.859e-030  2.196e-030
*    n2o5  Gas   4.367e-037  9.729e-038
*      *c  solid 1.449e+000  3.228e-001
*    *h2o liquid 0.000e+000  0.000e+000

     Total Gas   3.633e+001  8.093e+000
     Total Cond. 1.449e+000  3.228e-001
```

The Products at room temperature and pressure

Reference state = reactants
H(R) = H-62.84, E(R) = E-62.82, 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	890.4281	298.0	-1377.09	-1398.64	1.788	890.4209

Product concentrations

	Name		(mol/kg)	(mol gas/mol explosive)
*	n2	Gas	1.318e+001	2.937e+000
*	h2o	Gas	8.023e+000	1.787e+000
*	co2	Gas	7.781e+000	1.733e+000
*	co	Gas	3.126e+000	6.963e-001
*	h2	Gas	2.150e+000	4.789e-001
*	ch4	Gas	1.729e+000	3.850e-001
*	h3n	Gas	2.901e-001	6.462e-002
*	c2h6	Gas	1.835e-002	4.088e-003
*	ch2o2	Gas	1.735e-002	3.865e-003
*	ch2o	Gas	3.414e-003	7.605e-004
*	c2h4	Gas	2.713e-003	6.044e-004
*	ch3oh	Gas	2.294e-003	5.110e-004
*	chn	Gas	1.872e-003	4.171e-004
*	chno	Gas	1.277e-003	2.845e-004
*	ch3	Gas	2.276e-004	5.071e-005
*	c3h8	Gas	3.856e-005	8.590e-006
*	c3h6	Gas	2.064e-005	4.598e-006
*	c2h2	Gas	1.924e-005	4.286e-006
*	h	Gas	1.869e-005	4.163e-006
*	cho	Gas	1.205e-005	2.685e-006
*	h2n	Gas	4.527e-006	1.008e-006
*	ho	Gas	3.073e-006	6.846e-007
*	no	Gas	2.976e-007	6.630e-008
*	h4n2	Gas	8.554e-008	1.905e-008
*	h2n2	Gas	1.503e-008	3.349e-009
*	c2n2	Gas	1.418e-008	3.160e-009
*	cno	Gas	7.903e-009	1.760e-009
*	c3o2	Gas	7.845e-009	1.747e-009
*	ch2	Gas	2.639e-009	5.879e-010
*	c2h4o	Gas	1.957e-009	4.359e-010
*	h2o2	Gas	1.673e-009	3.726e-010
*	hno	Gas	1.621e-009	3.612e-010
*	cn	Gas	9.501e-010	2.117e-010
*	n2o	Gas	5.291e-010	1.179e-010
*	hn	Gas	3.304e-010	7.360e-011
*	c2h	Gas	1.520e-010	3.385e-011
*	o2	Gas	9.402e-011	2.094e-011
*	o	Gas	5.298e-011	1.180e-011
*	c2o	Gas	1.894e-011	4.219e-012
*	n	Gas	5.752e-012	1.281e-012
*	ho2	Gas	4.443e-012	9.898e-013
*	hno2	Gas	3.294e-012	7.338e-013
*	cn2	Gas	1.849e-012	4.119e-013
*	no2h	Gas	1.647e-012	3.669e-013
*	c2n	Gas	7.691e-013	1.713e-013
*	n3	Gas	3.898e-013	8.684e-014
*	no2	Gas	2.912e-013	6.487e-014
*	ch	Gas	4.700e-014	1.047e-014
*	cnn	Gas	2.758e-016	6.143e-017
*	c	Gas	1.288e-016	2.869e-017
*	c4n2	Gas	4.458e-018	9.931e-019
*	hno3	Gas	2.100e-018	4.678e-019
*	c3	Gas	1.701e-018	3.788e-019
*	c2	Gas	8.361e-019	1.863e-019
*	no3	Gas	3.135e-022	6.983e-023
*	o3	Gas	1.438e-022	3.203e-023
*	n2o3	Gas	6.317e-024	1.407e-024
*	c4	Gas	4.561e-025	1.016e-025
*	c5	Gas	1.419e-027	3.161e-028
*	n2o4	Gas	9.859e-030	2.196e-030

```
*    n2o5  Gas   4.367e-037  9.729e-038
*      *c  solid 1.449e+000  3.228e-001
*    *h2o liquid 0.000e+000  0.000e+000

     Total Gas   3.633e+001  8.093e+000
     Total Cond. 1.449e+000  3.228e-001
The mechanical energy of detonation =    -10.444 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.444 kJ/cc

JWL Tail Fit results:
Initial E0 =    -10.897, Final E0 =    -10.835
E0(V=infty) =    -10.835
C =      1.512,  omega =      0.391
Final fitting error = 0.000711

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

    20.000     -9.634     -9.634      0.024       0.023
    40.000     -9.919     -9.919      0.009       0.009
    80.000    -10.135    -10.136      0.003       0.003
   160.000    -10.302    -10.302      0.001       0.001

JWL Fit results:
E0(V=infty) =    -10.835
R[1] =      4.932, R[2] =      1.074, omega =      0.391
A    =   1170.029, B    =     12.172, C     =      1.512
Final fitting error = 0.012909

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

     0.767      3.832      3.832     32.879     34.163
     1.000     -1.229     -1.382     14.153     14.108
     2.200     -6.942     -6.919      1.514      1.674
     4.100     -8.327     -8.466      0.361      0.361
     6.500     -8.877     -8.961      0.148      0.123
    10.000     -9.231     -9.260      0.071      0.062
    20.000     -9.634     -9.634      0.024      0.023
    40.000     -9.919     -9.919      0.009      0.009
    80.000    -10.135    -10.136      0.003      0.003
   160.000    -10.302    -10.302      0.001      0.001
```

B.2 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 formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
RDX	98.70	98.98	97.53	16496	122.99	0.000	222.13	$C_3H_6N_6O_6$
Stearacid	1.30	1.02	2.47	-228967	302.30	0.000	284.47	$C_{18}H_{36}O_2$

```
Heat of formation =     62.836 cal/gm
Standard volume   =      0.560 cc/gm
Standard entropy  =      0.000 cal/k/gm
Standard energy   =     62.822 cal/gm

The elements and percent by mole
     c            14.762
```

```
     h             29.525
     n             27.809
     o             27.904
The average mol. wt. = 222.761 g/mol
Input>composition, rdx, 98.7, steacid, 1.3, weight
                                The Composition

Name      % wt. % mol % vol.   Heat of  Standard   Standard     Mol.  Formula
                              formation  volume     entropy      wt.
                              (cal/mol) (cc/mol)  (cal/K/mol)
RDX      98.70  98.98  97.53    16496    122.99     0.000      222.13  C3H6N6O6
Stearacid 1.30   1.02   2.47  -228967    302.30     0.000      284.47  C18H36O2

Heat of formation =     62.836 cal/gm
Standard volume   =      0.560 cc/gm
Standard entropy  =      0.000 cal/k/gm
Standard energy   =     62.822 cal/gm

The elements and percent by mole
     c             14.762
     h             29.525
     n             27.809
     o             27.904
The average mol. wt. = 222.761 g/mol
Input>standard run, rho, 1.784673
The hugoniot reference state:
P0 = 1.000000 ATM, V0 = 0.560327 cc/gm, E0 = 62.822270 cal/gm
Using  146576 ATM as a lower bound for the C-J pressure
Using  366441 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    =   8.77585e+003 m/s
The particle velocity =   2.12450e+003 m/s
The speed of sound    =   6.65135e+003 m/s

P0 =       1 atm, V0 =  0.56033 cc/gm, E0 =  62.82227 cal/gm

                          Reference state = reactants
                H(R) = H-62.84, E(R) = E-62.82, 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.)  328389.9     0.4247   4147.7   3916.85    539.40    1.709    0.4044

Product concentrations
         Name    (mol/kg) (mol gas/mol explosive)
      h2o  Gas   1.414e+001  3.150e+000
       n2  Gas   1.333e+001  2.969e+000
      co2  Gas   5.699e+000  1.270e+000
       co  Gas   1.187e+000  2.644e-001
    ch2o2  Gas   7.668e-003  1.708e-003
       no  Gas   7.461e-003  1.662e-003
       o2  Gas   1.272e-003  2.834e-004
      ch4  Gas   9.146e-004  2.037e-004
     c2h4  Gas   6.513e-004  1.451e-004
       h2  Gas   2.591e-004  5.771e-005
    ch3oh  Gas   1.831e-004  4.079e-005
      h3n  Gas   8.204e-005  1.828e-005
     ch2o  Gas   3.534e-006  7.873e-007
      ch3  Gas   2.113e-009  4.707e-010
     c2h6  Gas   4.239e-011  9.442e-012
      no2  Gas   2.221e-013  4.948e-014
       *c  solid 7.257e+000  1.617e+000

     Total Gas   3.437e+001  7.657e+000
     Total Cond. 7.257e+000  1.617e+000
```

The C-J Adiabat

Reference state = reactants
H(R) = H-62.84, E(R) = E-62.82, 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.)	135993.8	0.5603	3259.6	1681.62	-163.81	1.709	0.5367

Product concentrations

Name		(mol/kg)	(mol gas/mol explosive)
h2o	Gas	1.404e+001	3.128e+000
n2	Gas	1.333e+001	2.969e+000
co2	Gas	4.593e+000	1.023e+000
co	Gas	3.489e+000	7.772e-001
ch4	Gas	3.032e-002	6.754e-003
ch2o2	Gas	1.568e-002	3.494e-003
h2	Gas	1.307e-002	2.912e-003
c2h4	Gas	6.803e-003	1.515e-003
h3n	Gas	2.775e-003	6.182e-004
ch3oh	Gas	1.339e-003	2.983e-004
no	Gas	8.007e-004	1.784e-004
ch2o	Gas	1.451e-004	3.231e-005
o2	Gas	1.757e-005	3.913e-006
ch3	Gas	8.612e-007	1.918e-007
c2h6	Gas	1.742e-007	3.881e-008
no2	Gas	1.481e-012	3.299e-013
*c	solid	6.010e+000	1.339e+000
Total	Gas	3.552e+001	7.913e+000
Total	Cond.	6.010e+000	1.339e+000

Reference state = reactants
H(R) = H-62.84, E(R) = E-62.82, 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.)	14433.4	1.2327	1804.8	-465.91	-896.79	1.709	1.2217

Product concentrations

Name		(mol/kg)	(mol gas/mol explosive)
n2	Gas	1.330e+001	2.962e+000
h2o	Gas	1.113e+001	2.480e+000
co	Gas	5.783e+000	1.288e+000
co2	Gas	4.912e+000	1.094e+000
ch4	Gas	1.053e+000	2.347e-001
h2	Gas	7.915e-001	1.763e-001
h3n	Gas	6.851e-002	1.526e-002
ch2o2	Gas	5.661e-003	1.261e-003
c2h4	Gas	4.740e-003	1.056e-003
ch2o	Gas	1.235e-003	2.750e-004
ch3oh	Gas	1.088e-003	2.423e-004
c2h6	Gas	5.853e-004	1.304e-004
ch3	Gas	2.187e-005	4.871e-006
no	Gas	1.807e-007	4.025e-008
o2	Gas	4.061e-011	9.047e-012
no2	Gas	2.679e-015	5.967e-016
*c	solid	2.386e+000	5.315e-001
Total	Gas	3.705e+001	8.253e+000
Total	Cond.	2.386e+000	5.315e-001

Reference state = reactants
H(R) = H-62.84, E(R) = E-62.82, 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.)	14264.1	1.2386	1800.0	-470.98	-898.84	1.709	1.2277

Product concentrations

Name		(mol/kg)	(mol gas/mol explosive)
n2	Gas	1.330e+001	2.962e+000
h2o	Gas	1.111e+001	2.475e+000
co	Gas	5.775e+000	1.286e+000
co2	Gas	4.927e+000	1.098e+000
ch4	Gas	1.061e+000	2.363e-001
h2	Gas	7.981e-001	1.778e-001
h3n	Gas	6.877e-002	1.532e-002
ch2o2	Gas	5.604e-003	1.248e-003
c2h4	Gas	4.671e-003	1.040e-003
ch2o	Gas	1.230e-003	2.740e-004
ch3oh	Gas	1.075e-003	2.394e-004
c2h6	Gas	5.941e-004	1.323e-004
ch3	Gas	2.167e-005	4.827e-006
no	Gas	1.720e-007	3.831e-008
o2	Gas	3.780e-011	8.421e-012
no2	Gas	2.532e-015	5.640e-016
*c	solid	2.372e+000	5.283e-001
Total	Gas	3.705e+001	8.253e+000
Total	Cond.	2.372e+000	5.283e-001

Reference state = reactants
H(R) = H-62.84, E(R) = E-62.82, 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.)	3492.9	2.2973	1335.4	-882.54	-1076.86	1.709	2.2863

Product concentrations

	Name		(mol/kg)	(mol gas/mol explosive)
*	n2	Gas	1.330e+001	2.962e+000
*	h2o	Gas	1.111e+001	2.475e+000
*	co	Gas	5.775e+000	1.286e+000
*	co2	Gas	4.927e+000	1.098e+000
*	ch4	Gas	1.061e+000	2.363e-001
*	h2	Gas	7.981e-001	1.778e-001
*	h3n	Gas	6.877e-002	1.532e-002
*	ch2o2	Gas	5.604e-003	1.248e-003
*	c2h4	Gas	4.671e-003	1.040e-003
*	ch2o	Gas	1.230e-003	2.740e-004
*	ch3oh	Gas	1.075e-003	2.394e-004
*	c2h6	Gas	5.941e-004	1.323e-004
*	ch3	Gas	2.167e-005	4.827e-006
*	no	Gas	1.720e-007	3.831e-008
*	o2	Gas	3.780e-011	8.421e-012
*	no2	Gas	2.532e-015	5.640e-016
*	*c	solid	2.372e+000	5.283e-001
	Total	Gas	3.705e+001	8.253e+000
	Total	Cond.	2.372e+000	5.283e-001

Reference state = reactants
H(R) = H-62.84, E(R) = E-62.82, 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.)	1454.8	3.6421	1115.7	-1021.13	-1149.44	1.709	3.6311

Product concentrations

	Name		(mol/kg)	(mol gas/mol explosive)
*	n2	Gas	1.330e+001	2.962e+000
*	h2o	Gas	1.111e+001	2.475e+000
*	co	Gas	5.775e+000	1.286e+000
*	co2	Gas	4.927e+000	1.098e+000
*	ch4	Gas	1.061e+000	2.363e-001
*	h2	Gas	7.981e-001	1.778e-001
*	h3n	Gas	6.877e-002	1.532e-002

```
*    ch2o2  Gas    5.604e-003  1.248e-003
*     c2h4  Gas    4.671e-003  1.040e-003
*     ch2o  Gas    1.230e-003  2.740e-004
*    ch3oh  Gas    1.075e-003  2.394e-004
*     c2h6  Gas    5.941e-004  1.323e-004
*      ch3  Gas    2.167e-005  4.827e-006
*       no  Gas    1.720e-007  3.831e-008
*       o2  Gas    3.780e-011  8.421e-012
*      no2  Gas    2.532e-015  5.640e-016
*       *c  solid  2.372e+000  5.283e-001

      Total Gas    3.705e+001  8.253e+000
      Total Cond.  2.372e+000  5.283e-001

                              Reference state = reactants
                    H(R) = H-62.84, E(R) = E-62.82, 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.)    700.9       5.6033     959.5  -1101.84   -1196.93     1.709     5.5922

Product concentrations
           Name    (mol/kg)  (mol gas/mol explosive)
*       n2  Gas    1.330e+001  2.962e+000
*      h2o  Gas    1.111e+001  2.475e+000
*       co  Gas    5.775e+000  1.286e+000
*      co2  Gas    4.927e+000  1.098e+000
*      ch4  Gas    1.061e+000  2.363e-001
*       h2  Gas    7.981e-001  1.778e-001
*      h3n  Gas    6.877e-002  1.532e-002
*    ch2o2  Gas    5.604e-003  1.248e-003
*     c2h4  Gas    4.671e-003  1.040e-003
*     ch2o  Gas    1.230e-003  2.740e-004
*    ch3oh  Gas    1.075e-003  2.394e-004
*     c2h6  Gas    5.941e-004  1.323e-004
*      ch3  Gas    2.167e-005  4.827e-006
*       no  Gas    1.720e-007  3.831e-008
*       o2  Gas    3.780e-011  8.421e-012
*      no2  Gas    2.532e-015  5.640e-016
*       *c  solid  2.372e+000  5.283e-001

      Total Gas    3.705e+001  8.253e+000
      Total Cond.  2.372e+000  5.283e-001

                              Reference state = reactants
                    H(R) = H-62.84, E(R) = E-62.82, 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.)    241.8      11.2065     765.0  -1185.92   -1251.53     1.709    11.1955

Product concentrations
           Name    (mol/kg)  (mol gas/mol explosive)
*       n2  Gas    1.330e+001  2.962e+000
*      h2o  Gas    1.111e+001  2.475e+000
*       co  Gas    5.775e+000  1.286e+000
*      co2  Gas    4.927e+000  1.098e+000
*      ch4  Gas    1.061e+000  2.363e-001
*       h2  Gas    7.981e-001  1.778e-001
*      h3n  Gas    6.877e-002  1.532e-002
*    ch2o2  Gas    5.604e-003  1.248e-003
*     c2h4  Gas    4.671e-003  1.040e-003
*     ch2o  Gas    1.230e-003  2.740e-004
*    ch3oh  Gas    1.075e-003  2.394e-004
*     c2h6  Gas    5.941e-004  1.323e-004
*      ch3  Gas    2.167e-005  4.827e-006
*       no  Gas    1.720e-007  3.831e-008
*       o2  Gas    3.780e-011  8.421e-012
*      no2  Gas    2.532e-015  5.640e-016
```

```
*      *c  solid 2.372e+000  5.283e-001

     Total Gas   3.705e+001  8.253e+000
     Total Cond. 2.372e+000  5.283e-001

                              Reference state = reactants
                   H(R) = H-62.84, E(R) = E-62.82, 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.)    89.9     22.4131    612.9  -1241.97  -1290.73    1.709   22.4020

Product concentrations
          Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.330e+001  2.962e+000
*      h2o  Gas   1.111e+001  2.475e+000
*       co  Gas   5.775e+000  1.286e+000
*      co2  Gas   4.927e+000  1.098e+000
*      ch4  Gas   1.061e+000  2.363e-001
*       h2  Gas   7.981e-001  1.778e-001
*      h3n  Gas   6.877e-002  1.532e-002
*    ch2o2  Gas   5.604e-003  1.248e-003
*     c2h4  Gas   4.671e-003  1.040e-003
*     ch2o  Gas   1.230e-003  2.740e-004
*    ch3oh  Gas   1.075e-003  2.394e-004
*     c2h6  Gas   5.941e-004  1.323e-004
*      ch3  Gas   2.167e-005  4.827e-006
*       no  Gas   1.720e-007  3.831e-008
*       o2  Gas   3.780e-011  8.421e-012
*      no2  Gas   2.532e-015  5.640e-016
*       *c  solid 2.372e+000  5.283e-001

     Total Gas   3.705e+001  8.253e+000
     Total Cond. 2.372e+000  5.283e-001

                              Reference state = reactants
                   H(R) = H-62.84, E(R) = E-62.82, 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.)    34.5     44.8261    489.3  -1282.94  -1320.40    1.709   44.8151

Product concentrations
          Name   (mol/kg) (mol gas/mol explosive)
*       n2  Gas   1.330e+001  2.962e+000
*      h2o  Gas   1.111e+001  2.475e+000
*       co  Gas   5.775e+000  1.286e+000
*      co2  Gas   4.927e+000  1.098e+000
*      ch4  Gas   1.061e+000  2.363e-001
*       h2  Gas   7.981e-001  1.778e-001
*      h3n  Gas   6.877e-002  1.532e-002
*    ch2o2  Gas   5.604e-003  1.248e-003
*     c2h4  Gas   4.671e-003  1.040e-003
*     ch2o  Gas   1.230e-003  2.740e-004
*    ch3oh  Gas   1.075e-003  2.394e-004
*     c2h6  Gas   5.941e-004  1.323e-004
*      ch3  Gas   2.167e-005  4.827e-006
*       no  Gas   1.720e-007  3.831e-008
*       o2  Gas   3.780e-011  8.421e-012
*      no2  Gas   2.532e-015  5.640e-016
*       *c  solid 2.372e+000  5.283e-001

     Total Gas   3.705e+001  8.253e+000
     Total Cond. 2.372e+000  5.283e-001

                              Reference state = reactants
                   H(R) = H-62.84, E(R) = E-62.82, 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.)	13.4	89.6523	388.5	-1314.21	-1343.37	1.709	89.6412

Product concentrations

	Name		(mol/kg)	(mol gas/mol explosive)
*	n2	Gas	1.330e+001	2.962e+000
*	h2o	Gas	1.111e+001	2.475e+000
*	co	Gas	5.775e+000	1.286e+000
*	co2	Gas	4.927e+000	1.098e+000
*	ch4	Gas	1.061e+000	2.363e-001
*	h2	Gas	7.981e-001	1.778e-001
*	h3n	Gas	6.877e-002	1.532e-002
*	ch2o2	Gas	5.604e-003	1.248e-003
*	c2h4	Gas	4.671e-003	1.040e-003
*	ch2o	Gas	1.230e-003	2.740e-004
*	ch3oh	Gas	1.075e-003	2.394e-004
*	c2h6	Gas	5.941e-004	1.323e-004
*	ch3	Gas	2.167e-005	4.827e-006
*	no	Gas	1.720e-007	3.831e-008
*	o2	Gas	3.780e-011	8.421e-012
*	no2	Gas	2.532e-015	5.640e-016
*	*c	solid	2.372e+000	5.283e-001
	Total	Gas	3.705e+001	8.253e+000
	Total	Cond.	2.372e+000	5.283e-001

The End of the Adiabat

Reference state = reactants
H(R) = H-62.84, E(R) = E-62.82, 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.)	4.7	194.5069	298.0	-1340.99	-1363.12	1.709	194.4959

Product concentrations

	Name		(mol/kg)	(mol gas/mol explosive)
*	n2	Gas	1.330e+001	2.962e+000
*	h2o	Gas	1.111e+001	2.475e+000
*	co	Gas	5.775e+000	1.286e+000
*	co2	Gas	4.927e+000	1.098e+000
*	ch4	Gas	1.061e+000	2.363e-001
*	h2	Gas	7.981e-001	1.778e-001
*	h3n	Gas	6.877e-002	1.532e-002
*	ch2o2	Gas	5.604e-003	1.248e-003
*	c2h4	Gas	4.671e-003	1.040e-003
*	ch2o	Gas	1.230e-003	2.740e-004
*	ch3oh	Gas	1.075e-003	2.394e-004
*	c2h6	Gas	5.941e-004	1.323e-004
*	ch3	Gas	2.167e-005	4.827e-006
*	no	Gas	1.720e-007	3.831e-008
*	o2	Gas	3.780e-011	8.421e-012
*	no2	Gas	2.532e-015	5.640e-016
*	*c	solid	2.372e+000	5.283e-001
	Total	Gas	3.705e+001	8.253e+000
	Total	Cond.	2.372e+000	5.283e-001

The Products at room temperature and pressure

Reference state = reactants
H(R) = H-62.84, E(R) = E-62.82, 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	907.7454	298.0	-1341.16	-1363.13	1.823	907.7344

Product concentrations

```
         Name   (mol/kg) (mol gas/mol explosive)
*      n2  Gas   1.330e+001  2.962e+000
*     h2o  Gas   1.111e+001  2.475e+000
*      co  Gas   5.775e+000  1.286e+000
*     co2  Gas   4.927e+000  1.098e+000
*     ch4  Gas   1.061e+000  2.363e-001
*      h2  Gas   7.981e-001  1.778e-001
*     h3n  Gas   6.877e-002  1.532e-002
*   ch2o2  Gas   5.604e-003  1.248e-003
*    c2h4  Gas   4.671e-003  1.040e-003
*    ch2o  Gas   1.230e-003  2.740e-004
*   ch3oh  Gas   1.075e-003  2.394e-004
*    c2h6  Gas   5.941e-004  1.323e-004
*     ch3  Gas   2.167e-005  4.827e-006
*      no  Gas   1.720e-007  3.831e-008
*      o2  Gas   3.780e-011  8.421e-012
*     no2  Gas   2.532e-015  5.640e-016
*      *c  solid 2.372e+000  5.283e-001

     Total Gas   3.705e+001  8.253e+000
     Total Cond. 2.372e+000  5.283e-001
The mechanical energy of detonation =    -10.179 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.179 kJ/cc

JWL Tail Fit results:
Initial E0 =    -10.638, Final E0 =    -10.583
E0(V=infty) =    -10.583
C =      1.536,  omega =      0.388
Final fitting error = 0.000603

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

    20.000     -9.345     -9.345      0.025      0.024
    40.000     -9.638     -9.637      0.009      0.009
    80.000     -9.860     -9.860      0.003      0.004
   160.000    -10.031    -10.031      0.001      0.001

JWL Fit results:
E0(V=infty) =    -10.583
R[1] =      4.766, R[2] =      1.068, omega =      0.388
A    =    995.590, B    =     10.948, C     =      1.536
Final fitting error = 0.009871

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

     0.758      4.028      4.028     33.274     34.012
     1.000     -1.223     -1.323     13.780     13.780
     2.200     -6.696     -6.685      1.462      1.586
     4.100     -8.041     -8.165      0.354      0.354
     6.500     -8.583     -8.659      0.147      0.125
    10.000     -8.938     -8.963      0.071      0.063
    20.000     -9.345     -9.345      0.025      0.024
    40.000     -9.638     -9.637      0.009      0.009
    80.000     -9.860     -9.860      0.003      0.004
   160.000    -10.031    -10.031      0.001      0.001
```

Appendix C Summary printouts

C.1 Density TMD (1.7847 g/cm^3)

C.1.1 Product library BKWS

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

                          The composition:
Name      % wt.  % mol  % vol  Heat of     Mol.   TMD
                             formation     wt.  (g/cc)
                             (cal/mol)
Stearacid  1.30   1.02   2.47  -228967   284.47   0.94  C18H36O2
RDX       98.70  98.98  97.53    16496   222.13   1.81  C3H6N6O6

Density = 1.7847 g/cc Mixture TMD = 1.7847 g/cc  % TMD = 100.0000

The C-J condition:
The pressure          =          32.88 GPa
The volume            =          0.430 cc/g
The density           =          2.327 g/cc
The energy            =           3.83 kJ/cc explosive
The temperature       =           4085 K
The shock velocity    =          8.891 mm/us
The particle velocity =          2.072 mm/us
The speed of sound    =          6.818 mm/us
Gamma                 =          3.290

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    -1.23
   2.20    -6.94     143       109       93       77       159
   4.10    -8.33     143       108       94       79       151
   6.50    -8.88     142       107       94       80       145
  10.00    -9.23     142       106       94       80       141
  20.00    -9.63     140       105       95       81       134
  40.00    -9.92     139       104       95       82       128
  80.00   -10.14     138       104       95       82       123
 160.00   -10.30

Freezing occurred at T =     1800.0 K and relative V =   2.196
The mechanical energy of detonation =    -10.444 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.444 kJ/cc

JWL Fit results:
E0   =    -10.835 kJ/cc
A    =   1170.03 GPa, B   =  12.17 GPa , C     =    1.51 GPa
R[1] =      4.93,    R[2] =   1.07,      omega =    0.39

RMS fitting error = 1.29 %
```

C.1.2 Product library BKWC

```
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)
RDX       98.70  98.98  97.53    16496   222.13   1.81 C3H6N6O6
Stearacid  1.30   1.02   2.47  -228967   284.47   0.94 C18H36O2
```

Density = 1.7847 g/cc Mixture TMD = 1.7847 g/cc % TMD = 100.0000

The C-J condition:

The pressure	=	33.27 GPa
The volume	=	0.425 cc/g
The density	=	2.355 g/cc
The energy	=	4.03 kJ/cc explosive
The temperature	=	4148 K
The shock velocity	=	8.776 mm/us
The particle velocity	=	2.125 mm/us
The speed of sound	=	6.651 mm/us
Gamma	=	3.131

Cylinder runs: % of standards

V/V0 (rel.)	Energy (kJ/cc)	TATB 1.83g/cc	PETN 1.76g/cc	HMX 1.89g/cc	CL-20 2.04g/cc	TRITON 1.70g/cc
1.00	-1.22					
2.20	-6.70	138	105	90	74	154
4.10	-8.04	138	104	91	76	146
6.50	-8.58	138	103	91	77	140
10.00	-8.94	137	103	91	78	136
20.00	-9.35	136	102	92	79	130
40.00	-9.64	135	101	92	79	125
80.00	-9.86	134	101	92	80	120
160.00	-10.03					

Freezing occurred at T = 1800.0 K and relative V = 2.210
The mechanical energy of detonation = -10.179 kJ/cc
The thermal energy of detonation = -0.000 kJ/cc
The total energy of detonation = -10.179 kJ/cc

JWL Fit results:
E0 = -10.583 kJ/cc
A = 995.59 GPa, B = 10.95 GPa , C = 1.54 GPa
R[1] = 4.77, R[2] = 1.07, omega = 0.39
RMS fitting error = 0.99 %

C.2 Density 1.702 g/cm^3

C.2.1 Product library BKWS

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)	
rdx	98.70	98.98	97.53	16496	222.13	1.81	c3h6n6o6
steacid	1.30	1.02	2.47	-228967	284.47	0.94	c18h36o2

Density = 1.7020 g/cc Mixture TMD = 1.7847 g/cc % TMD = 95.3676

The C-J condition:

The pressure	=	29.57 GPa
The volume	=	0.448 cc/g
The density	=	2.233 g/cc
The energy	=	3.52 kJ/cc explosive
The temperature	=	4140 K
The shock velocity	=	8.549 mm/us
The particle velocity	=	2.032 mm/us
The speed of sound	=	6.517 mm/us
Gamma	=	3.206

Cylinder runs: % of standards

V/V0 (rel.)	Energy (kJ/cc)	TATB 1.83g/cc	PETN 1.76g/cc	HMX 1.89g/cc	CL-20 2.04g/cc	TRITON 1.70g/cc

```
   1.00    -1.13
   2.20    -6.41     132      101       86       71      147
   4.10    -7.74     133      100       87       73      140
   6.50    -8.27     133      100       88       74      135
  10.00    -8.62     132       99       88       75      131
  20.00    -9.02     131       98       88       76      126
  40.00    -9.30     130       98       89       77      120
  80.00    -9.51     129       97       89       77      115
 160.00    -9.68

Freezing occurred at T =     1800.0 K and relative V =   2.279
The mechanical energy of detonation =     -9.825 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.825 kJ/cc

JWL Fit results:
E0   =  -10.132 kJ/cc
A    = 1007.40 GPa, B   =  11.73 GPa , C     =   1.76 GPa
R[1] =    4.96,    R[2] =   1.12,      omega =   0.43
RMS fitting error =   1.02 %
```

C.2.2 Product library BKWC

```
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)
rdx        98.70  98.98  97.53     16496   222.13     1.81 c3h6n6o6
steacid     1.30   1.02   2.47   -228967   284.47     0.94 c18h36o2

Density  =  1.7020 g/cc   Mixture TMD =  1.7847 g/cc   % TMD = 95.3676

The C-J condition:
The pressure          =          29.74 GPa
The volume            =          0.444 cc/g
The density           =          2.250 g/cc
The energy            =           3.62 kJ/cc explosive
The temperature       =           4191 K
The shock velocity    =          8.471 mm/us
The particle velocity =          2.063 mm/us
The speed of sound    =          6.408 mm/us
Gamma                 =          3.107

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    -1.11
   2.20    -6.16     127       97       83       68      141
   4.10    -7.46     128       97       84       71      135
   6.50    -7.99     128       96       85       72      131
  10.00    -8.33     128       96       85       73      127
  20.00    -8.73     127       95       86       74      122
  40.00    -9.02     126       95       86       74      117
  80.00    -9.24     125       95       86       75      112
 160.00    -9.41

Freezing occurred at T =     1800.0 K and relative V =   2.292
The mechanical energy of detonation =     -9.554 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.554 kJ/cc

JWL Fit results:
E0   =   -9.879 kJ/cc
A    =  884.93 GPa, B    = 10.23 GPa , C     =   1.75 GPa
R[1] =    4.80,     R[2] =  1.11,      omega =   0.43
RMS fitting error =   0.77 %
```

References

(1) North Atlantic Council (2002): STANAG 4488 PSC (Edition 1), "Explosive, Shock Sensitivity Tests" NATO/PfP, Unclassified Document NSA/0883-PPS/4488, 12 September.

(2) Skaaden Tore, Eriksen Svein, Larsen Øyvind (1984): “Fremstilling og testing av støpbare TNT-nitroguanidin ekxplosiver”, FFI/NOTAT-84/4043.

(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.