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English summary

Norway's main objective in the EDA project No B-0585-GEM2-GC "Formulation and Production of New Energetic Materials" was to synthesize different new energetic binders built of GA and BAMO polymers. Before starting experimentally work, Cheetah calculations with both BKWC and BKWS product libraries at standard conditions were performed to study what effects energetic binder/binder system had on the performance on different types of compositions.

Two classes of pressed compositions, one with filler content of 96 wt. % RDX or HMX and one with 92 wt. % RDX or HMX, have been studied to replace PBXW-11 and PBXN-9. The energetic binders we wanted to synthesize were GA/BAMO with different ratio between GA and BAMO. Calculations have been performed with both GAP and BAMO and of a mixture of these two binders. In addition, calculations with energetic binder and inert plasticizer have been performed.

Obtained detonation pressures and velocities for compositions with GAP, BAMO or GA/BAMO are both equal for these compositions. The ratio between GA/BAMO has only minor effect on both detonation velocity and detonation pressure. Changes occur first when an inert plasticizer is introduced. With inert plasticizer the detonation pressure drops by 1.6 GPa for the 96 wt. % HMX compositions and by 3 GPa for the 92 wt. % HMX compositions with the BKWS product library. With the BKWC product library the drop is 2.3 and 4.2 GPa respectively. The detonation velocity drops are 150 m/s and 300 m/s with BKWS and 240 m/s and 450 m/s with the BKWC product library for the respective compositions.

A composition with 92 wt. % HMX and energetic binder/plasticizer has equal or better performance than PBXW-11 (96 wt. % HMX, inert binder). Use of energetic binder in combination with inert plasticizer has only minor influence on detonation velocity and pressure for compositions with 96 wt. % filler. For compositions with 92 wt. % filler and energetic binder/inert plasticizer the detonation pressure increases by 1 GPa and the detonation velocity by +100 m/s. This trend is independent of filler.

For 87 wt. % HMX or RDX cast-cure compositions the effect of changing the binder system in PBXN-110 to energetic binders gives larger differences. The detonation pressure increases with 7.32 GPa (BKWC) and 4.94 GPa (BKWS) for HMX and slightly less (6.48/4.39) with RDX. The detonation velocity increase by 820 m/s (BKWC) and 508 m/s (BKWS) for HMX and 784/468 m/s for RDX. Compositions with energetic binders and inert plasticizer (DOA) have properties between those for PBXN-110 and compositions containing energetic binder systems.

The calculations have shown that compositions having energetic binder/binder systems increase the performance for both cast-cure and pressed compositions. The increased performance may also be used or utilized to reduce the filler content and thus reduce the sensitivity. For pressed compositions, the choice of ratio between GA and BAMO for the new polymers to be synthesised will be governed by the ability to coat crystals and give the press powder the required properties rather than the energy content, since the energy content is independent of the ratio.

Sammendrag

I EDA-prosjektet No B-0585-GEM2-GC “Formulation and Production of New Energetic Materials” hadde Norge som målsetting å syntetisere ulike nye energirike bindemidler oppbygd av GA- og BAMO-enheter. Før det eksperimentelle syntesearbeidet ble igangsatt, ble teoretiske beregninger med Cheetah utført. Beregninger ble utført med både BKWC- og BKWS-produktbibliotekene under standard betingelser. Hensikten var å studere hvilken effekt energirike bindemiddel/bindemiddelsystem har på virkningen til ulike komposisjoner. Pressbare komposisjoner med 96 vektprosent RDX eller HMX og med 92 vektprosent RDX eller HMX inngikk i studien, komposisjoner til erstatning for PBXW-11 og PBXN-9. PBXW-11 og PBXN-9 har et inert bindemiddelsystem av HYTEMP og DOA i forholdet 1/3. De energirike bindemidlene vi ønsket å studere, var GA/BAMO i forskjellige blandeforhold. Beregninger har vært utført for både GAP og BAMO samt en blanding av disse. I tillegg har beregninger vært utført med inert mykner.

Beregnet detonasjonstrykk og detonasjonshastighet med GAP, BAMO eller GA/BAMO avviker lite for disse komposisjonene. Blandingsforholdet mellom GAP/BAMO har kun ubetydelig innvirkning på både detonasjonshastigheten og detonasjonstrykket. Forskjeller oppstår først når en inert mykner blir anvendt. For komposisjoner med 96 vektprosent HMX gir inert mykner en reduksjon i detonasjonstrykket på 1.6 GPa, og for komposisjonene med 92 vektprosent HMX 3 GPa med BKWS. Med BKWC er reduksjonen i detonasjonstrykk henholdsvis 2.3 og 4.2 GPa. Detonasjonshastigheten faller med 150 m/s og 300 m/s med BKWS og 240 m/s og 450 m/s med BKWC for de samme kombinasjonene. For komposisjoner med RDX er trenden og størrelsesorden i reduksjonen i detonasjonshastighet og trykk som for de HMX-baserte komposisjonene med inert mykner.

For komposisjoner med 92 vektprosent HMX eller RDX er effekten av å bytte til energirikt bindemiddel en økt virkning lik eller bedre enn for PBXW-11 (96 vektprosent HMX/inert bindemiddel). Anvendelse av energirikt bindemiddel i komposisjoner med 96 vektprosent fyllstoff i kombinasjon med inert mykner har kun ubetydelig innvirkning på detonasjonshastigheten og detonasjonstrykket. For komposisjoner med 92 vektprosent fyllstoff oppnås en økning i detonasjonstrykket med 1 GPa og i detonasjonshastigheten med 100 m/s. Tendensen er den samme for både RDX og HMX.

For støpherdbare komposisjoner med 87 vektprosent HMX (RDX) er effekten av å skifte til energirikt bindemiddel betydelig. Detonasjonstrykket øker med 7.32 GPa (BKWC) og 4.94 GPa (BKWS) for HMX og noe mindre for RDX-komposisjonen, henholdsvis 6.48 og 4.39 GPa. Detonasjonshastigheten øker tilsvarende med 820 m/s (BKWC) og 508 m/s (BKWS) for HMX og med 784/468 m/s for RDX-komposisjonen. Komposisjoner som har energirikt bindemiddel og inert mykner (DOA), har egenskaper som ligger mellom PBXN-110 og komposisjoner med energirikt bindemiddelsystem.

Konklusjonen fra beregningene er at energirikt bindemiddel gir betydelig økning i virkningen for både støpherdbare og pressede komposisjoner. Den økte virkningen kan tas ut eller benyttes til reduksjon av fyllstoffinnhold og dermed følsomheten. Valg av forholdet mellom GA og BAMO i nye bindemiddel for pressede komposisjoner vil bli styrt av beleggingsegenskaper/konsistens siden energien er den samme.

Contents

Abbrevations

BAMO	3,3-Bis(azidomethyl)oxetane, $C_5H_8N_6O$
BKWC	Becker-Kistiakowsky-Wilson C (LLNL library)
BKWS	Becker-Kistiakowsky-Wilson S (Baer/Hobbs library)
DOA	Dioctyl adipate, $C_{22}H_{42}O_4$
ETPE	Energetic Thermoplastic Elastomers
GA	Glycidyl azide, $C_3H_5N_3O$
GAP	Glycidyl azide polymer, $(C_3H_5N_3O)_n$
GA/BAMO	Glycidyl azide- (3,3-bis(azidomethyl)oxetane) Copolymers
HMX	Octogen/1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane, $C_4H_8N_8O_8$
HTPB	Hydroxy -terminated polybutadiene, C_4H_6
HYTEMP	Used formula in the calculations, $C_{10}H_{15.46}O_{3.307}$
IPDI	Isophorone diisocyanate, $C_{12}H_{18}N_2O_2$
IM	Insensitive Munitions
pNIMMO	Poly-3-nitratomethyl-3-methyloxethan, $C_5H_9N_1O_4$
RDX	Hexogen/1,3,5 -trinitro-1,3,5-triazacyclohexane, $C_3H_6N_6O_6$
TMD	Theoretical Maximum Density

1 Introduction

Norway had as the main objective in the EDA project arrangement No B-0585-GEM2-GC "Formulation and Production of New Energetic Materials" to synthesize different new energetic binders built of GA and BAMO polymer units. New GA/BAMO ETPE polymers for coating of RDX and HMX crystals to produce granules. Granules with properties suitable for press filling of munition units or production of pressed charges.

Norway was the only country with the aim to use the new energetic binders to produce explosive charges. The other countries working with energetic binders Italy and Germany aimed at use theirs polymers as binders for propellants (1-4). The compositions we aimed at to produce should have high content of HMX (92-97 wt. %) or RDX. Primary application for the compositions would be as boosters or main fillings for shaped charges.

The new energetic binders would contain different ratio of GA/BAMO polymers. GA is the liquid/soft part and BAMO the solid/hard part in the final polymer. In the previous project a 75/25 ratio of GA/BAMO was study for cast-cure applications (2). This was the starting point for the new program. The new thermoplastic elastomers must have mechanical properties similar to inert energetic binders as Hytemp 4454.

Before the syntheses of the new energetic polymer took place thermochemical calculations of performance were performed for different combinations of binders and nitramines. These calculations were performed with Cheetah 2.0 (5). The Cheetah reactant library contains both GAP and BAMO polymers but not the combined binder. The library gives formula, density and Heat of Formation for reactants. Our new polymer is a mixture of BAMO and GAP and will have density and Heat of Formation not different from the building units. Heat of Formation, chemical composition and density of the (GA/BAMO) polymer to be synthesized was not known. Therefore the calculations were performed with a mechanical mixture of GAP and BAMO polymer. The difference in Heat of Formation, density and formula between this choice and the actual properties will be small. For all other ingredients as HMX, RDX, DOA, IPDI, HTPB etc. the properties given in the Cheetah 2.0 reactant library have been used in the calculations.

The objectives for Norway was to look on pressed compositions containing some few percentage binder/and or plasticizer. PBXW-11 or Comp 7 is one model compound to be replaced. PBXW-11 contains 96 wt. % HMX. A more insensitive composition is PBXN-9 (Comp 14) with 92 wt. % HMX and inert binder and plasticizer. With these two filler contents (92/96) of both HMX and RDX, different ratios between GA and BAMO, with and without inert plasticizer have standard calculations been performed. Total 28 different combinations, 14 with RDX and 14 with HMX have been included in the study.

We have also performed some calculations for cast-cure alternatives with 87 wt. % HMX or RDX. These compositions are equal to PBXN-110 with regard to solid content (6). The GA/BAMO elastomers contain chains with no end groups (2). These molecules will function as plasticizer in cast-cure systems.

Cheetah 2.0 contains two product libraries, BKWS EOS and BKWC EOS. Standard run calculations have been performed with both libraries for compositions based on either HMX or RDX. These calculations give in addition to performance also the detonation products at the equilibrium at 1 atm and room temperature, 298 K. This information is used to see if there are significant differences in the detonation products for the studied compositions.

2 Calculations

All calculations have been performed with Cheetah 2.0 (5). We have used two libraries. The BKWS EOS product library takes into consideration a larger number of products than the BKWC EOS product library. In the appendixes are summary printouts for all calculations with both libraries. The content of the studied compositions are given in the respective chapters. Calculations have been performed for 38 different combinations of binder system and filler. 19 of the combinations contain RDX as filler and the remaining 19 combinations have HMX as filler.

Compound	Formula	Molecule Weight	Density (g/cm^3)	Heat of formation (cal/mol)
BAMO	$C_5H_8N_6O$	168.16	1.30	100382
DOA	$C_{22}H_{42}O_4$	370.56	0.93	-290392
GAP	$C_3H_5N_3O$	99.09	1.29	33939
HMX	$C_4H_8N_8O_8$	296.17	1.91	17866
HTPB	C_4H_6	54.09	0.90	1195
HYTEMP*	$C_{10}H_{15.46}O_{3.307}$	188.60	1.00	-205067
IPDI	$C_{12}H1_8N_2O_2$	222.28	1.06	-88910
pNIMMO	$C_5H_9N_1O_4$	147.13	1.28	73853
RDX	$C_3H_6N_6O_6$	222.13	1.81	16496

*Used formula is for Hycar 4051. For HYTEMP 4454, ($C_{4.95}H_{7.95}O_{1.95}Cl_{0.05}$) we have not the heat of formation.

Table 2.1 Properties used for the ingredients included in the calculations.

In addition to the performance properties the detonation products have been calculated and are given in 3.2 for all compositions with both product libraries. The BKWC product library uses 17 products in the equilibrium calculations. The BKWS product library uses 63 products in the equilibrium calculations. Tables with the product content for RDX containing compositions are given in 3.3.3 and for HMX containing compositions in 3.2.2. In addition the BKWC products and most of the BKWS products at equilibrium are given as plots. For the BKWS products of very low content have been excluded from the plots.

3 Results

3.1 Performance

3.1.1 96 wt. % HMX compositions

To obtain satisfactory sensitivity properties compositions with higher solid content than 96 wt. % have not been included in this study as candidates to replace PBXW-11, or other similar pressed filled compositions with high content of HMX. PBXW-11 can normally be used both as booster and main charge filling. Table 3.1 gives the content of the compositions we have selected to be included in our study. In addition to HMX and PBXW-11 are six compositions all with energetic binder included. Of those six two have GA/BAMO (75/25) as binder, one is without plasticizer (COMP 3) and the other is with inert DOA plasticizer (COMP 4). For comparison two compositions with GAP–binder and two with BAMO binder have been included. For both GAP (COMP 5) and BAMO (COMP 6) has one composition inert plasticizer.

Ingredients	HMX	COMP 1	COMP 2	COMP 3	COMP 4	COMP 5	COMP 6	COMP 7
HMX	100	96	96	96	96	96	96	96
GAP		4		3	0.75	1		
BAMO			4	1	0.25		1	
HYTEMP								1
DOA					3	3	3	3

Table 3.1 Content of candidate compositions containing 96 wt. % HMX.

3.1.1.1 BKWS EOS library

Cheetah 2.0 contains two product libraries. Normally both are used to perform standard runs for explosive compositions. In this study both libraries have been used, and a comparison of the obtained properties is performed. The BKWS EOS product library takes into consideration a larger number of products than the BKWC EOS product library, but have poorer fit to experimentally determined detonation velocity for compositions containing C, H,N,O. Appendix A gives obtained standard run results for HMX and compositions with 96 wt. % HMX for both libraries.

Table 3.2 gives the performance data for the compositions in Table 3.1. Appendix A gives separate summary sheets for all compositions. The largest differences in detonation pressure, detonation velocity and temperature are obtained between the compositions with or without inert plasticizer. The difference in properties between compositions with inert or energetic binder is small.

The C-J condition	HMX	COMP 1	COMP 2	COMP 3	COMP 4	COMP 5	COMP 6	COMP 7
Pressure (GPa)	38.12	36.36	36.40	36.37	34.77	34.77	34.78	34.32
Volume (cc/g)	0.406	0.413	0.413	0.413	0.419	0.419	0.419	0.421
Density (g/cc)	2.406	2.423	2.424	2.423	2.385	2.385	2.386	2.376
Energy (kJ/cc)	4.30	4.15	4.16	4.15	3.99	3.99	3.99	3.94
Temperature (K)	4059	4013	4021	4015	3918	3917	3919	3892
Shock Velocity (m/s)	9415	9227	9230	9228	9079	9079	9080	9033
Particle velocity(m/s)	2125	2108	2109	2108	2084	2084	2084	2076
Speed of sound (m/s)	7290	7119	7121	7120	6995	6995	6996	6958
Gama	3.430	3.378	3.377	3.377	3.357	3.357	3.357	3.352
For freezing at T=1800 K and relative V= we have	2.095	2.093	2.098	2.094	2.055	2.055	2.056	2.042
Mechanical energy of detonation (kJ/cc)	-11.353	-10.992	-11.007	-10.996	-10.682	-10.627	-10631	-10.514
Thermal energy of detonation (kJ/cc)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Total energy of detonation (kJ/cc)	-11.353	-10.992	-11.007	-10.996	-10628	-10.627	-10.631	-10.514

Table 3.2 Results for the compositions in Table 3.1 calculated by Cheetah 2.0 using the BKWS EOS product library.

3.1.1.2 BKWC EOS library

By using the BKWC EOS product library the equilibrium contain fewer products than obtained by use of the BKWS EOS product library. This difference gives slightly different results for most of the detonation properties. The effect on specific properties is different for the different compositions.

The C-J condition	HMX	COMP 1	COMP 2	COMP 3	COMP 4	COMP 5	COMP 6	COMP 7
Pressure (GPa)	39.37	37.18	37.28	37.21	34.90	34.90	34.92	34.29
Volume (cc/g)	0.400	0.406	0.406	0.406	0.412	0.412	0.412	0.414
Density (g/cc)	2.503	2.464	2.465	2.464	2.428	2.428	2.428	2.418
Energy (kJ/cc)	4.70	4.49	4.50	4.49	4.24	4.24	4.24	4.17
Temperature (K)	4113	4075	4080	4076	3998	3998	3999	3978
Shock Velocity (m/s)	9301	9080	9088	9082	8.841	8840	8842	8778
Particle velocity (m/s)	2222	2190	2194	2191	2148	2148	2149	2134
Speed of sound (m/s)	7079	6889	6894	6890	6693	6693	6694	6645
Gama	3.186	3.145	3.143	3.144	3.116	3.116	3.115	3.114
For freezing at T=1800 K and relative V= we have	2.085	2.104	2.107	2.105	2.101	2.101	2.102	2.095
Mechanical energy of detonation (kJ/cc)	-11.112	-10.752	-10.770	-10.756	-10.375	-10.374	-10.378	-10.257
Thermal energy of detonation (kJ/cc)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Total energy of detonation (kJ/cc)	-11.112	-10.752	-10.770	-10.757	-10.375	-10.374	-10.378	-10.257

Table 3.3 Results for the compositions in Table 3.1 calculated by Cheetah 2.0 using the BKWC EOS product library.

The manual for Cheetah 2.0 indicates that for some types of compositions the difference between experimentally measured properties and calculated is smallest by using the BKWC product library. Table 3.3 contains a summary of the most important detonation properties for the compositions given in Table 3.1. Detonation pressure calculated with BKWC is about 1 GPa higher for HMX and the compositions with energetic binder compared with BKWS. For Comp 4-7 the detonation pressure is independent of product library. Calculated detonation velocity shows the same differences as the pressure for the two product libraries. We have to wait until experimentally results are available to decide which product library gives the best agreement for our compositions.

3.1.2 92 wt.% HMX compositions

Compositions containing 92 wt. % HMX is mainly candidates as pressed main fillings with reduced sensitivity compared to the compositions with 96 wt. % HMX given in 3.1.1. Our main candidates to substitute Comp 14 (PBXN-9) are Comp 10 and Comp 11. Comp 10 contains only energetic binder, while Comp 11 has 6 wt. % inert plasticizer. The content of the 92 wt. % HMX compositions included in this study is given in Table 3.4

Ingredients	HMX	COMP 8	COMP 9	COMP 10	COMP 11	COMP 12	COMP 13	COMP 14
HMX	100	92	92	92	92	92	92	92
GAP		8		6	1.50	2		
BAMO			8	2	0.50		2	
HYTEMP								2
DOA					6	6	6	6

Table 3.4 Content of 92 wt. % HMX compositions.

3.1.2.1 BKWS EOS library

For the compositions in Table 3.4 we first performed standard Cheetah runs with the BKWS EOS product library. The results are summarized in Table 3.5. Appendix B gives summary printout sheets for each composition. The results in Table 3.5 show that both detonation pressure and detonation velocity drop some few percentages compared with the results given in Table 3.2 for the 96 wt. % compositions. The drop in detonation pressure is 2-3 GPa and in detonation velocity 200-300 m/s. Again the main difference in properties is between compositions with and without energetic binder system.

The detonation pressure for the compositions containing 92 wt. % HMX and energetic binder system is equal to the pressure obtained for the 96 wt. % HMX compositions with inert plasticizer and PBXW-11 (Comp 7). Also the detonation velocity shows only minor differences for compositions with 92 wt. % HMX and energetic binder system compared with 96 wt. % HMX compositions with inert plasticizer and PBXW-11 (Comp 7).

The C-J condition	HMX	COMP 8	COMP 9	COMP 10	COMP 11	COMP 12	COMP 13	COMP 14
Pressure (GPa)	38.12	34.67	34.75	34.69	31.77	31.77	31.78	30.96
Volume (cc/g)	0.406	0.419	0.419	0.419	0.433	0.433	0.433	0.436
Density (g/cc)	2.406	2.384	2.386	2.384	2.312	2.311	2.312	2.294
Energy (kJ/cc)	4.30	3.99	4.00	3.99	3.69	3.68	3.69	3.60
Temperature (K)	4059	3967	3982	3971	3780	3779	3782	3729
Shock Velocity (m/s)	9415	9061	9067	9063	8784	8783	8785	8698
Particle velocity (m/s)	2125	2084	2.087	2085	2037	2037	2038	2021
Speed of sound (m/s)	7290	6977	6981	6978	6746	6746	6747	6677
Gama	3.430	3.347	3.346	3.347	3.311	3.311	3.311	3.303
For freezing at T=1800 K and relative V= we have	2.095	2.091	2.102	2.094	2.009	2.009	2.011	1.981
Mechanical energy of detonation (kJ/cc)	-11.353	-10.645	-10.674	-10.653	-9.985	-9.957	-9.963	-9.747
Thermal energy of detonation (kJ/cc)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Total energy of detonation (kJ/cc)	-11.353	-10.645	-10.674	-10.653	-9.958	-9.957	-9.963	-9.747

Table 3.5 Results for the 92 wt. % HMX compositions calculated with Cheetah 2.0 and the BKWS EOS product library.

3.1.2.2 BKWC EOS library

Table 3.6 summaries the results obtained from Cheetah 2.0 standard runs by using the BKWC EOS product library. Appendix B gives summary printout for each composition.

The C-J condition	HMX	COMP 8	COMP 9	COMP 10	COMP 11	COMP 12	COMP 13	COMP 14
Pressure (GPa)	39.37	35.11	35.30	35.16	30.89	30.88	30.92	29.79
Volume (cc/g)	0.400	0.412	0.412	0.412	0.425	0.425	0.425	0.429
Density (g/cc)	2.503	2.425	2.427	2.425	2.352	2.351	2.352	2.332
Energy (kJ/cc)	4.70	4.27	4.29	4.27	3.78	3.78	3.79	3.65
Temperature (K)	4113	4034	4045	4037	3877	3877	3879	3829
Shock Velocity (m/s)	9301	8871	8888	8875	8426	8425	8429	8311
Particle velocity (m/s)	2222	2156	2162	2158	2065	2064	2066	2035
Speed of sound (m/s)	7079	6715	6725	6718	6362	6361	6363	6276
Gama	3.186	3.114	3.110	3.113	3.081	3.081	3.080	3.084
For freezing at T=1800 K and relative V= we have	2.085	2.120	2.127	2.122	2.104	2.103	2.105	2.086
Mechanical energy of detonation (kJ/cc)	-11.112	-10.408	-10.444	-10.417	-9.701	-9.699	9.707	-9.483
Thermal energy of detonation (kJ/cc)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Total energy of detonation (kJ/cc)	-11.112	-10.408	-10.445	-10.417	-9.701	-9.699	-9.707	-9.483

Table 3.6 Results for the 92 wt. % HMX compositions calculated with Cheetah 2.0 and the BKWC EOS product library.

The results show a similar or larger drop in both detonation pressure and velocity compared with the properties for the 96 wt. % HMX compositions as was observed by use of the BKWS EOS product library.

3.1.3 Comparison 96 wt. % and 92 wt. % HMX

In Figure 3.1 detonation velocity and pressure from Table 3.2, Table 3.3,Table 3.5 and Table 3.6 have been plotted. The figure visualizes the differences discussed above between the different product libraries and the contents of filler.

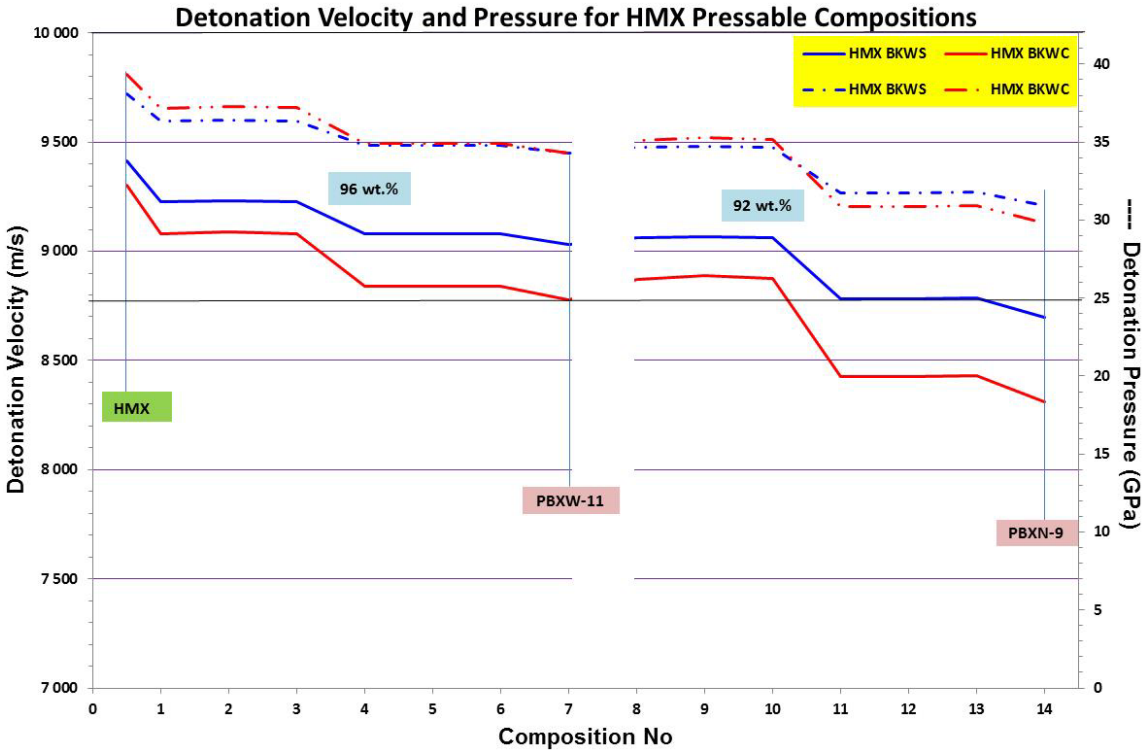

Figure 3.1 Plot of detonation velocity and pressure for HMX and HMX based pressed compositions.

3.1.4 96 wt. % RDX containing compositions

Table 3.7 gives the content for some RDX compositions with and without energetic binder/plasticizer. All compositions contain 96 wt. % RDX. The compositions in Table 3.7 are equal to the compositions in Table 3.1 except for the filler which has been changed from HMX to RDX. Compositions 15-17 have energetic binder/plasticizer. All the compositions 18-20 have energetic binder and inert plasticizer, while for Comp 21 both the binder and the plasticizer are inert.

Ingredients	RDX	COMP 15	COMP 16	COMP 17	COMP 18	COMP 19	COMP 20	COMP 21
RDX	100	96	96	96	96	96	96	96
GAP		4		3	0.75	1		
BAMO			4	1	0.25		1	
HYTEMP								1
DOA					3	3	3	3

Table 3.7 Content of some RDX compositions with 96 wt. % solid content.

The compositions with RDX filler are cheaper alternatives than the similar compositions with HMX.

3.1.4.1 BKWS EOS library

Table 3.8 summarises the results obtained for Cheetah 2.0 standard runs by using the BKWS EOS product library. Appendix C gives a summary printout for each composition. For the compositions

The C-J condition	RDX	COMP 15	COMP 16	COMP 17	COMP 18	COMP 19	COMP 20	COMP 21
Pressure (GPa)	33.78	32.55	32.59	32.56	31.19	31.19	31.20	30.80
Volume (cc/g)	0.426	0.431	0.431	0.431	0.438	0.438	0.438	0.439
Density (g/cc)	2.348	2.320	2.321	2.320	2.285	2.285	2.285	2.276
Energy (kJ/cc)	3.90	3.80	3.81	3.80	3.66	3.66	3.66	3.61
Temperature (K)	4154	4103	4111	4105	4002	4002	4004	3975
Shock Velocity (m/s)	9000	8853	8856	8854	8720	8720	8721	8679
Particle velocity (m/s)	2078	2068	2069	2069	2045	2045	2045	2037
Speed of sound (m/s)	6922	6785	6787	6785	6675	6675	6676	6642
Gama	3.331	3.280	3.280	3.280	3.264	3.264	3.264	3.261
For freezing at T=1800 K and relative V= we have	2.225	2.215	2.221	2.216	2.172	2.171	2.173	2.157
Mechanical energy of detonation (kJ/cc)	-10,695	-10.391	-10.404	-10.394	-10.057	-10.056	-10.060	-9.952
Thermal energy of detonation (kJ/cc)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Total energy of detonation (kJ/cc)	-10.695	-10.391	-10.404	-10.394	-10.057	-10.056	-10.060	-9.952

Table 3.8 Results for the 96 wt. % RDX compositions calculated with Cheetah 2.0 and the BKWS EOS product library.

with inert plasticizer the obtained detonation pressures and velocities fall in the same range as we obtained for compositions with 92 wt. % HMX in Table 3.5. For RDX compositions with energetic binder and plasticizer the detonation velocities are about 200 m/s lower and the detonation pressure is reduced by approximately 2 GPa. Compared with the properties of 96 wt. % HMX compositions the detonation pressure difference increased to approximately 4 GPa and for the detonation velocity to 400±50 m/s.

3.1.4.2 BKWC EOS library

Table 3.9 summarises the properties for the compositions in Table 3.7 obtained by performing standard Cheetah runs with the BKWC EOS product library. Appendix C gives a summary printout for each composition. By comparing the results in Table 3.9 with the results in Table 3.8 the largest differences both in detonation pressure and detonation velocity are observed between the most and the less energetic compositions. For detonation pressure the difference goes from 32.56 to 30.80 GPa in Table 3.8 compared to from 33.12 to 30.52 GPa in Table 3.9. Detonation velocity calculated with BKWC gives a difference of approximately 200 m/s between

compositions with energetic binders and compositions with inert plasticizer. With the BKWS library this difference is only 130 m/s.

The C-J condition	RDX	COMP 15	COMP 16	COMP 17	COMP 18	COMP 19	COMP 20	COMP 21
Pressure (GPa)	34.74	33.03	33.12	33.06	31.05	31.05	31.07	30.52
Volume (cc/g)	0.421	0.426	0.426	0.426	0.432	0.432	0.432	0.434
Density (g/cc)	2.378	2.347	2.348	2.347	2.313	2.313	2.313	2.304
Energy (kJ/cc)	4.18	4.00	4.02	4.01	3.78	3.78	3.79	3.72
Temperature (K)	4209	4160	4165	4161	4075	4074	4076	4049
Shock Velocity (m/s)	8942	8755	8764	8757	8534	8533	8535	8475
Particle velocity (m/s)	2151	2122	2125	2123	2080	2080	2081	2067
Speed of sound (m/s)	6791	6633	6639	6634	6454	6453	6455	6.409
Gama	3.157	3.125	3.124	3.125	3.102	3.103	3.102	3.101
For freezing at T=1800 K and relative V= we have	2.214	2.223	2.227	2.224	2.214	2.214	2.215	2.206
Mechanical energy of detonation (kJ/cc)	-10.434	-10.134	-10.151	-10.138	-9.790	-9.789	-9.793	-9.681
Thermal energy of detonation (kJ/cc)	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000
Total energy of detonation (kJ/cc)	-10.434	-10.134	-10.151	-10.138	-9.790	-9.789	-9.793	-9.681

Table 3.9 Results for the 96 wt. % RDX compositions calculated with Cheetah 2.0 and the BKWC EOS product library.

3.1.5 92 wt. % RDX containing compositions

Table 3.10 gives the content for the study compositions with RDX filler content of 92 wt. %. All compositions are copies of the compositions given in Table 3.4 with the only difference that HMX is replaced with RDX.

Ingredients	RDX	COMP 22	COMP 23	COMP 24	COMP 25	COMP 26	COMP 27	COMP 28
RDX	100	92	92	92	92	92	92	92
GAP		8		6	1.50	2		
BAMO			8	2	0.50		2	
HYTEMP								2
DOA					6	6	6	6

Table 3.10 Content of the RDX compositions with 92 wt. % solid content.

3.1.5.1 BKWS library

Table 3.11 summaries the properties for the compositions in Table 3.10 obtained by performing standard Cheetah runs with the BKWS EOS product library. Appendix D gives summary printout for each composition.

The results in Table 3.11 shows a reduction of 1-3 GPa in detonation pressure and 100-300 m/s in detonation velocity for the 92 wt.% RDX compositions compared with the 96 wt.% RDX

compositions. The largest reduction is found for Comp 28 having inert binder/plasticizer (HYTEMP/DOA).The detonation pressure is reduced by 2.8 GPa and the velocity by 290 m/s.

The C-J condition	RDX	COMP 22	COMP 23	COMP 24	COMP 25	COMP 26	COMP 27	COMP 28
Pressure (GPa)	33.78	31.24	31.31	31.26	28.73	28.72	28.74	28.01
Volume (cc/g)	0.426	0.437	0.437	0.437	0.450	0.450	0.450	0.454
Density (g/cc)	2.348	2.287	2.289	2.288	2.220	2.220	2.221	2.204
Energy (kJ/cc)	3.90	3.67	3.68	3.67	3.39	3.39	3.39	3.31
Temperature (K)	4154	4049	4064	4052	3852	3851	3855	3799
Shock Velocity (m/s)	9000	8720	8725	8721	8467	8467	8468	8389
Particle velocity (m/s)	2078	2047	2049	2047	2001	2000	2001	1985
Speed of sound (m/s)	6922	6673	6676	6.674	6467	6467	6468	6404
Gama	3.331	3.260	3.259	3.259	3.232	3.233	3.232	3.227
For freezing at T=1800 K and relative V= we have	2.225	2.204	2.216	2.207	2.113	2.112	2.115	2.082
Mechanical energy of detonation (kJ/cc)	-10.695	-10.096	-10.123	-10.103	-9.464	-9.462	-9.469	-9.268
Thermal energy of detonation (kJ/cc)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Total energy of detonation (kJ/cc)	-10.695	-10.096	-10.123	-10.103	-9.464	-9.462	-9.469	9.268

Table 3.11 Results for the 92 wt. % RDX compositions calculated with Cheetah 2.0 and the BKWS EOS product library.

3.1.5.2 BKWC EOS library

Table 3.12 summaries the properties for the compositions in Table 3.10 obtained by performing standard Cheetah runs with the BKWC EOS product library. Appendix D gives summary printout for each composition.

The C-J condition	RDX	COMP 22	COMP 23	COMP 24	COMP 25	COMP 26	COMP 27	COMP 28
Pressure (GPa)	34.74	31.39	31.55	31.43	27.69	27.68	27.71	26.72
Volume (cc/g)	0.421	0.432	0.432	0.432	0.445	0.445	0.445	0.449
Density (g/cc)	2.378	2.315	2.317	2.315	2.247	2.247	2.247	2.229
Energy (kJ/cc)	4.18	3.83	3.85	3.83	3.40	3.40	3.40	3.28
Temperature (K)	4209	4109	4121	4112	3939	3938	3941	3887
Shock Velocity (m/s)	8942	8576	8593	8581	8158	8157	8160	8048
Particle velocity (m/s)	2151	2091	2097	2092	2001	2001	2002	1973
Speed of sound (m/s)	6791	6485	6496	6488	6156	6155	6158	6074
Gama	3.157	3.101	3.098	3.101	3.076	3.076	3.075	3.078
For freezing at T=1800 K and relative V= we have	2.214	2.231	2.239	2.233	2.201	2.201	2.203	2.180
Mechanical energy of detonation (kJ/cc)	-10.434	-9.846	-9.880	-9.854	-9.197	-9.195	-9.203	-8.995
Thermal energy of detonation (kJ/cc)	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000
Total energy of detonation (kJ/cc)	-10.434	-9.846	-9.880	-9.854	-9.197	-9.195	-9.203	-8.995

Table 3.12 Results for the 92 wt. % RDX compositions calculated with Cheetah 2.0 and the BKWC EOS product library.

Compared with the results given in Table 3.11 the BKWC EOS product library gives equal detonation pressure for the compositions with energetic binder/plasticizer, but lower detonation pressure for compositions with inert binder/plasticizer. The detonation velocity is lower for all compositions. Highest reduction is 341 m/s obtained for Comp 28.

3.1.6 Comparison 96 wt. % and 92 wt. % RDX

In Figure 3.2 detonation velocities and detonation pressures from Table 3.2,Table 3.3,Table 3.5 and Table 3.6 have been plotted. The figure visualizes the differences being discussed above between the different product libraries and the content of filler.

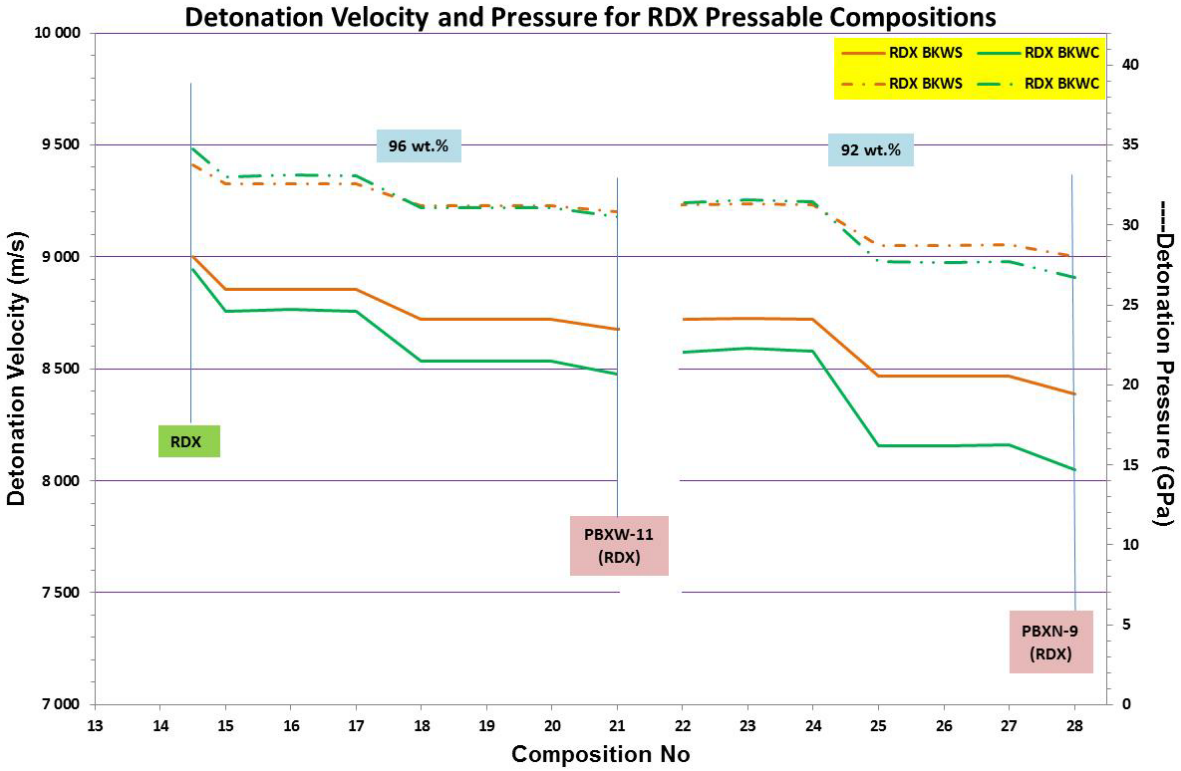

Figure 3.2 Plot of detonation velocity and pressure for RDX and RDX based pressed compositions.

3.1.7 87 wt. % HMX cast-cure compositions

In addition to Comp 1-28, which are all press filled compositions, Cheetah 2.0 standard run calculations have been carried out on 5 cast-cured 87 wt.% HMX compositions. They contain 5 different combinations of different polymers/plasticizer. The content of these compositions is given in the top of Table 3.13. The lower part of the table gives the accompanying results for both the BKWC and the BKWS EOS product library. The model composition is a simplified version of PBXN-110. The choice of 87 wt. % filler content was done to increase the probability for the compositions to be castable. The volume of the binder is largely decreased for energetic binders compared with inert HTPB polymer since the density is significantly higher.

Independent of which product library we use Comp 33 has significantly higher detonation pressure than Comp 29. Also for the detonation velocity large differences are obtained. Between Comp 29 and Comp 33 with the BKWC product library a difference in detonation velocity of 820 m/s is observed.

Comp 33 can compete with several of the pressed 92 wt. % HMX compositions in Table 3.4 either in detonation velocity or in detonation pressure. From Table 3.13 we can see that Comp 30 containing pNIMMO has slightly higher performance with regard both to detonation pressure and velocity than Comp 31 and Comp 32 based on GAP and BABO respectively. Comp 33 with energetic binder/plasticizer has significantly highest performance.

CONTENT	COMP 29		COMP30		COMP 31		COMP 32		COMP 33	
HTPB	5									
pNIMMO			5							
GAP					5				8	
BAMO							5		3	
DOA	7		7		7		7			
IPDI	1		1		1		1		2	
HMX	87		87		87		87		87	
The C-J condition EOS product library	BKWC	BKWS	BKWC	BKWS	BKWC	BKWS	BKWC	BKWS	BKWC	BKWS
Pressure (GPa)	24.53	27.15	28.09	29.84	27.68	29.30	27.77	29.34	31.85	32.09
Volume (cc/g)	0.450	0.457	0.437	0.444	0.438	0.445	0.438	0.445	0.423	0.430
Density (g/cc)	2.221	2.190	2.288	2.250	2.284	2.249	2.285	2.250	2.363	2.324
Energy (kJ/cc)	3.02	3.20	3.48	3.51	3.40	3.43	3.41	3.43	3.90	3.73
Temperature (K)	3664	3547	3867	3748	3774	3671	3781	3679	3947	3871
Shock Velocity (m/s)	7714	8294	8118	8588	8087	8528	8097	8531	8534	8802
Particle velocity (m/s)	1900	1955	2010	2018	1986	1995	1990	1995	2092	2044
Speed of sound (m/s)	5813	6338	6108	6570	6101	6533	6107	6536	6442	6758
Gama	3.060	3.242	3.038	3.255	3.071	3.276	3.069	3.275	3.080	3.307
For freezing at T=1800 K and relative V= we have	2.103	1.936	2.193	2.055	2.098	1.973	2.103	1.979	2.132	2.071
Mechanical energy of detonation (kJ/cc)	-8.683	-8.940	-9.409	-9.695	-9.148	-9.398	-9.168	-9.414	-9.854	-10.087
Thermal energy of detonation (kJ/cc)	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000
Total energy of detonation (kJ/cc)	-8.683	-8.940	-9.409	-9.695	-9.148	-9.398	-9.168	-9.414	-9.854	-10.087

Table 3.13 Results for the 87 wt. % HMX compositions calculated with Cheetah 2.0 and both the BKWC EOS and BKWS EOS product library.

3.1.8 87 wt.% RDX cast-cure compositions

Table 3.14 gives content and results for standard Cheetah 2.0 runs for compositions containing 87 wt.% RDX. Appendix F gives summary printout of each composition. The compositions in Table 3.14 are equal to the compositions given in Table 3.13 except that HMX has been substituted with

RDX. From the results in Table 3.14 more or less the same conclusions can be drawn as for the HMX compositions in Table 3.13.

CONTENT	COMP 34		COMP35		COMP 36		COMP 37		COMP 38	
HTPB	5									
PNIMMO			5							
GAP					5				8	
BAMO							5		3	
DOA	7		7		7		7			
IPDI	1		1		1		1		2	
RDX	87		87		87		87		87	
The C-J condition EOS product library	BKWC	BKWS	BKWC	BKWS	BKWC	BKWS	BKWC	BKWS	BKWC	BKWS
Pressure (GPa)	22.22	24.77	25.42	27.21	25.01	26.70	25.09	26.73	28.70	29.16
Volume (cc/g)	0.469	0.474	0.456	0.461	0.457	0.462	0.456	0.462	0.442	0.447
Density (g/cc)	2.132	2.111	2.194	2.168	2.190	2.166	2.191	2.167	2.263	2.236
Energy (kJ/cc)	2.74	2.96	3.15	3.25	3.07	3.17	3.08	3.17	3.52	3.44
Temperature (K)	3708	3603	3917	3811	3825	3733	3832	374	4008	3941
Shock Velocity (m/s)	7491	8033	7883	8309	7849	8249	7859	8253	8275	8501
Particle velocity (m/s)	1846	1919	1954	1984	1929	1960	1932	1960	2031	2008
Speed of sound (m/s)	5644	6114	5929	6325	5920	6290	5926	6292	6245	6492
Gama	3.057	3.185	3.035	3.186	3.068	3.210	3.067	3.210	3.075	3.233
For freezing at T=1800 K and relative V= we have	2.178	2.023	2.279	2.150	2.182	2.065	2.188	2.072	2.230	2.172
Mechanical energy of detonation (kJ/cc)	-8.287	-8.545	-8.960	-9.249	-8.715	-8.971	-8.734	-8.986	-9.366	-9.608
Thermal energy of detonation (kJ/cc)	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000
Total energy of detonation (kJ/cc)	-8.287	-8.545	-8.960	-9.249	-8.715	-8.971	-8.734	-8.986	-9.366	-9.608

Table 3.14 Content and properties of cast-cure compositions containing 87 wt. % RDX.

3.1.9 Comparison between HMX and RDX cast-cure compositions

Table 3.15 shows detonation velocities and pressures for the 87 wt. % cast-cure compositions. In addition the differences between HMX and RDX compositions are given. HMX compositions with energetic binder have 2.6-2.7 GPa higher detonation pressure than analogue RDX compositions independent of product library. For PBXN-110 the difference is 2.3 GPa and for the composition with energetic binder/plasticizer 3 GPa. The detonation velocity for HMX compositions is 223 to 301 m/s higher than for analogue RDX compositions. The BKWS product libray gives approximately 40 m/s higher difference in detonation velocity than the BKWC product library.

Composition	COMP 29/COMP34		COMP 30/COMP35		COMP 31/COMP36		COMP 32/COMP37		COMP 33/COMP38	
EOS product library	BKWC	BKWS	BKWC	BKWS	BKWC	BKWS	BKWC	BKWS	BKWC	BKWS
Pressure HMX (GPa)	24.53	27.15	28.09	29.84	27.68	29.30	27.77	29.34	31.85	32.09
Pressure RDX (GPa)	22.22	24.77	25.42	27.21	25.01	26.70	25.09	26.73	28.70	29.16
Pres. difference (GPa)	**2.31**	**2.38**	**2.67**	**2.63**	**2.67**	**2.60**	**2.68**	**2.61**	**3.15**	**2.93**
Shock Velocity HMX (m/s)	7714	8294	8118	8588	8087	8528	8097	8531	8534	8802
Shock Velocity RDX (m/s)	7491	8033	7883	8309	7849	8249	7859	8253	8275	8501
Velocity Difference (m/s)	**223**	**261**	**235**	**279**	**238**	**279**	**238**	**278**	**259**	**301**

Table 3.15 Detonation velocities and pressures for cast-cure compositions.

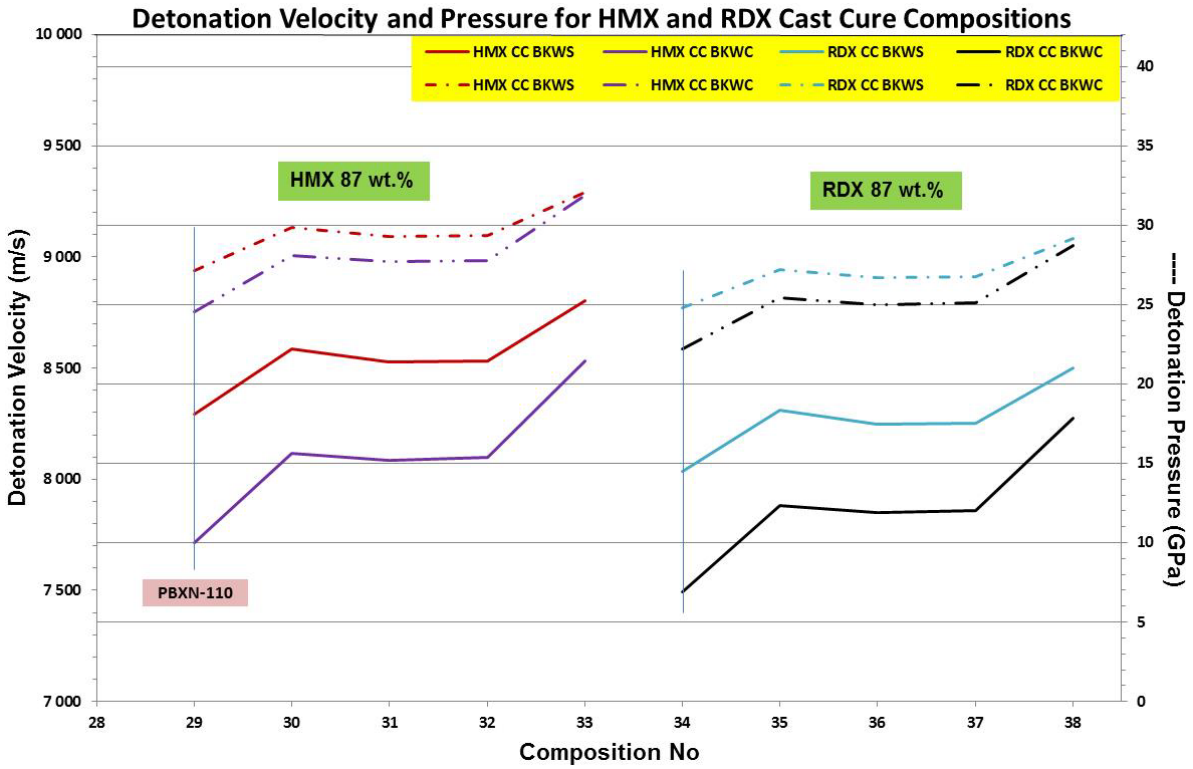

Figure 3.3 Plot of detonation velocity and pressure for HMX and RDX based cast-cure compositions.

For cast-cure compositions with 87 wt. % HMX or RDX the effect of changing the binder in PBXN-110 to an energetic binder (COMP 33/38) give large differences. For HMX compositions the detonation pressure increases with 7.32 GPa (BKWC) or 4.94 GPa (BKWS) and for compositions with RDX slightly less (6.48 GPa/4.39GPa). The detonation velocity increases by 820 m/s (BKWC) and 508 m/s (BKWS) for HMX and 784 m/s/468 m/s for RDX. Compositions with energetic binders and inert plasticizer (DOA) have properties between PBXN-110 and compositions containing an energetic binder system.

3.1.10 All compositions

Figure 3.4 shows a plot of detonation velocity and pressure for all compositions in this study.

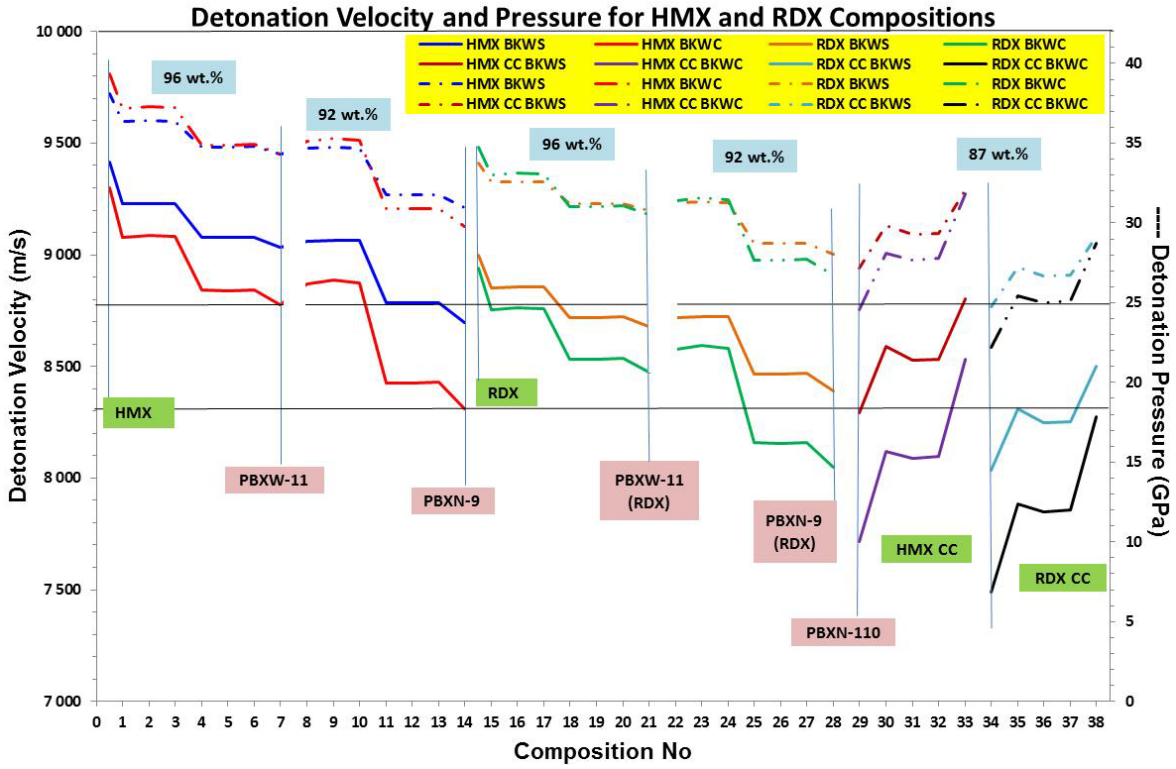

Figure 3.4 Plot of detonation velocity and pressure for HMX and RDX based compositions.

3.2 Detonation products

The detonation products at room temperature and pressure have been calculated by Cheetah 2.0 by use of both the BKWC and the BKWS product library. As mentioned above the BKWC library use 17 products and BKWS use 63 products in the chemical equilibrium calculations.

3.2.1 BKWC

3.2.1.1 Pressed HMX compositions

14 compositions with HMX have been studied. Contents for the 7 compositions with 96 wt. % HMX are given in Table 3.1 and for the 7 compositions with 92 wt. % HMX in Table 3.4. Table 3.16 and Table 3.17 give the concentration of the 17 products that the BKWC product library use in the equilibrium calculations at 1 atm and 298 K. Figure 3.5 shows a plot of the concentrations of all detonation products for all pressed HMX compositions and HMX itself.

The product with highest the concentration is N_2 gas followed by H_2O gas except for PBXN-9 where they change positions. The level of CO_2 gas is slightly higher than the level of CO gas for HMX and compositions with 96 wt. % HMX and energetic binder/plasticizer. For all other compositions the order is changed with higher CO gas content. The product C solid had a concentration of 2.78 mol/kg for pure HMX and increased to 6.58 mol/kg for PBXN-9.

For PBXN-9 C solid is the third most common product. For the other products the concentrations are low and do not change significantly by the content of the compositions.

		HMX	COMP 1	COMP 2	COMP 3	COMP 4	COMP 5	COMP 6	COMP 7
N_2	Gas	1.348e+01	1.354e+01	1.365e+01	1.357e+01	1.309e+01	1.308e+01	1.311e+01	1.293e+01
CO_2	Gas	5.396e+00	4.966e+00	4.921e+00	4.955e+00	4.698e+00	4.701e+00	4.690e+00	4.685e+00
H_2O	Gas	1.158e+01	1.164e+01	1.157e+01	1.162e+01	1.213e+01	1.213e+01	1.211e+01	1.222e+01
CO	Gas	4.630e+00	4.753e+00	4.742e+00	4.750e+00	4.811e+00	4.811e+00	4.809e+00	4.825e+00
H_2	Gas	4.706e-01	5.634e-01	5.656e-01	5.639e-01	6.497e-01	6.495e-01	6.503e-01	6.613e-01
CH_4	Gas	6.860e-01	8.368e-01	8.389e-01	8.374e-01	1.012e+00	1.012e+00	1.013e+00	1.037e+00
H_3N	Gas	4.778e-02	5.626e-02	5.662e-02	5.635e-02	6.406e-02	6.404e-02	6.415e-02	6.491e-02
CH_2O_2	Gas	5.529e-03	5.460e-03	5.414e-03	5.448e-03	5.569e-03	5.572e-03	5.560e-03	5.610e-03
C_2H_6	Gas	2.291e-04	3.325e-04	3.350e-04	3.331e-04	4.569e-04	4.566e-04	4.576e-04	4.759e-04
CH_2O	Gas	7.642e-04	8.747e-04	8.745e-04	8.746e-04	9.736e-04	9.736e-04	9.736e-04	9.888e-04
CH_3OH	Gas	8.561e-04	9.612e-04	9.581e-04	9.605e-04	1.101e-03	1.102e-03	1.101e-03	1.124e-03
C_2H_4	Gas	2.955e-03	3.619e-03	3.629e-03	3.621e-03	4.381e-03	4.380e-03	4.384e-03	4.491e-03
CH_3	Gas	9.015e-06	1.204e-05	1.212e-05	1.206e-05	1.496e-05	1.495e-05	1.498e-05	1.537e-05
NO	Gas	1.816e-07	1.747e-07	1.746e-07	1.747e-07	1.672e-07	1.672e-07	1.671e-07	1.659e-07
O_2	Gas	4.714e-11	4.204e-11	4.160e-11	4.193e-11	3.918e-11	3.920e-11	3.910e-11	3.900e-11
NO_2	Gas	1.765e-15	1.831e-15	1.831e-15	1.831e-15	1.801e-15	1.801e-15	1.801e-15	1.797e-15
*C	solid	2.781e+00	3.605e+00	3.638e+00	3.614e+00	4.510e+00	4.508e+00	4.515e+00	4.712e+00
Total	Gas	3.630e+01	3.637e+01	3.636e+01	3.636e+01	3.646e+01	3.646e+01	3.646e+01	3.644e+01
Total	Cond.	2.781e+00	3.605e+00	3.638e+00	3.614e+00	4.510e+00	4.508e+00	4.515e+00	4.712e+00

Table 3.16 Detonation product concentrations (mol/kg) for HMX pressed compositions.

		HMX	COMP 8	COMP 9	COMP 10	COMP 11	COMP 12	COMP 13	COMP 14
N_2	Gas	1.348e+01	1.360e+01	1.382e+01	1.366e+01	1.270e+01	1.269e+01	1.274e+01	1.238e+01
CO_2	Gas	5.396e+00	4.571e+00	4.483e+00	4.549e+00	4.115e+00	4.120e+00	4.100e+00	4.100e+00
H_2O	Gas	1.158e+01	1.166e+01	1.152e+01	1.162e+01	1.254e+01	1.255e+01	1.252e+01	1.274e+01
CO	Gas	4.630e+00	4.849e+00	4.826e+00	4.843e+00	4.891e+00	4.893e+00	4.887e+00	4.896e+00
H_2	Gas	4.706e-01	6.635e-01	6.693e-01	6.650e-01	8.411e-01	8.406e-01	8.427e-01	8.600e-01
CH_4	Gas	6.860e-01	1.004e+00	1.010e+00	1.006e+00	1.396e+00	1.395e+00	1.398e+00	1.449e+00
H_3N	Gas	4.778e-02	6.531e-02	6.621e-02	6.553e-02	8.122e-02	8.114e-02	8.145e-02	8.247e-02
CH_2O_2	Gas	5.529e-03	5.360e-03	5.265e-03	5.337e-03	5.514e-03	5.520e-03	5.496e-03	5.587e-03
C_2H_6	Gas	2.291e-04	4.673e-04	4.751e-04	4.693e-04	8.020e-04	8.010e-04	8.049e-04	8.487e-04
CH_2O	Gas	7.642e-04	9.853e-04	9.852e-04	9.853e-04	1.169e-03	1.169e-03	1.169e-03	1.192e-03
CH_3OH	Gas	8.561e-04	1.065e-03	1.059e-03	1.064e-03	1.349e-03	1.349e-03	1.347e-03	1.394e-03
C_2H_4	Gas	2.955e-03	4.360e-03	4.388e-03	4.367e-03	6.071e-03	6.068e-03	6.080e-03	6.298e-03
CH_3	Gas	9.015e-06	1.565e-05	1.591e-05	1.572e-05	2.241e-05	2.238e-05	2.248e-05	2.315e-05
NO	Gas	1.816e-07	1.680e-07	1.676e-07	1.679e-07	1.541e-07	1.542e-07	1.541e-07	1.520e-07
O_2	Gas	4.714e-11	3.760e-11	3.677e-11	3.739e-11	3.310e-11	3.315e-11	3.295e-11	3.296e-11
NO_2	Gas	1.765e-15	1.876e-15	1.875e-15	1.876e-15	1.769e-15	1.769e-15	1.770e-15	1.746e-15
*C	solid	2.781e+00	4.407e+00	4.468e+00	4.422e+00	6.166e+00	6.163e+00	6.175e+00	6.581e+00
Total	Gas	3.630e+01	3.642e+01	3.641e+01	3.642e+01	3.659e+01	3.659e+01	3.658e+01	3.653e+01
Total	Cond.	2.781e+00	4.407e+00	4.468e+00	4.422e+00	6.166e+00	6.163e+00	6.175e+00	6.581e+00

Table 3.17 Detonation product concentrations (mol/kg) for HMX pressed compositions.

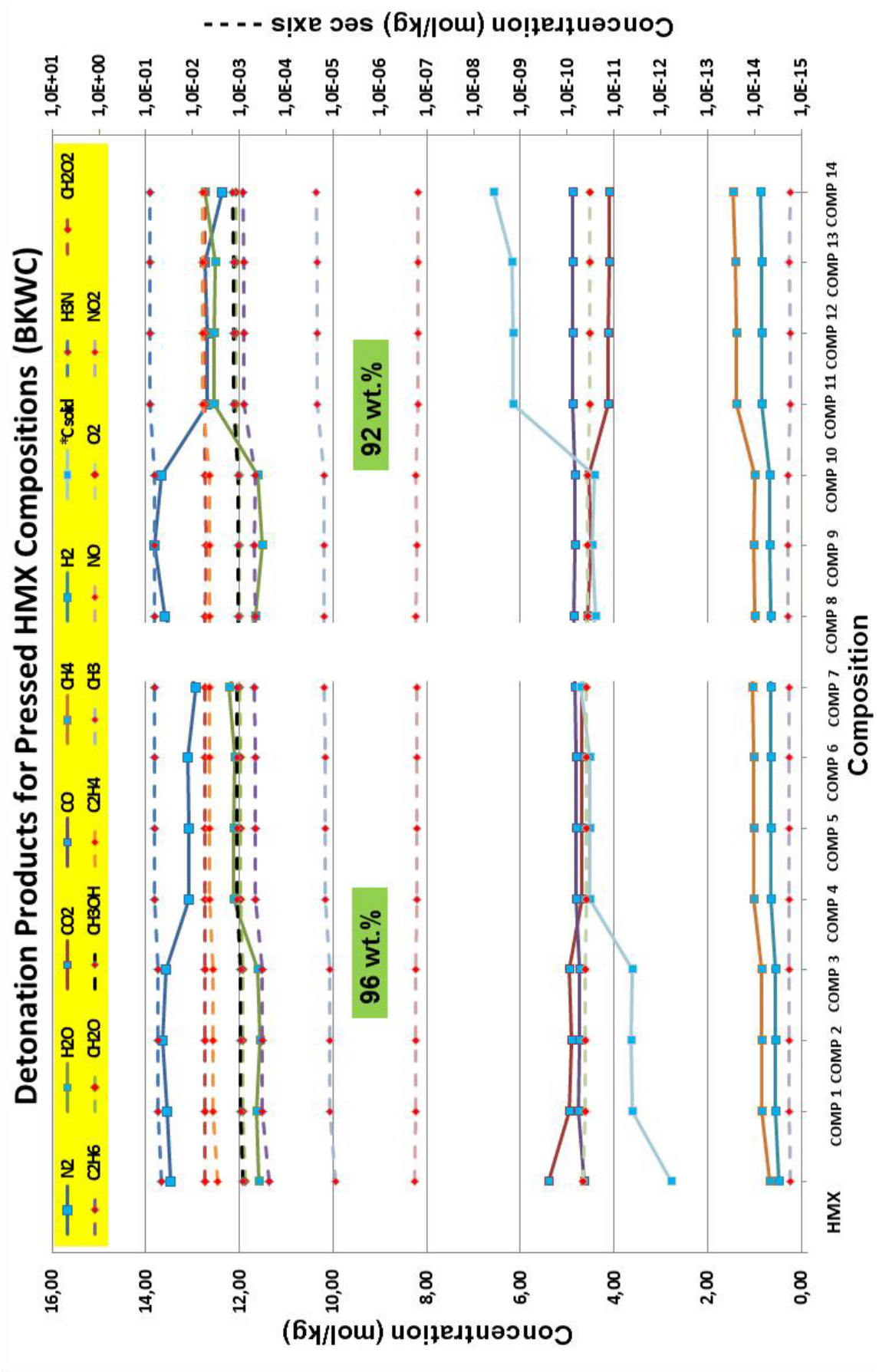

Figure 3.5 Plot of the detonation products for HMX pressed compositions.

3.2.1.2 Pressed RDX compositions

Table 3.7 gives the content of the pressed RDX compositions with 96 wt. % RDX, and Table 3.10 the compositions with 92 wt. % RDX. Table 3.18 gives the detonation products for the compositions in Table 3.7 and Table 3.19 gives the detonation products for the compositions in Table 3.10. Figure 3.6 shows a plot of the detonation products for all pressed RDX compositions.

Name		RDX	COMP 15	COMP 16	COMP 17	COMP 18	COMP 19	COMP 20	COMP 21
N_2	Gas	1.347e+01	1.354e+01	1.364e+01	1.356e+01	1.308e+01	1.308e+01	1.310e+01	1.293e+01
CO_2	Gas	5.196e+00	4.813e+00	4.769e+00	4.802e+00	4.586e+00	4.588e+00	4.578e+00	4.577e+00
H_2O	Gas	1.082e+01	1.087e+01	1.081e+01	1.086e+01	1.132e+01	1.132e+01	1.131e+01	1.142e+01
CO	Gas	5.787e+00	5.823e+00	5.812e+00	5.820e+00	5.841e+00	5.842e+00	5.839e+00	5.847e+00
H_2	Gas	7.244e-01	8.228e-01	8.261e-01	8.236e-01	9.210e-01	9.208e-01	9.218e-01	9.326e-01
CH_4	Gas	9.251e-01	1.077e+00	1.079e+00	1.078e+00	1.267e+00	1.266e+00	1.267e+00	1.293e+00
H_3N	Gas	6.237e-02	7.044e-02	7.087e-02	7.055e-02	7.831e-02	7.828e-02	7.840e-02	7.905e-02
CH_2O_2	Gas	5.589e-03	5.473e-03	5.423e-03	5.460e-03	5.571e-03	5.574e-03	5.561e-03	5.613e-03
C_2H_6	Gas	4.752e-04	6.234e-04	6.275e-04	6.244e-04	8.093e-04	8.089e-04	8.104e-04	8.354e-04
CH_2O	Gas	1.153e-03	1.255e-03	1.254e-03	1.255e-03	1.361e-03	1.361e-03	1.361e-03	1.376e-03
CH_3OH	Gas	9.784e-04	1.066e-03	1.061e-03	1.065e-03	1.200e-03	1.201e-03	1.200e-03	1.223e-03
C_2H_4	Gas	4.069e-03	4.753e-03	4.764e-03	4.756e-03	5.595e-03	5.594e-03	5.598e-03	5.710e-03
CH_3	Gas	1.872e-05	2.288e-05	2.305e-05	2.292e-05	2.710e-05	2.708e-05	2.714e-05	2.760e-05
NO	Gas	1.778e-07	1.714e-07	1.713e-07	1.714e-07	1.646e-07	1.646e-07	1.646e-07	1.634e-07
O_2	Gas	4.023e-11	3.653e-11	3.614e-11	3.643e-11	3.447e-11	3.449e-11	3.440e-11	3.439e-11
NO_2	Gas	2.606e-15	2.590e-15	2.590e-15	2.590e-15	2.505e-15	2.505e-15	2.505e-15	2.491e-15
*C	solid	1.581e+00	2.444e+00	2.476e+00	2.452e+00	3.334e+00	3.332e+00	3.339e+00	3.539e+00
Total	Gas	3.700e+01	3.703e+01	3.702e+01	3.703e+01	3.711e+01	3.711e+01	3.711e+01	3.708e+01
Total	Cond.	1.581e+00	2.444e+00	2.476e+00	2.452e+00	3.334e+00	3.332e+00	3.339e+00	3.539e+00

Table 3.18 Detonation products concentrations in mol/kg for RDX pressed compositions.

Name		RDX	COMP 22	COMP 23	COMP 24	COMP 25	COMP 26	COMP 27	COMP 28
N_2	Gas	1.347e+01	1.360e+01	1.381e+01	1.365e+01	1.269e+01	1.268e+01	1.273e+01	1.238e+01
CO_2	Gas	5.196e+00	4.457e+00	4.371e+00	4.436e+00	4.065e+00	4.070e+00	4.050e+00	4.058e+00
H_2O	Gas	1.082e+01	1.090e+01	1.076e+01	1.086e+01	1.173e+01	1.174e+01	1.170e+01	1.193e+01
CO	Gas	5.787e+00	5.836e+00	5.812e+00	5.830e+00	5.803e+00	5.805e+00	5.799e+00	5.792e+00
H_2	Gas	7.244e-01	9.255e-01	9.335e-01	9.275e-01	1.119e+00	1.118e+00	1.121e+00	1.136e+00
CH_4	Gas	9.251e-01	1.241e+00	1.247e+00	1.243e+00	1.651e+00	1.651e+00	1.653e+00	1.705e+00
H_3N	Gas	6.237e-02	7.890e-02	7.988e-02	7.914e-02	9.452e-02	9.444e-02	9.477e-02	9.556e-02
CH_2O_2	Gas	5.589e-03	5.338e-03	5.236e-03	5.312e-03	5.489e-03	5.495e-03	5.469e-03	5.567e-03
C_2H_6	Gas	4.752e-04	8.021e-04	8.137e-04	8.050e-04	1.259e-03	1.258e-03	1.263e-03	1.317e-03
CH_2O	Gas	1.153e-03	1.353e-03	1.352e-03	1.353e-03	1.543e-03	1.543e-03	1.543e-03	1.563e-03
CH_3OH	Gas	9.784e-04	1.151e-03	1.142e-03	1.149e-03	1.422e-03	1.423e-03	1.420e-03	1.467e-03
C_2H_4	Gas	4.069e-03	5.494e-03	5.523e-03	5.501e-03	7.318e-03	7.315e-03	7.327e-03	7.550e-03
CH_3	Gas	1.872e-05	2.754e-05	2.798e-05	2.765e-05	3.652e-05	3.648e-05	3.664e-05	3.729e-05
NO	Gas	1.778e-07	1.653e-07	1.650e-07	1.652e-07	1.526e-07	1.526e-07	1.526e-07	1.506e-07
O_2	Gas	4.023e-11	3.321e-11	3.247e-11	3.302e-11	2.989e-11	2.994e-11	2.976e-11	2.987e-11
NO_2	Gas	2.606e-15	2.557e-15	2.556e-15	2.557e-15	2.353e-15	2.353e-15	2.353e-15	2.313e-15
*C	solid	1.581e+00	3.293e+00	3.354e+00	3.308e+00	5.045e+00	5.041e+00	5.054e+00	5.467e+00
Total	Gas	3.700e+01	3.704e+01	3.703e+01	3.704e+01	3.718e+01	3.718e+01	3.717e+01	3.711e+01
Total	Cond.	1.581e+00	3.293e+00	3.354e+00	3.308e+00	5.045e+00	5.041e+00	5.054e+00	5.467e+00

Table 3.19 Detonation products concentrations in mol/kg for RDX pressed compositions.

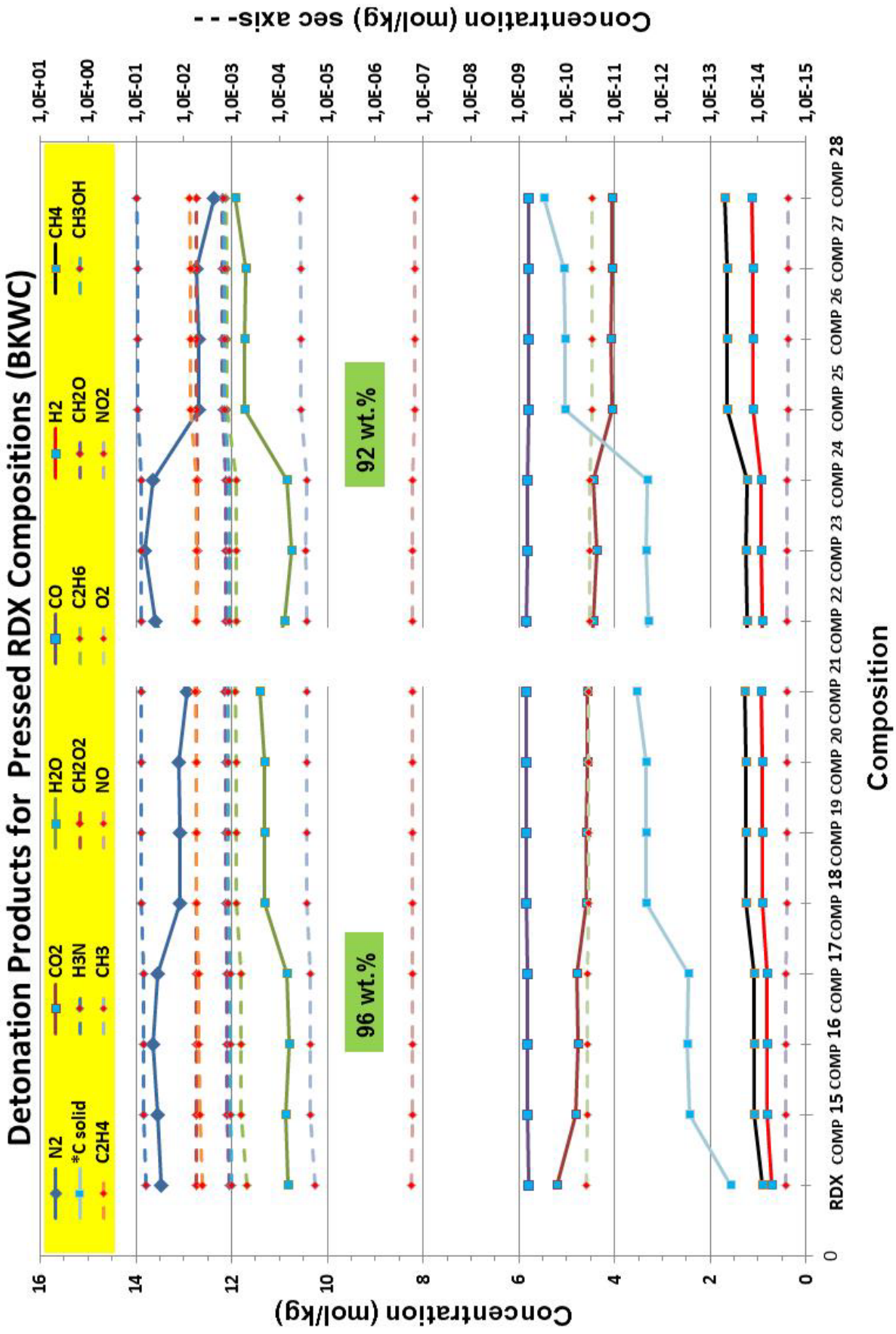

Figure 3.6 Plot of detonation product concentrations for different RDX pressed compositions.

The concentration of the different detonation products for the RDX compositions is slightly different from equal HMX compositions. The order of the major detonation products with respect to concentration is nearly the same. However, RDX-compositions give higher concentration of CO gas and lower concentration of solid C than the equal HMX-compositions. This change have also influence on the concentration of H_2O gas, which is lower for RDX compared with HMX-compositions. For the remaining products the differences are small.

3.2.1.3 Cast-cure compositions

Table 3.13 gives the content of the HMX cast-cure compositions. Table 3.20 gives the obtained concentrations of the detonation products at 1 atm and 298 K for these compositions. The concentrations of the main detonation products depend on the binder. Composition 29 with HTPB binder has a concentration of solid C of 9.6 mol/kg compared to only 2.78 mol/kg for HMX. The content of N_2 gas for Comp 29 is 11.74 mol/kg compared with 13.48 mol/kg for HMX. Figure 3.7 shows plot of the concentrations for all detonation products for cast-cure HMX compositions. Composition 29 (PBXN-110) with inert binder and Comp 33 containing only energetic binder are the two compositions with largest differences in the content of N_2 gas, CO_2 gas, H_2O gas and solid C.

Name		**COMP 29**	**COMP 30**	**COMP 31**	**COMP 32**	**COMP 33**
N_2	Gas	1.174e+01	1.191e+01	1.250e+01	1.264e+01	1.355e+01
CO_2	Gas	3.251e+00	3.839e+00	3.641e+00	3.594e+00	4.013e+00
H_2O	Gas	1.287e+01	1.253e+01	1.266e+01	1.256e+01	1.171e+01
CO	Gas	4.957e+00	5.481e+00	4.892e+00	4.877e+00	4.920e+00
H_2	Gas	1.252e+00	1.160e+00	1.016e+00	1.022e+00	8.304e-01
CH_4	Gas	2.280e+00	1.888e+00	1.765e+00	1.774e+00	1.306e+00
H_3N	Gas	1.150e-01	1.007e-01	9.695e-02	9.792e-02	8.038e-02
CH_2O_2	Gas	5.251e-03	5.600e-03	5.339e-03	5.275e-03	5.185e-03
C_2H_6	Gas	1.922e-03	1.478e-03	1.215e-03	1.231e-03	7.550e-04
CH_2O	Gas	1.534e-03	1.547e-03	1.323e-03	1.323e-03	1.151e-03
CH_3OH	Gas	1.804e-03	1.606e-03	1.544e-03	1.538e-03	1.236e-03
C_2H_4	Gas	1.002e-02	8.324e-03	7.712e-03	7.754e-03	5.702e-03
CH_3	Gas	4.216e-05	3.791e-05	3.021e-05	3.058e-05	2.241e-05
NO	Gas	1.316e-07	1.439e-07	1.438e-07	1.436e-07	1.570e-07
O_2	Gas	2.458e-11	2.873e-11	2.847e-11	2.803e-11	3.180e-11
NO_2	Gas	1.665e-15	2.037e-15	1.716e-15	1.716e-15	1.879e-15
***C**	solid	9.623e+00	6.909e+00	7.635e+00	7.661e+00	5.884e+00
Total	Gas	3.649e+01	3.693e+01	3.659e+01	3.659e+01	3.642e+01
Total	Cond.	9.623e+00	6.909e+00	7.635e+00	7.661e+00	5.884e+00

Table 3.20 Detonation product concentrations in mol/kg for cast-cure HMX compositions.

Table 3.14 gives the content of the RDX cast-cure compositions. Table 3.21 gives the obtained concentrations of the detonation products at 1 atm and 298 K. The variation in concentrations of the main detonation products are as for HMX based compositions and depends on the binder. Composition 34 with HTPB binder has a concentration of solid C of 8.6 (9.6) mol/kg compared to only 1.58 (2.78) mol/kg for RDX (HMX in brackets). The content of N_2 gas for Comp 34 is 11.73

mol/kg compared with 13.47 mol/kg for RDX. Figure 3.7 shows a plot of the concentrations for all detonation products for cast-cure compositions with RDX.

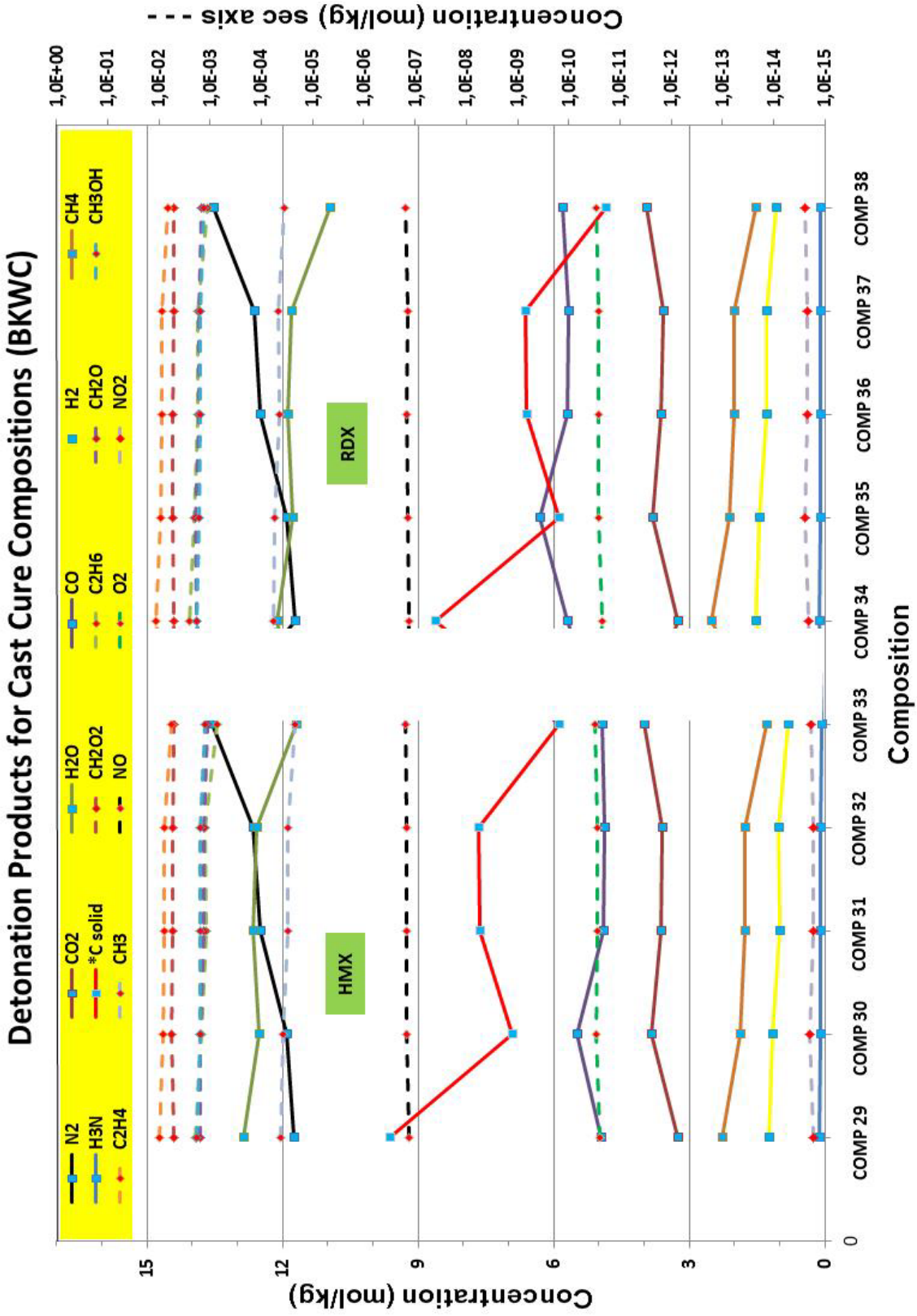

Figure 3.7 Detonation products at room temperature and pressure in mol/kg for cast-cure compositions obtained by use of the BKWC product library.

N_2	Gas	1.173e+01	1.191e+01	1.250e+01	1.263e+01	1.354e+01
CO_2	Gas	3.262e+00	3.806e+00	3.628e+00	3.581e+00	3.949e+00
H_2O	Gas	1.211e+01	1.177e+01	1.189e+01	1.179e+01	1.096e+01
CO	Gas	5.700e+00	6.309e+00	5.692e+00	5.677e+00	5.793e+00
H_2	Gas	1.533e+00	1.444e+00	1.287e+00	1.295e+00	1.094e+00
CH_4	Gas	2.513e+00	2.117e+00	2.006e+00	2.014e+00	1.535e+00
H_3N	Gas	1.257e-01	1.115e-01	1.089e-01	1.099e-01	9.292e-02
CH_2O_2	Gas	5.202e-03	5.503e-03	5.302e-03	5.236e-03	5.131e-03
C_2H_6	Gas	2.580e-03	2.043e-03	1.744e-03	1.764e-03	1.162e-03
CH_2O	Gas	1.877e-03	1.907e-03	1.669e-03	1.670e-03	1.498e-03
CH_3OH	Gas	1.827e-03	1.635e-03	1.592e-03	1.585e-03	1.296e-03
C_2H_4	Gas	1.122e-02	9.487e-03	8.913e-03	8.953e-03	6.826e-03
CH_3	Gas	5.979e-05	5.505e-05	4.539e-05	4.592e-05	3.585e-05
NO	Gas	1.313e-07	1.427e-07	1.430e-07	1.428e-07	1.552e-07
O_2	Gas	2.301e-11	2.650e-11	2.624e-11	2.584e-11	2.872e-11
NO_2	Gas	2.083e-15	2.532e-15	2.201e-15	2.200e-15	2.452e-15
***C**	solid	8.631e+00	5.881e+00	6.603e+00	6.631e+00	4.842e+00
Total	Gas	3.700e+01	3.749e+01	3.713e+01	3.712e+01	3.698e+01
Total	Cond.	8.631e+00	5.881e+00	6.603e+00	6.631e+00	4.842e+00

Table 3.21 Detonation product concentrations in mol/kg for cast cure RDX compositions.

Composition 34 (PBXN-110 with HMX replaced by RDX) with inert binder and Comp 38 containing only energetic binder are the two compositions having larges differences in the content of N_2 gas, CO_2 gas, H_2O gas and solid C.

Comparing the detonation product concentrations for compositions with HMX with compositions with RDX three products H_2O gas, solid Carbon and CO gas have different concentrations. The first two have highest concentrations for HMX-based compositions, while RDX-compositions give higher concentration of CO gas than the HMX compositions. For the remaining detonation products the concentrations are the same in these two types of compositions.

3.2.2 BKWS

3.2.2.1 Pressed HMX compositions

14 compositions with HMX have been studied. Contents for the 7 compositions with 96 wt. % HMX are given in Table 3.1 and for the 7 compositions with 92 wt. % HMX in Table 3.4. Table 3.22 and Table 3.23 give the concentrations of the 63 products that the BKWS product library use in the equilibrium calculations at 1 atm and 298 K. Figure 3.8 shows a plot of the concentrations of major detonation products for HMX itself and all pressed HMX compositions. Figure 3.9 shows a plot of the remaining detonation products with concentrations between 8.0 E-10 mol/kg and 1.0 E-29 mol/kg. Only N_2O_5 with concentration of 1.0E-27 mol/kg is not shown.

The detonation product with the highest concentration is N_2 gas followed by H_2O gas and CO_2 gas. The level of other main detonation products, CO gas, H_2 gas and CH_4 gas, for HMX compositions with 96 wt.% HMX and 92 wt.% HMX is nearly constant. The product C solid has

a higher concentration for compositions with 92 wt. % HMX than for 96 wt.% HMX compositions. For pure HMX the C solid concentration is 1.4 mol/kg and increase to 5.32 mol/kg for PBXN-9. For PBXN-9 C solid is the fourth most common detonation product. The concentrations of the other detonation products are low, and do not change significantly by the content of the compositions.

Name		HMX	COMP 1	COMP 2	COMP 3	COMP 4	COMP 5	COMP 6	COMP 7
CH	Gas	2.907e-14	3.208e-14	3.233e-14	3.217e-14	3.235e-14	3.233e-14	3.242e-14	3.215e-14
CNN	Gas	1.637e-16	1.793e-16	1.678e-16	1.803e-16	1.680e-16	1.678e-16	1.687e-16	1.640e-16
C	Gas	8.139e-17	8.828e-17	8.665e-17	8.855e-17	8.672e-17	8.665e-17	8.692e-17	8.579e-17
HNO_3	Gas	3.368e-18	2.965e-18	2.943e-18	2.951e-18	2.939e-18	2.943e-18	2.928e-18	2.966e-18
C_3	Gas	6.148e-19	7.289e-19	6.919e-19	7.336e-19	6.930e-19	6.919e-19	6.965e-19	6.773e-19
C_2	Gas	4.459e-19	4.965e-19	4.823e-19	4.986e-19	4.828e-19	4.823e-19	4.843e-19	4.759e-19
C_4N_2	Gas	3.827e-19	5.745e-19	4.797e-19	5.845e-19	4.819e-19	4.797e-19	4.883e-19	4.508e-19
NO_3	Gas	6.265e-22	5.247e-22	5.129e-22	5.216e-22	5.122e-22	5.129e-22	5.099e-22	5.169e-22
O_3	Gas	2.009e-22	1.786e-22	1.749e-22	1.778e-22	1.747e-22	1.749e-22	1.741e-22	1.759e-22
N_2O_3	Gas	9.323e-24	8.208e-24	7.711e-24	8.183e-24	7.705e-24	7.711e-24	7.688e-24	7.678e-24
C_4	Gas	8.796e-26	1.155e-25	1.057e-25	1.167e-25	1.060e-25	1.057e-25	1.068e-25	1.021e-25
C_5	Gas	1.090e-28	1.664e-28	1.443e-28	1.691e-28	1.449e-28	1.443e-28	1.467e-28	1.368e-28
N_2O_4	Gas	2.800e-29	2.161e-29	2.074e-29	2.144e-29	2.070e-29	2.074e-29	2.057e-29	2.093e-29
N_2O_5	Gas	1.216e-36	9.202e-37	8.680e-37	9.121e-37	8.661e-37	8.680e-37	8.603e-37	8.756e-37
***C**	Solid	1.400e+00	2.267e+00	3.164e+00	2.275e+00	3.166e+00	3.164e+00	3.172e+00	3.372e+00
***H_2O**	Liquid	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
Total	Gas	3.565e+01	3.572e+01	3.575e+01	3.572e+01	3.575e+01	3.575e+01	3.575e+01	3.571e+01
Total	Cond.	1.400e+00	2.267e+00	3.164e+00	2.275e+00	3.166e+00	3.164e+00	3.172e+00	3.372e+00

Table 3.22 Detonation products concentrations for pressed HMX compositions at room temperature and pressure.

Name		HMX	COMP 8	COMP 9	COMP 10	COMP 11	COMP 12	COMP 13	COMP 14
N_2	Gas	1.335e+01	1.347e+01	1.369e+01	1.353e+01	1.255e+01	1.254e+01	1.259e+01	1.223e+01
CO_2	Gas	8.258e+00	7.447e+00	7.324e+00	7.417e+00	7.140e+00	7.148e+00	7.118e+00	7.161e+00
H_2O	Gas	8.196e+00	8.305e+00	8.196e+00	8.278e+00	9.094e+00	9.101e+00	9.072e+00	9.266e+00
CO	Gas	2.252e+00	2.414e+00	2.439e+00	2.421e+00	2.258e+00	2.256e+00	2.262e+00	2.211e+00
H_2	Gas	1.717e+00	1.976e+00	1.989e+00	1.979e+00	2.155e+00	2.154e+00	2.159e+00	2.163e+00
CH_4	Gas	1.527e+00	1.788e+00	1.779e+00	1.786e+00	2.194e+00	2.195e+00	2.193e+00	2.258e+00
H_3N	Gas	3.006e-01	3.263e-01	3.256e-01	3.262e-01	3.730e-01	3.730e-01	3.729e-01	3.790e-01
CH_2O_2	Gas	2.040e-02	1.877e-02	1.825e-02	1.864e-02	2.028e-02	2.032e-02	2.018e-02	2.085e-02
C_2H_6	Gas	1.795e-02	2.138e-02	2.101e-02	2.129e-02	2.951e-02	2.954e-02	2.943e-02	3.114e-02
CH_2O	Gas	2.772e-03	3.015e-03	3.009e-03	3.014e-03	3.185e-03	3.185e-03	3.185e-03	3.201e-03
CH_3OH	Gas	2.421e-03	2.552e-03	2.497e-03	2.538e-03	3.111e-03	3.115e-03	3.099e-03	3.237e-03
C_2H_4	Gas	2.030e-03	2.500e-03	2.507e-03	2.502e-03	2.988e-03	2.987e-03	2.991e-03	3.044e-03
CHN	Gas	1.130e-03	1.381e-03	1.424e-03	1.392e-03	1.309e-03	1.307e-03	1.317e-03	1.264e-03
CHNO	Gas	1.065e-03	1.118e-03	1.126e-03	1.120e-03	1.076e-03	1.076e-03	1.078e-03	1.060e-03
CH_3	Gas	1.749e-04	2.086e-04	2.097e-04	2.089e-04	2.380e-04	2.379e-04	2.383e-04	2.405e-04
C_3H_8	Gas	3.020e-05	4.063e-05	4.012e-05	4.050e-05	6.012e-05	6.016e-05	6.001e-05	6.375e-05
H	Gas	1.399e-05	1.600e-05	1.622e-05	1.606e-05	1.641e-05	1.640e-05	1.646e-05	1.626e-05
C_3H_6	Gas	1.199e-05	1.684e-05	1.699e-05	1.688e-05	2.147e-05	2.146e-05	2.152e-05	2.195e-05
C_2H_2	Gas	1.025e-05	1.336e-05	1.371e-05	1.345e-05	1.367e-05	1.365e-05	1.375e-05	1.339e-05
CHO	Gas	8.252e-06	9.237e-06	9.327e-06	9.259e-06	9.028e-06	9.022e-06	9.047e-06	8.895e-06
H_2N	Gas	4.140e-06	4.557e-06	4.590e-06	4.565e-06	4.852e-06	4.849e-06	4.860e-06	4.848e-06
HO	Gas	2.757e-06	2.837e-06	2.827e-06	2.835e-06	2.892e-06	2.892e-06	2.890e-06	2.897e-06
NO	Gas	3.233e-07	3.043e-07	3.035e-07	3.041e-07	2.899e-07	2.899e-07	2.897e-07	2.874e-07

H_4N_2	Gas	1.119e-07	1.156e-07	1.145e-07	1.153e-07	1.379e-07	1.379e-07	1.377e-07	1.416e-07
H_2N_2	Gas	1.703e-08	1.748e-08	1.755e-08	1.750e-08	1.838e-08	1.837e-08	1.840e-08	1.837e-08
CNO	Gas	7.571e-09	7.396e-09	7.421e-09	7.403e-09	6.903e-09	6.902e-09	6.909e-09	6.793e-09
C_2N_2	Gas	6.966e-09	8.823e-09	9.289e-09	8.938e-09	7.353e-09	7.328e-09	7.429e-09	6.857e-09
C_3O_2	Gas	2.886e-09	3.643e-09	3.775e-09	3.676e-09	2.970e-09	2.963e-09	2.991e-09	2.792e-09
H_2O_2	Gas	2.237e-09	1.982e-09	1.915e-09	1.965e-09	2.186e-09	2.190e-09	2.172e-09	2.265e-09
CH_2	Gas	1.884e-09	2.240e-09	2.267e-09	2.247e-09	2.399e-09	2.397e-09	2.405e-09	2.392e-09
HNO	Gas	1.598e-09	1.594e-09	1.593e-09	1.594e-09	1.576e-09	1.576e-09	1.576e-09	1.568e-09
C_2H_4O	Gas	1.195e-09	1.498e-09	1.507e-09	1.501e-09	1.680e-09	1.679e-09	1.683e-09	1.691e-09
CN	Gas	6.332e-10	7.295e-10	7.511e-10	7.349e-10	6.665e-10	6.652e-10	6.704e-10	6.413e-10
N_2O	Gas	5.765e-10	5.417e-10	5.442e-10	5.423e-10	4.937e-10	4.935e-10	4.942e-10	4.833e-10
HN	Gas	2.654e-10	2.966e-10	3.017e-10	2.979e-10	2.940e-10	2.936e-10	2.950e-10	2.887e-10
O_2	Gas	1.184e-10	1.014e-10	9.889e-11	1.008e-10	9.987e-11	1.000e-10	9.939e-11	1.012e-10
C_2H	Gas	7.435e-11	9.696e-11	1.003e-10	9.778e-11	9.302e-11	9.281e-11	9.365e-11	8.978e-11
O	Gas	5.154e-11	5.030e-11	5.009e-11	5.025e-11	4.928e-11	4.929e-11	4.924e-11	4.914e-11
C_2O	Gas	8.521e-12	1.060e-11	1.096e-11	1.069e-11	9.223e-12	9.202e-12	9.285e-12	8.776e-12
HO_2	Gas	5.097e-12	4.619e-12	4.512e-12	4.592e-12	4.727e-12	4.733e-12	4.706e-12	4.807e-12
N	Gas	4.994e-12	5.299e-12	5.387e-12	5.321e-12	5.045e-12	5.040e-12	5.062e-12	4.933e-12
HNO_2	Gas	3.708e-12	3.379e-12	3.328e-12	3.366e-12	3.297e-12	3.300e-12	3.288e-12	3.307e-12
NO_2H	Gas	1.628e-12	1.547e-12	1.534e-12	1.544e-12	1.481e-12	1.481e-12	1.479e-12	1.473e-12
CN_2	Gas	1.435e-12	1.573e-12	1.619e-12	1.584e-12	1.406e-12	1.403e-12	1.414e-12	1.348e-12
NO_2	Gas	4.016e-13	3.336e-13	3.263e-13	3.318e-13	3.187e-13	3.191e-13	3.173e-13	3.206e-13
N_3	Gas	3.957e-13	3.987e-13	4.080e-13	4.010e-13	3.554e-13	3.549e-13	3.571e-13	3.421e-13
C_2N	Gas	3.622e-13	4.653e-13	4.873e-13	4.707e-13	4.029e-13	4.017e-13	4.066e-13	3.795e-13
CH	Gas	2.907e-14	3.526e-14	3.606e-14	3.546e-14	3.509e-14	3.504e-14	3.525e-14	3.435e-14
CNN	Gas	1.637e-16	1.957e-16	2.041e-16	1.978e-16	1.680e-16	1.676e-16	1.695e-16	1.585e-16
C	Gas	8.139e-17	9.545e-17	9.783e-17	9.604e-17	9.046e-17	9.032e-17	9.090e-17	8.786e-17
HNO_3	Gas	3.368e-18	2.610e-18	2.506e-18	2.584e-18	2.598e-18	2.605e-18	2.579e-18	2.664e-18
C_3	Gas	6.148e-19	8.581e-19	9.037e-19	8.693e-19	7.456e-19	7.431e-19	7.533e-19	7.000e-19
C_2	Gas	4.459e-19	5.506e-19	5.689e-19	5.551e-19	5.080e-19	5.069e-19	5.112e-19	4.883e-19
C_4N_2	Gas	3.827e-19	8.467e-19	9.721e-19	8.765e-19	5.413e-19	5.364e-19	5.564e-19	4.537e-19
NO_3	Gas	6.265e-22	4.402e-22	4.194e-22	4.350e-22	4.301e-22	4.314e-22	4.261e-22	4.428e-22
O_3	Gas	2.009e-22	1.586e-22	1.527e-22	1.571e-22	1.535e-22	1.539e-22	1.524e-22	1.566e-22
N_2O_3	Gas	9.323e-24	7.222e-24	7.037e-24	7.176e-24	6.446e-24	6.456e-24	6.416e-24	6.432e-24
C_4	Gas	8.796e-26	1.499e-25	1.629e-25	1.531e-25	1.184e-25	1.177e-25	1.203e-25	1.070e-25
C_5	Gas	1.090e-28	2.494e-28	2.837e-28	2.576e-28	1.712e-28	1.698e-28	1.756e-28	1.462e-28
N_2O_4	Gas	2.800e-29	1.674e-29	1.566e-29	1.646e-29	1.594e-29	1.601e-29	1.574e-29	1.656e-29
N_2O_5	Gas	1.216e-36	6.977e-37	6.485e-37	6.851e-37	6.411e-37	6.441e-37	6.322e-37	6.653e-37
***C**	Solid	1.400e+00	3.123e+00	3.188e+00	3.139e+00	4.904e+00	4.900e+00	4.915e+00	5.320e+00
***H_2O**	Liquid	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
Total	Gas	3.565e+01	3.578e+01	3.579e+01	3.578e+01	3.583e+01	3.583e+01	3.583e+01	3.574e+01
Total	Cond.	1.400e+00	3.123e+00	3.188e+00	3.139e+00	4.904e+00	4.900e+00	4.915e+00	5.320e+00

Table 3.23 Concentrations of detonation products for pressed HMX compositions at room temperature and pressure.

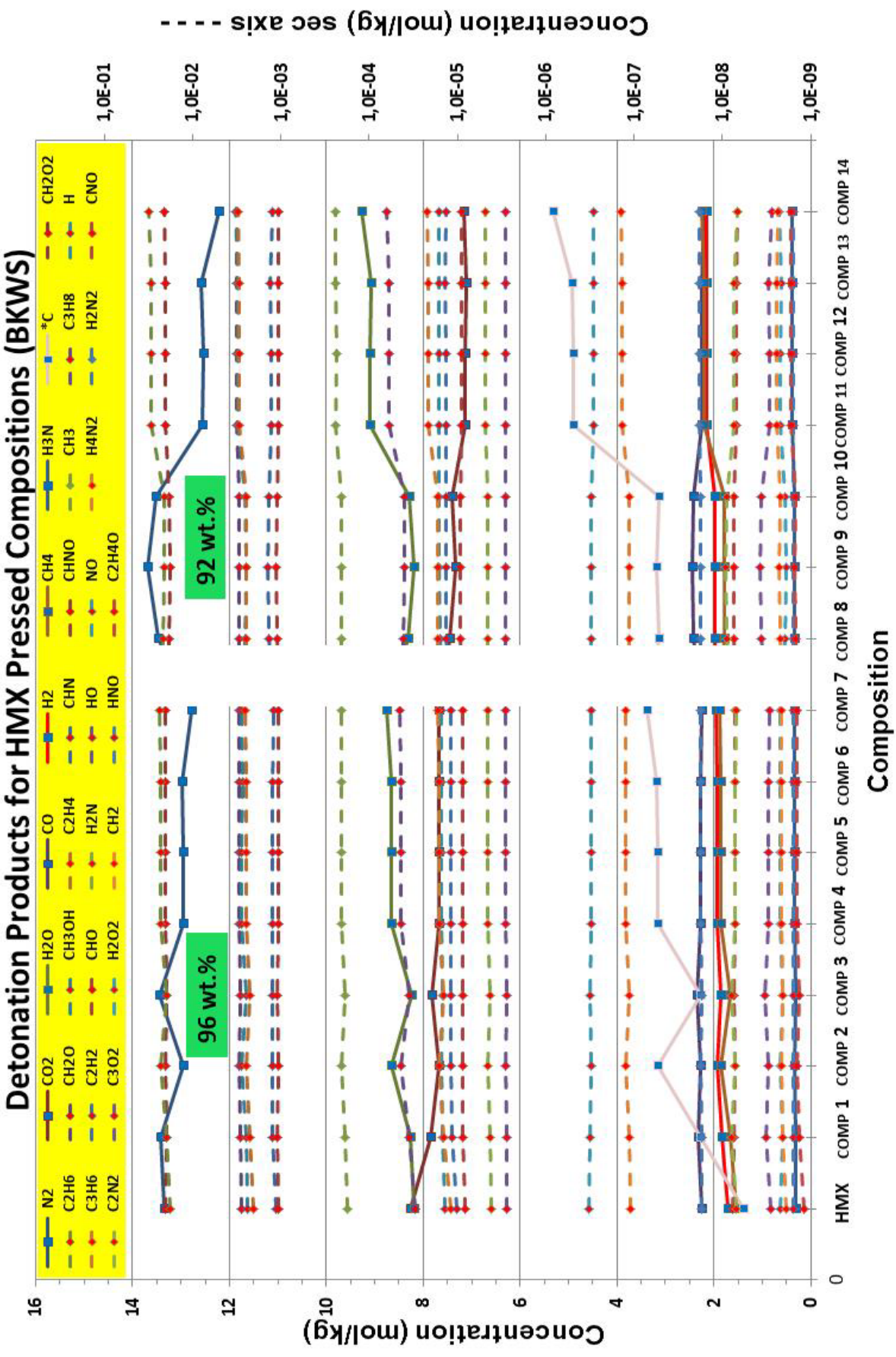

Figure 3.8 Plot of concentrations of main detonation products for pressed HMX compositions.

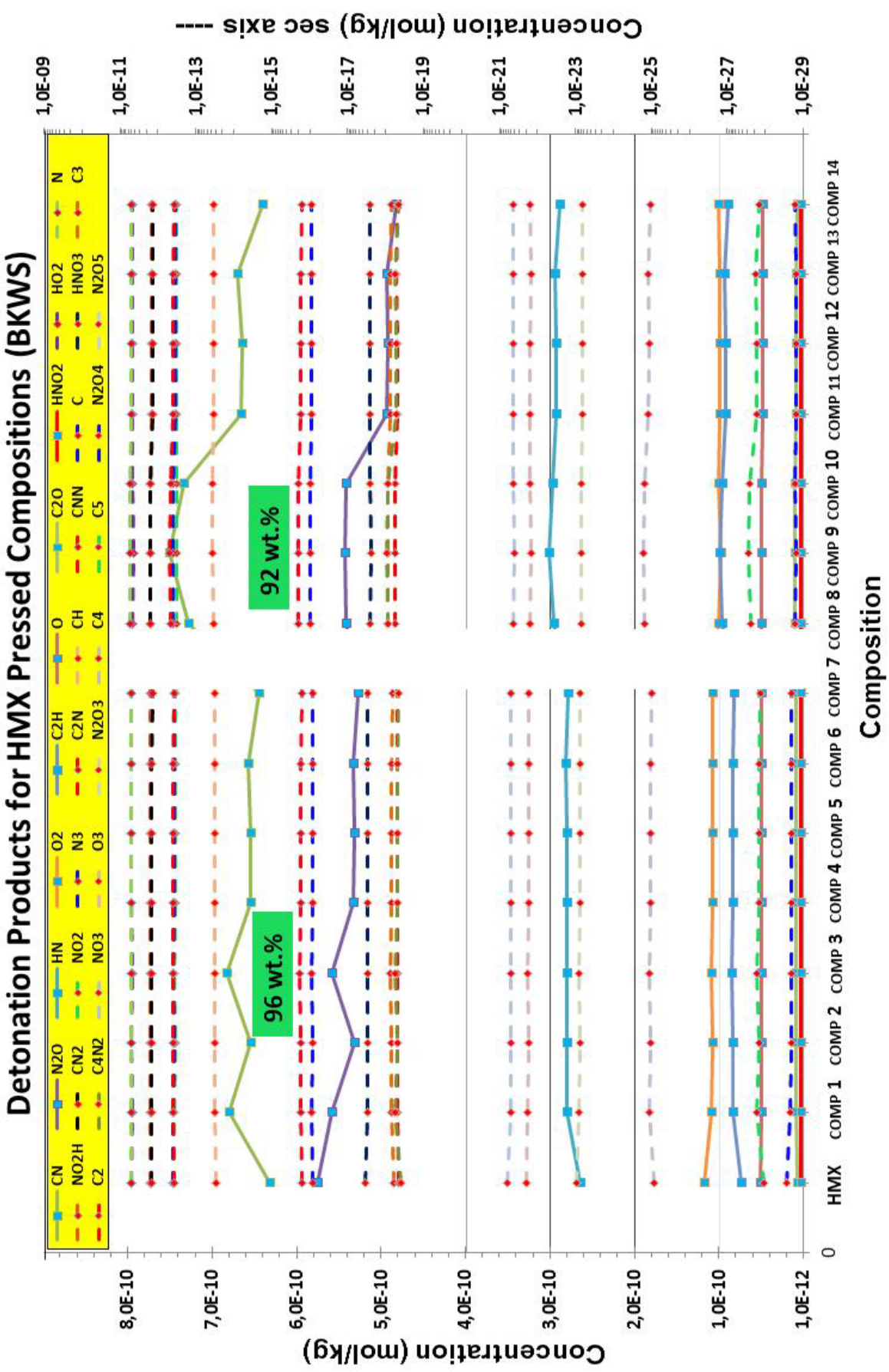

Figure 3.9 Plot of concentrations of minor detonation products for pressed HMX compositions.

3.2.2.2 Pressed RDX compositions

The content of the 14 RDX compositions is given in Table 3.7 for compositions having RDX content of 96 wt. % and in Table 3.10 for compositions with 92 wt. % RDX. Table 3.24 and Table 3.25 give the concentrations of the 63 products the BKWS product library use in the equilibrium calculations at 1 atm and 298 K. Figure 3.10 shows a plot of the concentrations for major detonation products for RDX itself and all pressed RDX compositions. Figure 3.11 shows a plot of detonation products with concentration between 1.0 E-4 mol/kg and 1.0 E-11 mol/kg, while Figure 3.12 shows a plot of the remaining detonation products with concentration down to 1.0 E-25 mol/kg.

The detonation product with the highest concentration is N_2 (g) followed by H_2O (g) and CO_2 (g). The levels of CO (g), H_2 (g) and CH_4 (g) for RDX compositions with 96 wt. % RDX and 92 wt. % RDX are nearly constant. The product C solid is higher for the compositions with 92.wt% RDX than the ones with 96 wt. %. For pure RDX the concentration is 0.66 mol/kg and increases to 4.67 mol/kg for PBXN-9 (RDX). For PBXN-9 (RDX) C solid is the fourth most common detonation product. For the other detonation products the concentrations are low and do not change significantly by the content of the compositions.

Name		RDX	COMP 15	COMP 16	COMP 17	COMP 18	COMP 19	COMP 21	COMP 21
N_2	Gas	1.337e+01	1.343e+01	1.353e+01	1.345e+01	1.297e+01	1.296e+01	1.299e+01	1.281e+01
CO_2	Gas	7.999e+00	7.610e+00	7.546e+00	7.594e+00	7.463e+00	7.467e+00	7.452e+00	7.476e+00
H_2O	Gas	7.777e+00	7.850e+00	7.797e+00	7.836e+00	8.243e+00	8.247e+00	8.233e+00	8.328e+00
CO	Gas	3.196e+00	3.226e+00	3.240e+00	3.230e+00	3.134e+00	3.133e+00	3.136e+00	3.109e+00
H_2	Gas	2.063e+00	2.183e+00	2.190e+00	2.185e+00	2.291e+00	2.290e+00	2.292e+00	2.299e+00
CH_4	Gas	1.588e+00	1.713e+00	1.708e+00	1.712e+00	1.911e+00	1.911e+00	1.910e+00	1.942e+00
H_3N	Gas	2.733e-01	2.865e-01	2.862e-01	2.864e-01	3.076e-01	3.076e-01	3.075e-01	3.104e-01
CH_2O_2	Gas	1.706e-02	1.656e-02	1.633e-02	1.650e-02	1.728e-02	1.729e-02	1.723e-02	1.752e-02
C_2H_6	Gas	1.613e-02	1.775e-02	1.759e-02	1.771e-02	2.104e-02	2.105e-02	2.101e-02	2.165e-02
CH_2O	Gas	3.337e-03	3.431e-03	3.425e-03	3.429e-03	3.549e-03	3.549e-03	3.548e-03	3.566e-03
CH_3OH	Gas	2.133e-03	2.208e-03	2.184e-03	2.202e-03	2.454e-03	2.455e-03	2.449e-03	2.506e-03
C_2H_4	Gas	2.508e-03	2.742e-03	2.744e-03	2.743e-03	3.024e-03	3.024e-03	3.025e-03	3.062e-03
CHN	Gas	1.873e-03	1.995e-03	2.023e-03	2.002e-03	1.958e-03	1.956e-03	1.963e-03	1.931e-03
CHNO	Gas	1.287e-03	1.299e-03	1.303e-03	1.300e-03	1.282e-03	1.282e-03	1.283e-03	1.275e-03
CH_3	Gas	2.145e-04	2.308e-04	2.312e-04	2.309e-04	2.482e-04	2.482e-04	2.483e-04	2.501e-04
C_3H_8	Gas	3.281e-05	3.780e-05	3.752e-05	3.773e-05	4.667e-05	4.669e-05	4.661e-05	4.826e-05
H	Gas	1.835e-05	1.925e-05	1.936e-05	1.928e-05	1.956e-05	1.956e-05	1.959e-05	1.951e-05
C_3H_6	Gas	1.848e-05	2.122e-05	2.127e-05	2.123e-05	2.433e-05	2.432e-05	2.434e-05	2.473e-05
C_2H_2	Gas	1.874e-05	2.049e-05	2.073e-05	2.055e-05	2.093e-05	2.091e-05	2.098e-05	2.081e-05
CHO	Gas	1.210e-05	1.244e-05	1.248e-05	1.245e-05	1.238e-05	1.238e-05	1.239e-05	1.233e-05
H_2N	Gas	4.372e-	4.566e-06	4.581e-06	4.570e-06	4.731e-06	4.730e-06	4.734e-06	4.736e-06
HO	Gas	3.054e-06	3.072e-06	3.066e-06	3.071e-06	3.113e-06	3.113e-06	3.112e-06	3.119e-06
NO	Gas	3.033e-07	2.954e-07	2.951e-07	2.953e-07	2.885e-07	2.885e-07	2.884e-07	2.873e-07
H_4N_2	Gas	7.921e-08	8.243e-08	8.206e-08	8.234e-08	9.039e-08	9.041e-08	9.032e-08	9.165e-08
H_2N_2	Gas	1.457e-08	1.492e-08	1.495e-08	1.493e-08	1.534e-08	1.534e-08	1.535e-08	1.534e-08
CNO	Gas	8.093e-09	7.960e-09	7.972e-09	7.963e-09	7.707e-09	7.706e-09	7.709e-09	7.651e-09
C_2N_2	Gas	1.476e-08	1.572e-08	1.609e-08	1.581e-08	1.449e-08	1.447e-08	1.456e-08	1.407e-08
C_3O_2	Gas	8.367e-09	8.680e-09	8.808e-09	8.712e-09	7.958e-09	7.950e-09	7.981e-09	7.777e-09
H_2O_2	Gas	1.637e-09	1.572e-09	1.546e-09	1.566e-09	1.655e-09	1.657e-09	1.650e-09	1.684e-09
CH_2	Gas	2.544e-09	2.716e-09	2.731e-09	2.720e-09	2.828e-09	2.827e-09	2.831e-09	2.831e-09

HNO	Gas	1.624e-09	1.617e-09	1.616e-09	1.617e-09	1.614e-09	1.614e-09	1.614e-09	1.612e-09
C_2H_4O	Gas	1.855e-09	2.007e-09	2.009e-09	2.008e-09	2.155e-09	2.154e-09	2.155e-09	2.173e-09
CN	Gas	9.670e-10	1.007e-09	1.021e-09	1.011e-09	9.671e-10	9.663e-10	9.697e-10	9.514e-10
N_2O	Gas	5.450e-10	5.296e-10	5.308e-10	5.299e-10	5.065e-10	5.064e-10	5.067e-10	5.015e-10
HN	Gas	3.272e-10	3.405e-10	3.432e-10	3.412e-10	3.404e-10	3.402e-10	3.409e-10	3.380e-10
O_2	Gas	9.604e-11	9.013e-11	8.906e-11	8.986e-11	8.942e-11	8.949e-11	8.921e-11	8.993e-11
C_2H	Gas	1.515e-10	1.645e-10	1.670e-10	1.651e-10	1.625e-10	1.624e-10	1.630e-10	1.605e-10
O	Gas	5.359e-11	5.279e-11	5.268e-11	5.276e-11	5.229e-11	5.230e-11	5.227e-11	5.223e-11
C_2O	Gas	1.969e-11	2.065e-11	2.095e-11	2.072e-11	1.946e-11	1.944e-11	1.952e-11	1.910e-11
HO_2	Gas	4.460e-12	4.279e-12	4.229e-12	4.266e-12	4.339e-12	4.342e-12	4.329e-12	4.376e-12
N	Gas	5.798e-12	5.911e-12	5.959e-12	5.923e-12	5.776e-12	5.773e-12	5.784e-12	5.717e-12
HNO_2	Gas	3.345e-12	3.207e-12	3.182e-12	3.201e-12	3.181e-12	3.183e-12	3.176e-12	3.189e-12
NO_2H	Gas	1.680e-12	1.628e-12	1.620e-12	1.626e-12	1.602e-12	1.602e-12	1.600e-12	1.601e-12
CN_2	Gas	1.893e-12	1.942e-12	1.969e-12	1.949e-12	1.844e-12	1.842e-12	1.849e-12	1.810e-12
NO_2	Gas	2.998e-13	2.787e-13	2.757e-13	2.779e-13	2.722e-13	2.724e-13	2.717e-13	2.728e-13
N_3	Gas	3.996e-13	4.004e-13	4.050e-13	4.015e-13	3.787e-13	3.785e-13	3.796e-13	3.720e-13
C_2N	Gas	7.925e-13	8.490e-13	8.671e-13	8.534e-13	7.972e-13	7.961e-13	8.004e-13	7.779e-13
CH	Gas	4.647e-14	4.950e-14	5.000e-14	4.962e-14	4.968e-14	4.964e-14	4.977e-14	4.931e-14
CNN	Gas	2.848e-16	2.989e-16	3.048e-16	3.003e-16	2.790e-16	2.787e-16	2.801e-16	2.722e-16
C	Gas	1.299e-16	1.362e-16	1.377e-16	1.366e-16	1.331e-16	1.330e-16	1.334e-16	1.315e-16
HNO_3	Gas	2.146e-18	1.945e-18	1.907e-18	1.936e-18	1.944e-18	1.946e-18	1.937e-18	1.966e-18
C_3	Gas	1.750e-18	1.919e-18	1.964e-18	1.930e-18	1.809e-18	1.806e-18	1.817e-18	1.764e-18
C_2	Gas	8.486e-19	9.017e-19	9.152e-19	9.050e-19	8.714e-19	8.705e-19	8.739e-19	8.577e-19
C_4N_2	Gas	4.923e-18	6.053e-18	6.437e-18	6.147e-18	4.999e-18	4.979e-18	5.058e-18	4.662e-18
NO_3	Gas	3.247e-22	2.848e-22	2.784e-22	2.832e-22	2.806e-22	2.810e-22	2.794e-22	2.839e-22
O_3	Gas	1.491e-22	1.350e-22	1.325e-22	1.344e-22	1.329e-22	1.330e-22	1.324e-22	1.341e-22
N_2O_3	Gas	6.681e-24	5.997e-24	5.921e-24	5.978e-24	5.679e-24	5.683e-24	5.665e-24	5.671e-24
C_4	Gas	4.796e-25	5.538e-25	5.747e-25	5.589e-25	5.016e-25	5.004e-25	5.052e-25	4.822e-25
C_5	Gas	1.540e-27	1.918e-27	2.030e-27	1.946e-27	1.639e-27	1.633e-27	1.657e-27	1.542e-27
N_2O_4	Gas	1.039e-29	8.598e-30	8.334e-30	8.532e-30	8.358e-30	8.375e-30	8.309e-30	8.481e-30
N_2O_5	Gas	4.691e-37	3.784e-37	3.654e-37	3.752e-37	3.622e-37	3.630e-37	3.598e-37	3.676e-37
***C**	Solid	6.596e-01	1.561e+00	1.594e+00	1.569e+00	2.465e+00	2.463e+00	2.471e+00	2.674e+00
***H_2O**	Liquid	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
Total	Gas	3.631e+01	3.634e+01	3.635e+01	3.634e+01	3.637e+01	3.637e+01	3.637e+01	3.632e+01
Total	Cond.	6.596e-01	1.561e+00	1.594e+00	1.569e+00	2.465e+00	2.463e+00	2.471e+00	2.674e+00

Table 3.24 Detonation product concentrations in mol/kg for pressed RDX compositions.

Name		RDX	COMP 22	COMP 23	COMP 24	COMP 25	COMP 26	COMP 27	COMP 28
N_2	Gas	1.337e+01	1.348e+01	1.370e+01	1.354e+01	1.257e+01	1.256e+01	1.261e+01	1.225e+01
CO_2	Gas	7.999e+00	7.230e+00	7.105e+00	7.199e+00	6.964e+00	6.972e+00	6.941e+00	6.994e+00
H_2O	Gas	7.777e+00	7.909e+00	7.802e+00	7.882e+00	8.675e+00	8.682e+00	8.653e+00	8.846e+00
CO	Gas	3.196e+00	3.250e+00	3.277e+00	3.257e+00	3.034e+00	3.032e+00	3.039e+00	2.972e+00
H_2	Gas	2.063e+00	2.306e+00	2.320e+00	2.310e+00	2.506e+00	2.505e+00	2.509e+00	2.514e+00
CH_4	Gas	1.588e+00	1.844e+00	1.834e+00	1.841e+00	2.256e+00	2.257e+00	2.254e+00	2.321e+00
H_3N	Gas	2.733e-01	2.999e-01	2.993e-01	2.997e-01	3.427e-01	3.427e-01	3.426e-01	3.484e-01
CH_2O_2	Gas	1.706e-02	1.604e-02	1.558e-02	1.592e-02	1.743e-02	1.747e-02	1.734e-02	1.796e-02
C_2H_6	Gas	1.613e-02	1.946e-02	1.913e-02	1.938e-02	2.682e-02	2.684e-02	2.674e-02	2.829e-02
CH_2O	Gas	3.337e-03	3.518e-03	3.505e-03	3.515e-03	3.717e-03	3.718e-03	3.715e-03	3.738e-03
CH_3OH	Gas	2.133e-03	2.278e-03	2.229e-03	2.266e-03	2.785e-03	2.789e-03	2.774e-03	2.900e-03
C_2H_4	Gas	2.508e-03	2.988e-03	2.994e-03	2.990e-03	3.557e-03	3.556e-03	3.560e-03	3.622e-03
CHN	Gas	1.873e-03	2.120e-03	2.181e-03	2.135e-03	2.002e-03	1.998e-03	2.014e-03	1.932e-03
CHNO	Gas	1.287e-03	1.309e-03	1.316e-03	1.310e-03	1.263e-03	1.262e-03	1.264e-03	1.245e-03
CH_3	Gas	2.145e-04	2.477e-04	2.488e-04	2.480e-04	2.815e-04	2.814e-04	2.818e-04	2.844e-04
C_3H_8	Gas	3.281e-05	4.331e-05	4.272e-05	4.316e-05	6.397e-05	6.401e-05	6.384e-05	6.786e-05
H	Gas	1.835e-05	2.016e-05	2.041e-05	2.022e-05	2.057e-05	2.055e-05	2.062e-05	2.036e-05
C_3H_6	Gas	1.848e-05	2.423e-05	2.438e-05	2.426e-05	3.075e-05	3.074e-05	3.081e-05	3.143e-05
C_2H_2	Gas	1.874e-05	2.232e-05	2.285e-05	2.245e-05	2.269e-05	2.266e-05	2.280e-05	2.221e-05
CHO	Gas	1.210e-05	1.275e-05	1.284e-05	1.277e-05	1.245e-05	1.244e-05	1.247e-05	1.227e-05
H_2N	Gas	4.372e-	4.761e-06	4.794e-06	4.769e-06	5.063e-06	5.061e-06	5.071e-06	5.060e-06
HO	Gas	3.054e-06	3.085e-06	3.071e-06	3.082e-06	3.147e-06	3.147e-06	3.144e-06	3.154e-06
NO	Gas	3.033e-07	2.876e-07	2.868e-07	2.874e-07	2.748e-07	2.748e-07	2.746e-07	2.726e-07
H_4N_2	Gas	7.921e-08	8.568e-08	8.491e-08	8.549e-08	1.025e-07	1.026e-07	1.024e-07	1.055e-07
H_2N_2	Gas	1.457e-08	1.526e-08	1.533e-08	1.528e-08	1.608e-08	1.607e-08	1.610e-08	1.608e-08
CNO	Gas	8.093e-09	7.822e-09	7.843e-09	7.828e-09	7.315e-09	7.313e-09	7.320e-09	7.202e-09
C_2N_2	Gas	1.476e-08	1.670e-08	1.752e-08	1.690e-08	1.387e-08	1.382e-08	1.400e-08	1.294e-08
C_3O_2	Gas	8.367e-09	8.961e-09	9.225e-09	9.026e-09	7.303e-09	7.289e-09	7.347e-09	6.880e-09
H_2O_2	Gas	1.637e-09	1.508e-09	1.457e-09	1.495e-09	1.676e-09	1.680e-09	1.665e-09	1.740e-09
CH_2	Gas	2.544e-09	2.893e-09	2.925e-09	2.901e-09	3.083e-09	3.081e-09	3.090e-09	3.071e-09
HNO	Gas	1.624e-09	1.609e-09	1.606e-09	1.608e-09	1.596e-09	1.596e-09	1.596e-09	1.589e-09
C_2H_4O	Gas	1.855e-09	2.162e-09	2.167e-09	2.164e-09	2.425e-09	2.424e-09	2.427e-09	2.443e-09
CN	Gas	9.670e-10	1.047e-09	1.076e-09	1.054e-09	9.528e-10	9.511e-10	9.580e-10	9.163e-10
N_2O	Gas	5.450e-10	5.144e-10	5.164e-10	5.149e-10	4.713e-10	4.711e-10	4.717e-10	4.621e-10
HN	Gas	3.272e-10	3.539e-10	3.596e-10	3.553e-10	3.500e-10	3.496e-10	3.511e-10	3.437e-10
O_2	Gas	9.604e-11	8.454e-11	8.245e-11	8.401e-11	8.377e-11	8.390e-11	8.337e-11	8.500e-11
C_2H	Gas	1.515e-10	1.779e-10	1.835e-10	1.793e-10	1.694e-10	1.691e-10	1.705e-10	1.634e-10
O	Gas	5.359e-11	5.196e-11	5.172e-11	5.190e-11	5.091e-11	5.092e-11	5.086e-11	5.078e-11
C_2O	Gas	1.969e-11	2.158e-11	2.222e-11	2.174e-11	1.870e-11	1.866e-11	1.881e-11	1.780e-11
HO_2	Gas	4.460e-12	4.099e-12	4.001e-12	4.074e-12	4.220e-12	4.226e-12	4.201e-12	4.299e-12
N	Gas	5.798e-12	6.023e-12	6.120e-12	6.047e-12	5.719e-12	5.713e-12	5.737e-12	5.589e-12
HNO_2	Gas	3.345e-12	3.070e-12	3.020e-12	3.058e-12	3.022e-12	3.025e-12	3.013e-12	3.038e-12
NO_2H	Gas	1.680e-12	1.575e-12	1.558e-12	1.571e-12	1.519e-12	1.520e-12	1.516e-12	1.516e-12
CN_2	Gas	1.893e-12	1.991e-12	2.047e-12	2.005e-12	1.778e-12	1.775e-12	1.788e-12	1.705e-12
NO_2	Gas	2.998e-13	2.589e-13	2.533e-13	2.575e-13	2.494e-13	2.498e-13	2.484e-13	2.515e-13
N_3	Gas	3.996e-13	4.012e-13	4.104e-13	4.035e-13	3.586e-13	3.581e-13	3.603e-13	3.454e-13
C_2N	Gas	7.925e-13	9.069e-13	9.465e-13	9.167e-13	7.806e-13	7.784e-13	7.872e-13	7.351e-13
CH	Gas	4.647e-14	5.260e-14	5.369e-14	5.287e-14	5.202e-14	5.195e-14	5.223e-14	5.089e-14
CNN	Gas	2.848e-16	3.130e-16	3.256e-16	3.161e-16	2.682e-16	2.675e-16	2.703e-16	2.531e-16
C	Gas	1.299e-16	1.425e-16	1.458e-16	1.433e-16	1.341e-16	1.339e-16	1.348e-16	1.301e-16
HNO_3	Gas	2.146e-18	1.761e-18	1.690e-18	1.743e-18	1.779e-18	1.783e-18	1.765e-18	1.830e-18
C_3	Gas	1.750e-18	2.097e-18	2.199e-18	2.122e-18	1.804e-18	1.798e-18	1.821e-18	1.692e-18

C_2	Gas	8.486e-19	9.557e-19	9.852e-19	9.630e-19	8.747e-19	8.729e-19	8.799e-19	8.399e-19
C_4N_2	Gas	4.923e-18	7.379e-18	8.357e-18	7.612e-18	4.666e-18	4.628e-18	4.783e-18	3.919e-18
NO_3	Gas	3.247e-22	2.499e-22	2.384e-22	2.470e-22	2.478e-22	2.485e-22	2.455e-22	2.558e-22
O_3	Gas	1.491e-22	1.222e-22	1.176e-2	1.210e-22	1.195e-22	1.198e-22	1.187e-22	1.223e-22
N_2O_3	Gas	6.681e-24	5.380e-24	5.236e-24	5.344e-24	4.880e-24	4.888e-24	4.856e-24	4.889e-24
C_4	Gas	4.796e-25	6.356e-25	6.852e-25	6.477e-25	4.954e-25	4.930e-25	5.029e-25	4.474e-25
C_5	Gas	1.540e-27	2.367e-27	2.658e-27	2.437e-27	1.598e-27	1.586e-27	1.635e-27	1.365e-27
N_2O_4	Gas	1.039e-29	7.122e-30	6.675e-30	7.008e-30	6.945e-30	6.973e-30	6.859e-30	7.249e-30
N_2O_5	Gas	4.691e-37	3.054e-37	2.839e-37	2.999e-37	2.886e-37	2.899e-37	2.846e-37	3.014e-37
***C**	Solid	6.596e-01	2.453e+00	2.519e+00	2.470e+00	4.248e+00	4.244e+00	4.259e+00	4.670e+00
***H_2O**	Liquid	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
Total	Gas	3.631e+01	3.637e+01	3.639e+01	3.638e+01	3.640e+01	3.640e+01	3.641e+01	3.630e+01
Total	Cond.	6.596e-01	2.453e+00	2.519e+00	2.470e+00	4.248e+00	4.244e+00	4.259e+00	4.670e+00

Table 3.25 Detonation products concentrations in mol/kg for pressed RDX compositions.

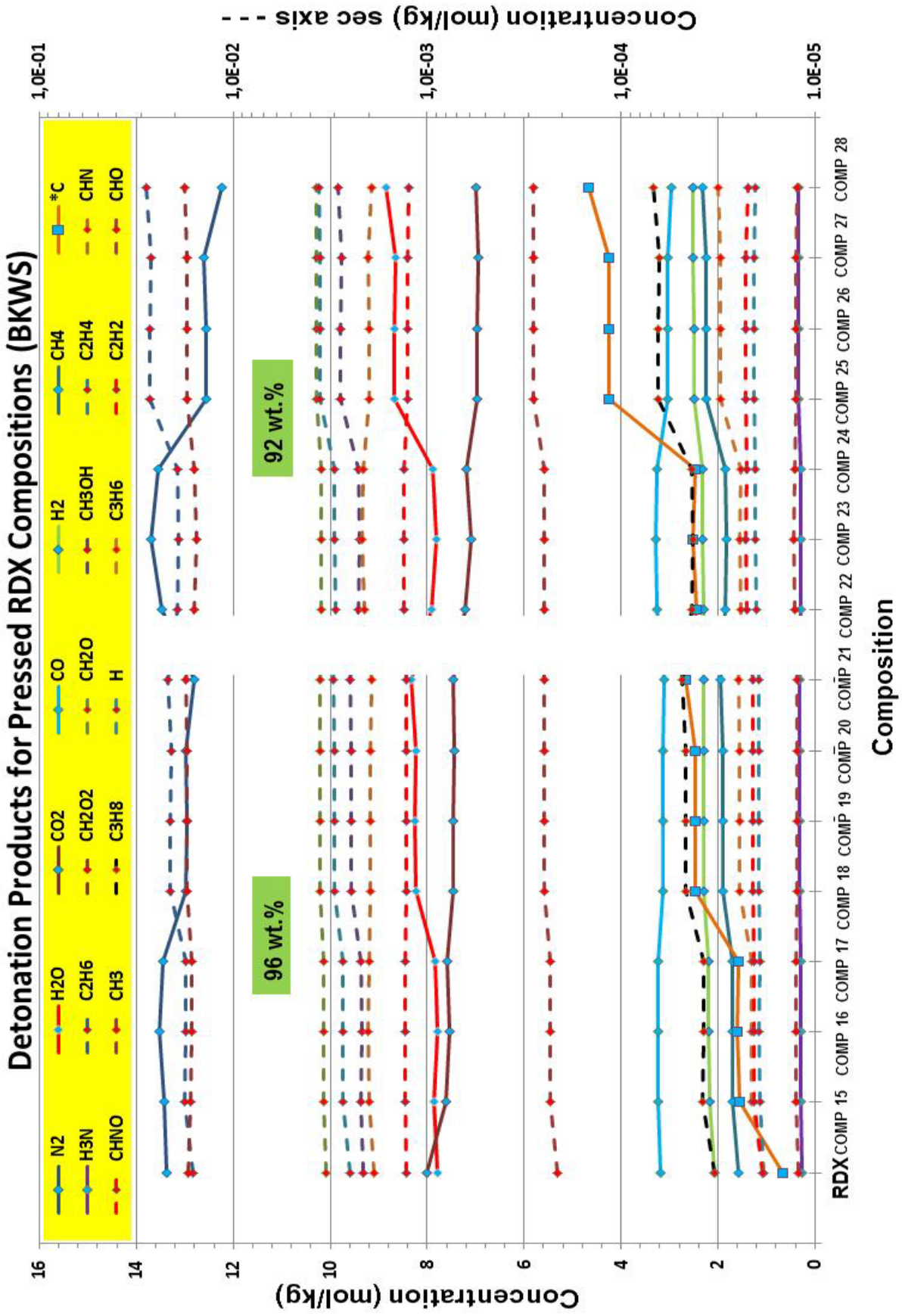

Figure 3.10 Detonation products and concentrations for some pressed RDX compositions.

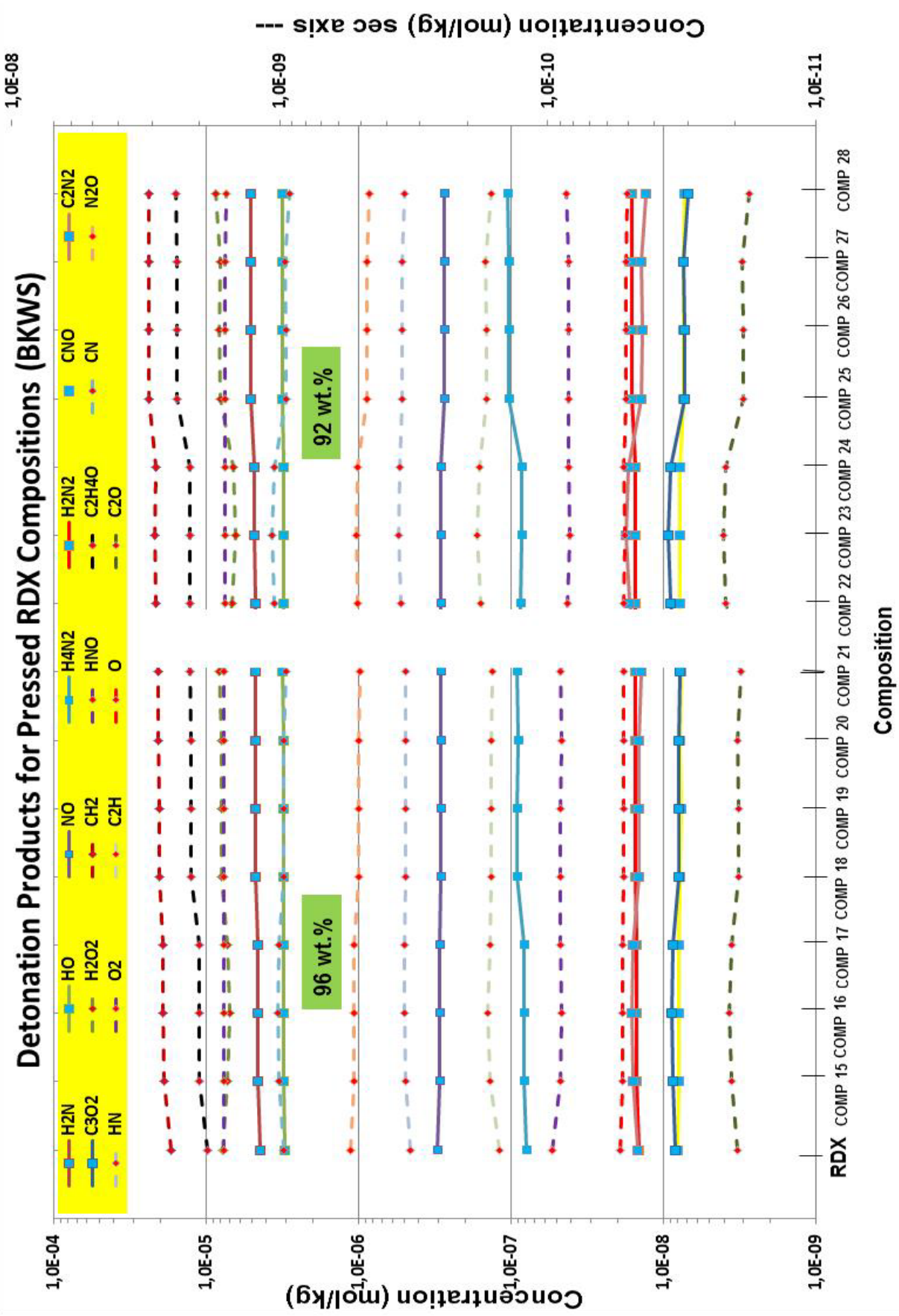

Figure 3.11 Detonation products and concentrations for some pressed RDX compositions.

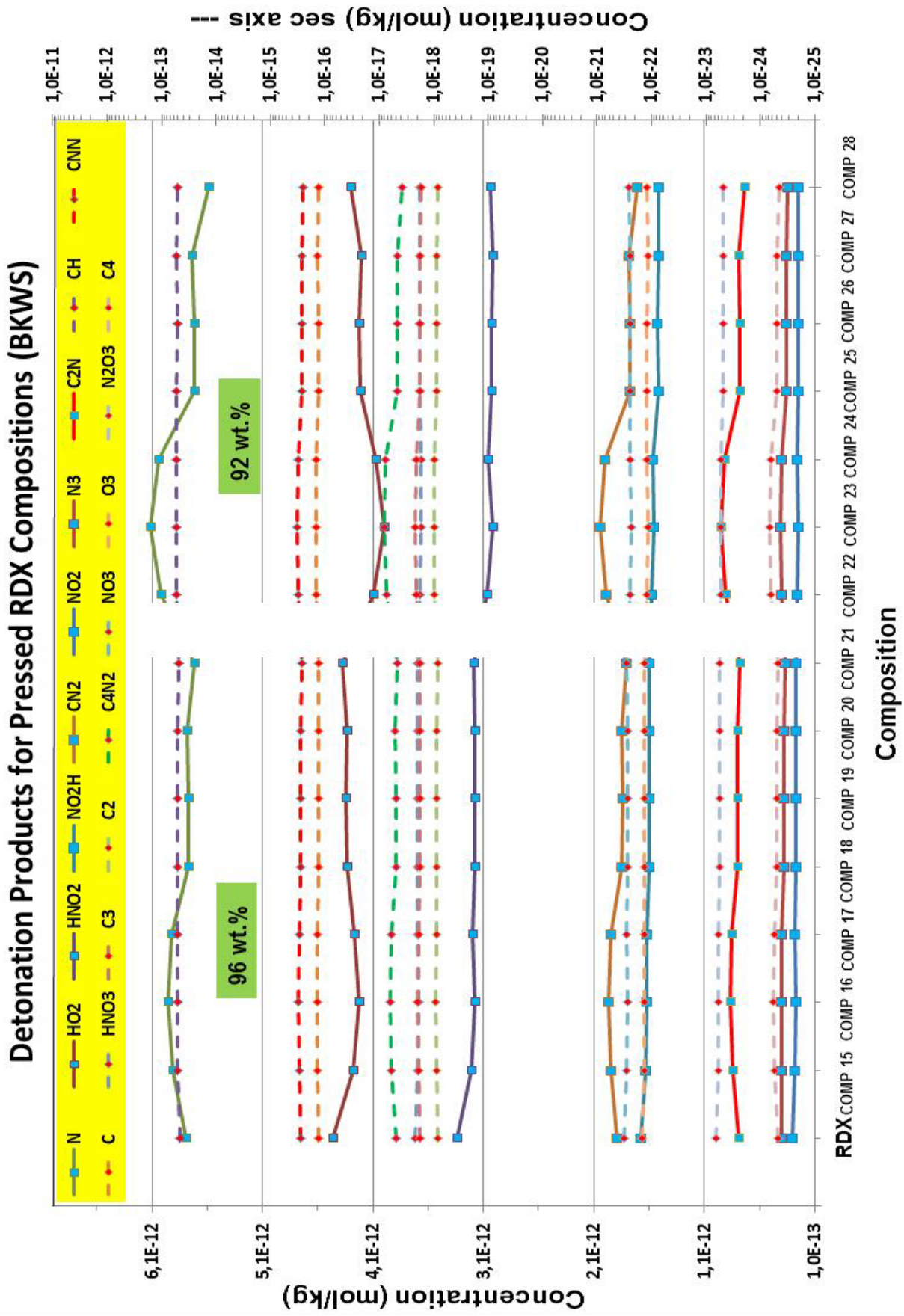

Figure 3.12 Detonation products and concentrations for some pressed RDX compositions.

3.2.2.3 Cast-cure compositions

Table 3.13 gives the content of the cast-cure compositions containing HMX and Table 3.26 gives the obtained concentrations of the detonation products at 1 atm and 298 K. The variation in the main detonation products concentrations depends on the binder. Composition 29 with HTPB binder has a concentration of solid C of 8.69 mol/kg compared to only 1.40 mol/kg for HMX. In addition the concentration of N_2 gas is significantly lower. Figure 3.13 shows a plot of the concentrations for major detonation products for cast-cure HMX compositions, while Figure 3.14 shows plot of the concentrations for minor detonation products. Composition 29 (PBXN-110) with inert binder and Comp 33 containing only energetic binder, are the two compositions having the largest differences in the concentrations of N_2 gas, CO_2 gas, H_2O gas and solid C.

Table 3.14 gives the content of the RDX cast-cure compositions. Table 3.26 gives the obtained concentrations of the detonation products at 1 atm and 298 K. Compared with the product concentrations obtained for the pressed compositions. The variation in main detonation product concentrations are as for HMX based compositions and dependent on the binder. Composition 34 with HTPB binder has a concentration of solid C of 8.09 (8.69) mol/kg compared to only 0.6 (1.4) mol/kg for RDX. Composition 34 (PBXN-110 with HMX replaced with RDX) with inert binder and Comp 38 containing only energetic binder are the two compositions with the largest differences in the concentration of N_2 gas, CO_2 gas, H_2O gas and solid C.

Comparing compositions with HMX and RDX, the three products, H_2O gas, solid C and CO gas, have different concentrations. For the remaining detonation products the concentrations are the same.

Name		COMP 29	COMP 30	COMP 31	COMP 32	COMP 33	COMP 34	COMP 35	COMP 36	COMP 37	COMP38
N_2	Gas	1.158e+01	1.177e+01	1.235e+01	1.248e+01	1.341e+01	1.159e+01	1.179e+01	1.236e+01	1.250e+0	1.342e+01
CO_2	Gas	6.184e+00	6.849e+00	6.621e+00	6.547e+00	6.863e+00	6.060e+00	6.681e+00	6.477e+00	6.402e+0	6.676e+00
H_2O	Gas	9.690e+00	9.352e+00	9.308e+00	9.234e+00	8.430e+00	9.276e+00	8.948e+00	8.906e+00	8.832e+0	8.049e+00
CO	Gas	2.241e+00	2.609e+00	2.253e+00	2.269e+00	2.468e+00	2.908e+00	3.354e+00	2.949e+00	2.966e+0	3.225e+00
H_2	Gas	2.571e+00	2.500e+00	2.345e+00	2.358e+00	2.174e+00	2.928e+00	2.844e+00	2.686e+00	2.699e+0	2.496e+00
CH_4	Gas	2.907e+00	2.543e+00	2.492e+00	2.487e+00	2.027e+00	2.966e+00	2.598e+00	2.550e+00	2.545e+0	2.079e+00
H_3N	Gas	4.330e-01	3.813e-01	4.021e-01	4.021e-01	3.502e-01	4.005e-01	3.535e-01	3.717e-01	3.716e-01	3.238e-01
CH_2O	Gas	1.957e-02	1.942e-02	1.967e-02	1.931e-02	1.785e-02	1.712e-02	1.694e-02	1.713e-02	1.682e-02	1.545e-02
C_2H_6	Gas	4.340e-02	3.415e-02	3.497e-02	3.466e-02	2.496e-02	3.967e-02	3.134e-02	3.197e-02	3.169e-02	2.287e-02
CH_2O	Gas	3.512e-03	3.646e-03	3.319e-03	3.317e-03	3.172e-03	4.016e-03	4.138e-03	3.817e-03	3.811e-03	3.638e-03
CH_3O	Gas	3.722e-03	3.300e-03	3.343e-03	3.301e-03	2.699e-03	3.364e-03	2.981e-03	3.017e-03	2.978e-03	2.429e-03
C_2H_4	Gas	4.053e-03	3.742e-03	3.435e-03	3.447e-03	2.906e-03	4.708e-03	4.332e-03	4.019e-03	4.031e-03	3.408e-03
CHN	Gas	1.461e-03	1.645e-03	1.399e-03	1.430e-03	1.540e-03	2.120e-03	2.355e-03	2.059e-03	2.100e-03	2.264e-03
CHN	Gas	1.059e-03	1.156e-03	1.075e-03	1.080e-03	1.135e-03	1.218e-03	1.317e-03	1.243e-03	1.248e-03	1.307e-03
CH_3	Gas	3.031e-04	2.877e-04	2.663e-04	2.676e-04	2.362e-04	3.501e-04	3.316e-04	3.098e-04	3.111e-04	2.754e-04
C_3H_8	Gas	1.035e-04	8.082e-05	7.645e-05	7.607e-05	5.154e-05	1.084e-04	8.427e-05	8.063e-05	8.017e-05	5.435e-05
H	Gas	1.860e-05	1.918e-05	1.749e-05	1.765e-05	1.737e-05	2.265e-05	2.331e-05	2.146e-05	2.164e-05	5.435e-05
C_3H_6	Gas	3.428e-05	3.170e-05	2.656e-05	2.679e-05	2.138e-05	4.672e-05	4.265e-05	3.675e-05	3.700e-05	2.957e-05
C_2H_2	Gas	1.731e-05	1.916e-05	1.534e-05	1.563e-05	1.564e-05	2.698e-05	2.948e-05	2.432e-05	2.473e-05	2.484e-05
CHO	Gas	9.618e-06	1.094e-05	9.294e-06	9.360e-06	9.754e-06	1.275e-05	1.432e-05	1.245e-05	1.252e-05	1.303e-05
H_2N	Gas	5.402e-06	5.138e-06	5.148e-06	5.178e-06	4.872e-06	5.594e-06	5.316e-06	5.346e-06	5.375e-06	5.061e-06
HO	Gas	2.958e-06	3.088e-06	2.915e-06	2.909e-06	2.872e-06	3.182e-06	3.309e-06	3.145e-06	3.137e-06	3.092e-06

NO	Gas	2.575e-07	2.690e-07	2.760e-07	2.756e-07	2.895e-07	2.459e-07	2.565e-07	2.629e-07	2.625e-07	2.750e-07
H_4N_2	Gas	1.564e-07	1.258e-07	1.476e-07	1.469e-07	1.216e-07	1.201e-07	9.701e-08	1.125e-07	1.121e-07	9.247e-08
H_2N_2	Gas	1.885e-08	1.713e-08	1.889e-08	1.896e-08	1.793e-08	1.673e-08	1.522e-08	1.671e-08	1.678e-08	1.584e-08
CNO	Gas	6.239e-09	6.793e-09	6.632e-09	6.647e-09	7.169e-09	6.574e-09	7.124e-09	6.995e-09	7.009e-09	7.540e-09
C_2N_2	Gas	7.583e-09	9.670e-09	7.668e-09	7.942e-09	9.851e-09	1.325e-08	1.651e-08	1.367e-08	1.413e-08	1.751e-08
C_3O_2	Gas	3.039e-09	4.672e-09	3.005e-09	3.080e-09	3.978e-09	6.708e-09	9.921e-09	6.823e-09	6.964e-09	8.939e-09
H_2O_2	Gas	2.072e-09	1.971e-09	2.100e-09	2.054e-09	1.849e-09	1.638e-09	1.559e-09	1.648e-09	1.612e-09	1.441e-09
CH_2	Gas	2.906e-09	2.934e-09	2.631e-09	2.654e-09	2.506e-09	3.615e-09	3.636e-09	3.302e-09	3.329e-09	3.154e-09
HNO	Gas	1.514e-09	1.566e-09	1.554e-09	1.555e-09	1.579e-09	1.529e-09	1.573e-09	1.571e-09	1.570e-09	1.589e-09
C_2H_4	Gas	2.192e-09	2.301e-09	1.889e-09	1.900e-09	1.730e-09	3.012e-09	3.106e-09	2.633e-09	2.643e-09	2.399e-09
$\hat{C}N$	Gas	6.876e-10	7.815e-10	6.875e-10	7.013e-10	7.812e-10	9.417e-10	1.061e-09	9.520e-10	9.700e-10	1.083e-09
N_2O	Gas	4.183e-10	4.449e-10	4.637e-10	4.653e-10	5.118e-10	4.018e-10	4.249e-10	4.447e-10	4.460e-10	4.878e-10
HN	Gas	3.142e-10	3.233e-10	3.071e-10	3.109e-10	3.162e-10	3.656e-10	3.746e-10	3.597e-10	3.638e-10	3.705e-10
O_2	Gas	8.440e-11	8.844e-11	9.145e-11	8.992e-11	9.101e-11	7.239e-11	7.589e-11	7.793e-11	7.664e-11	7.716e-11
C_2H	Gas	1.122e-10	1.326e-10	1.024e-10	1.048e-10	1.124e-10	1.900e-10	2.211e-10	1.766e-10	1.805e-10	1.944e-10
O	Gas	4.672e-11	4.951e-11	4.801e-11	4.787e-11	4.904e-11	4.810e-11	5.095e-11	4.945e-11	4.929e-11	5.048e-11
C_2O	Gas	9.855e-12	1.328e-11	9.565e-12	9.787e-12	1.168e-11	1.835e-11	2.413e-11	1.821e-11	1.858e-11	2.216e-11
HO_2	Gas	4.317e-12	4.474e-12	4.481e-12	4.413e-12	4.314e-12	3.905e-12	4.033e-12	4.040e-12	3.977e-12	3.863e-12
N	Gas	5.001e-12	5.228e-12	5.098e-12	5.154e-12	5.445e-12	5.584e-12	5.833e-12	5.713e-12	5.775e-12	6.113e-12
HNO_2	Gas	2.883e-12	3.063e-12	3.090e-12	3.060e-12	3.145e-12	2.667e-12	2.809e-12	2.853e-12	2.823e-12	2.876e-12
NO_2H	Gas	1.322e-12	1.461e-12	1.403e-12	1.396e-12	1.471e-12	1.351e-12	1.473e-12	1.436e-12	1.426e-12	1.489e-12
CN_2	Gas	1.350e-12	1.493e-12	1.413e-12	1.441e-12	1.632e-12	1.660e-12	1.821e-12	1.750e-12	1.783e-12	2.020e-12
NO_2	Gas	2.531e-13	2.630e-13	2.856e-13	2.814e-13	2.932e-13	2.043e-13	2.121e-13	2.286e-13	2.253e-13	2.329e-13
N_3	Gas	3.126e-13	3.238e-13	3.449e-13	3.505e-13	3.942e-13	3.151e-13	3.249e-13	3.478e-13	3.533e-13	3.962e-13
C_2N	Gas	4.385e-13	5.556e-13	4.274e-13	4.410e-13	5.265e-13	7.846e-13	9.745e-13	7.807e-13	8.038e-13	9.614e-13
CH	Gas	4.088e-14	4.482e-14	3.792e-14	3.852e-14	3.941e-14	5.772e-14	6.280e-14	5.424e-14	5.502e-14	5.652e-14
CNN	Gas	1.686e-16	2.022e-16	1.727e-16	1.778e-16	2.122e-16	2.542e-16	2.997e-16	2.644e-16	2.717e-16	3.239e-16
C	Gas	9.866e-17	1.118e-16	9.501e-17	9.660e-17	1.038e-16	1.396e-16	1.572e-16	1.360e-16	1.381e-16	1.491e-16
HNO_3	Gas	1.993e-18	2.034e-18	2.269e-18	2.209e-18	2.202e-18	1.428e-18	1.451e-18	1.607e-18	1.565e-18	1.538e-18
C_3	Gas	8.850e-19	1.196e-18	8.184e-19	8.476e-19	1.018e-18	1.926e-18	2.543e-18	1.830e-18	1.890e-18	2.282e-18
C_2	Gas	5.676e-19	6.795e-19	5.402e-19	5.523e-19	6.143e-19	9.162e-19	1.085e-18	8.864e-19	9.049e-19	1.012e-18
C_4N_2	Gas	7.383e-19	1.608e-18	6.537e-19	7.183e-19	1.254e-18	4.891e-18	9.831e-18	4.646e-18	5.061e-18	8.800e-18
NO_3	Gas	2.989e-22	2.968e-22	3.587e-22	3.473e-22	3.497e-22	1.845e-22	1.838e-22	2.173e-22	2.106e-22	2.094e-22
O_3	Gas	1.186e-22	1.288e-22	1.339e-22	1.305e-22	1.345e-22	9.531e-23	1.031e-22	1.067e-22	1.040e-22	1.060e-22
N_2O_3	Gas	4.494e-24	4.986e-24	5.447e-24	5.355e-24	5.991e-24	3.521e-24	3.864e-24	4.230e-24	4.156e-24	4.576e-24
C_4	Gas	1.552e-25	2.547e-25	1.369e-25	1.448e-25	1.969e-25	5.466e-25	8.582e-25	5.043e-25	5.309e-25	7.245e-25
C_5	Gas	2.603e-28	5.664e-28	2.140e-28	2.335e-28	3.802e-28	1.852e-27	3.741e-27	1.635e-27	1.770e-27	2.888e-27
N_2O_4	Gas	9.281e-30	9.031e-30	1.223e-29	1.170e-29	1.198e-29	4.482e-30	4.374e-30	5.748e-30	5.505e-30	5.524e-30
N_2O_5	Gas	3.482e-37	3.644e-37	4.735e-37	4.509e-37	4.812e-37	1.730e-37	1.801e-37	2.293e-37	2.184e-37	2.273e-37
***C**	Solid	8.687e+00	6.039e+00	6.488e+00	6.524e+00	4.704e+00	8.092e+00	5.412e+00	5.884e+00	5.920e+0	4.084e+00
***H_2O**	Liquid	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+0	0.000e+00
Total	Gas	3.568e+01	3.607e+01	3.584e+01	3.585e+01	3.578e+01	3.620e+01	3.663e+01	3.637e+01	3.638e+0	3.632e+01
Total	Cond	8.687e+00	6.039e+00	6.488e+00	6.524e+00	4.704e+00	8.092e+00	5.412e+00	5.884e+00	5.920e+0	4.084e+00

Table 3.26 Detonation products concentrations in mol/kg for cast-cure compositions.

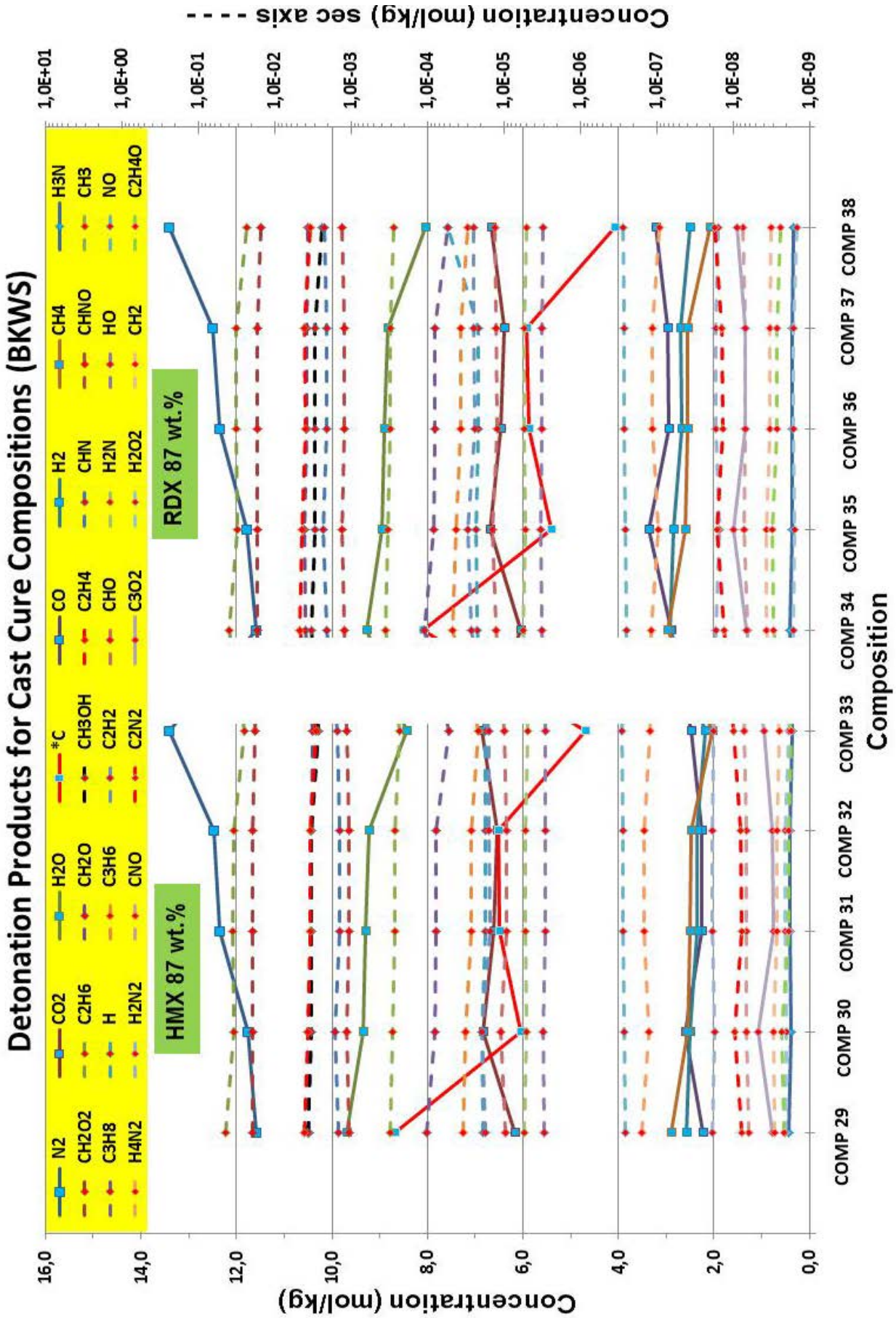

Figure 3.13 Main detonation products and concentrations for cast-cure compositions.

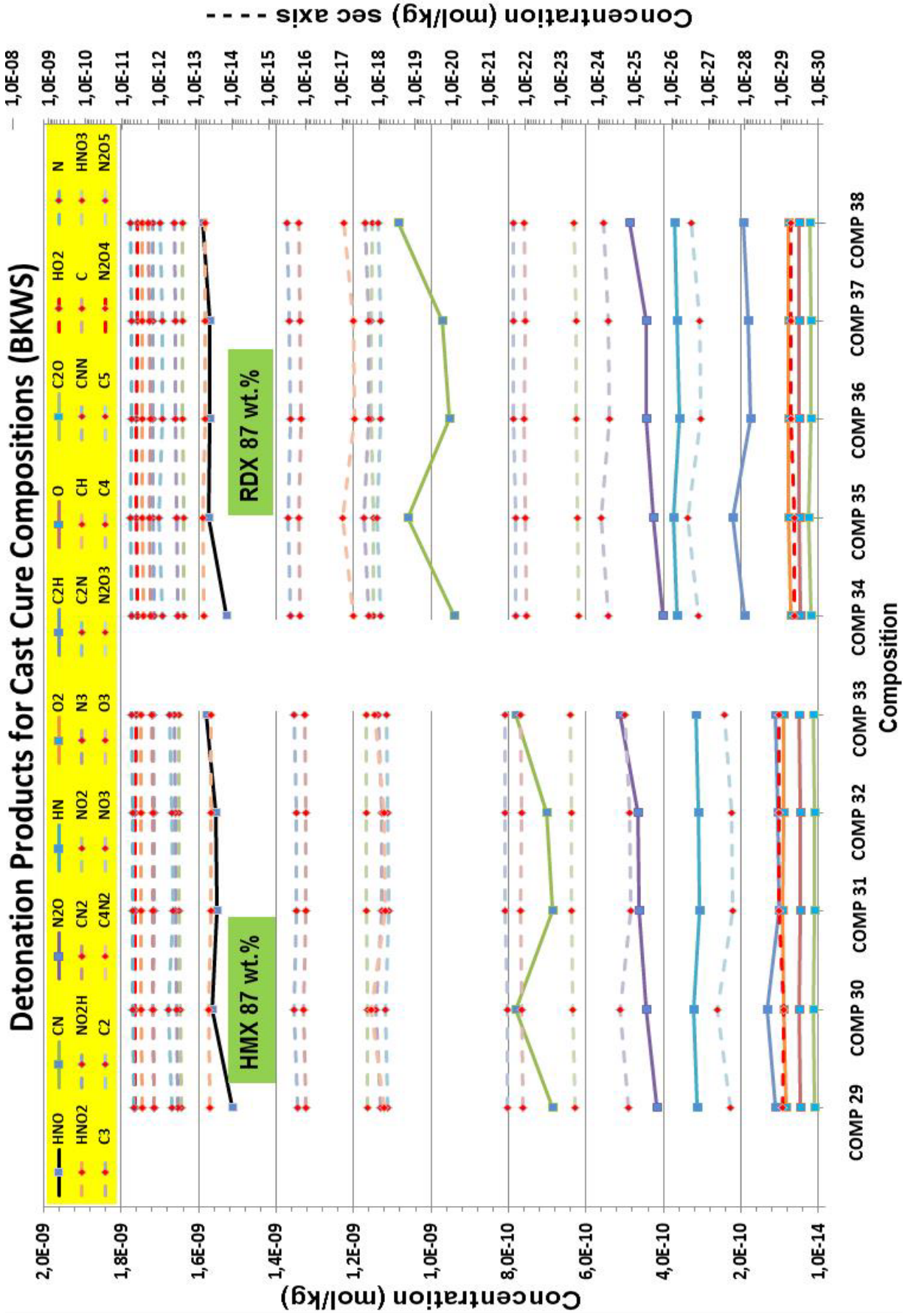

Figure 3.14 Minor detonation products and concentrations for cast-cure compositions.

4 Summary

Cheetah calculations with both BKWC and BKWS product libraries at standard conditions have been performed to study what effect energetic binder/binder system has on performance on different type of compositions.

Two classes of pressed compositions, one with filler content 96 wt.% RDX or HMX and one with 92 wt.% RDX or HMX have been studied. Compositions to be replaced are PBXW-11 and PBXN-9 with respectively 96 and 92 wt.% HMX. Both compositions have an inert binder system of HYTEMP and DOA ratio 1/3. The energetic binder we want to study is GA/BAMO with different ratios. Calculations have been performed with both GAP and BAMO and a mixture of these two. In addition the same calculations with inert plasticizer have been performed.

Detonation pressure and velocity for compositions with GAP, BAMO or GA/BAMO are both equal for these compositions. The ratio between GAP/BAMO has only minor effect on both detonation velocity and pressure. Changes occurred when an inert plasticizer was introduced. For the 96 wt.% HMX compositions the detonation pressure dropped ~2 GPa and for the 92 wt.% HMX compositions 3 GPa with the BKWS and 4 GPa with the BKWC product library with inert plasticizer. The detonation velocity dropped 100-200 m/s and 300 and 400 m/s for the respective compositions and conditions. For compositions with RDX filler the drop in detonation velocity and pressure show the same trend and size as for equivalent HMX compositions.

A composition with 92 wt.% HMX and energetic binder/plasticizer has equal or better performance than PBXW-11 (96 wt.% HMX, inert binder). Use of energetic binder in combination with inert plasticizer has only small influence on detonation velocity and pressure for 96 wt.% compositions, while for the 92 wt.% compositions it increases the detonation pressure by 1 GPa and the detonation velocity by +100 m/s. This trend is the same independent of filler.

For cast-cure compositions with 87 wt.% HMX or RDX the effect of changing to an energetic binder for PBXN-110 give larger differences. The detonation pressure increases with 7.32 GPa (BKWC) and 4.94 GPa (BKWS) for HMX and slightly less (6.48/4.39) with RDX . The detonation velocity increases by 820 m/s (BKWC) and 508 m/s (BKWS) for HMX and 784/468 m/s for RDX. Compositions with energetic binder and inert plasticizer (DOA) have properties between PBXN-110 and compositions containing an energetic binder system.

Detonation products for all study compositions at 298 K and 1 atm have been determined with both the BKWC and the BKWS product libraries. BKWC and BKWS take into consideration respectively 17 and 63 products. For the main product concentrations both for RDX and HMX the largest difference between BKWC and BKWS results is observed in the content of water, CO_2 and CO. BKWC gives 50% higher concentrations of water and CO and 50 % lower concentrations of CO_2 (gas) than BKWS. The concentration of C(solid) increases with lower content of filler (RDX/HMX) (87>92>96) with both product libraries.

References

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

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Appendix Cheetah summary printout 96 wt. % HMX

A.1 HMX

A.1.1 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     Mol.    TMD
                              formation     wt.    (g/cc)
                              (cal/mol)
HMX      100.00 100.00 100.00    17866   296.17     1.91 C4H8N8O8

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)
HMX      100.00 100.00 100.00    17866   296.17     1.91 C4H8N8O8

Density = 1.9050 g/cc  Mixture TMD = 1.9050 g/cc % TMD = 100.0000

The C-J condition:
The pressure          =          38.12 GPa
The volume            =          0.406 cc/g
The density           =          2.460 g/cc
The energy            =          4.30 kJ/cc explosive
The temperature       =          4059 K
The shock velocity    =          9.415 mm/us
The particle velocity =          2.125 mm/us
The speed of sound    =          7.290 mm/us
Gamma                 =          3.430

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    -1.38
   2.20    -7.79     161      123      104       86      179
   4.10    -9.26     159      120      104       88      168
   6.50    -9.82     158      118      104       88      161
  10.00   -10.18     156      117      104       89      155
  20.00   -10.59     154      116      104       89      148
  40.00   -10.87     152      114      104       89      141
  80.00   -11.08     150      113      103       90      135
 160.00   -11.25

Freezing occurred at T =     1800.0 K and relative V =   2.095
The mechanical energy of detonation =    -11.353 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -11.353 kJ/cc

JWL Fit results:
E0   =      -11.682 kJ/cc
A    =     1608.58 GPa, B =  14.83 GPa,   C  =   1.84 GPa
R[1] =        5.11   R[2] =   1.15,    omega =   0.44
RMS fitting error =   1.15 %
```

A.1.2 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      100.00 100.00 100.00    17866   296.17     1.91 C4H8N8O8

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      100.00 100.00 100.00    17866   296.17     1.91 C4H8N8O8

Density = 1.9050 g/cc Mixture TMD = 1.9050 g/cc  % TMD = 100.0000

The C-J condition:
The pressure          =          39.37 GPa
The volume            =          0.400 cc/g
The density           =          2.503 g/cc
The energy            =          4.70 kJ/cc explosive
The temperature       =          4113 K
The shock velocity    =          9.301 mm/us
The particle velocity =          2.222 mm/us
The speed of sound    =          7.079 mm/us
Gamma                 =          3.186

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    -1.41
   2.20    -7.59     157      120      102       84      174
   4.10    -9.00     155      117      102       85      163
   6.50    -9.56     153      115      101       86      156
  10.00    -9.91     152      114      101       86      151
  20.00   -10.32     150      113      101       87      144
  40.00   -10.61     148      112      101       87      137
  80.00   -10.83     147      111      101       88      131
 160.00   -11.00

Freezing occurred at T =     1800.0 K and relative V =   2.085
The mechanical energy of detonation =    -11.112 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -11.112 kJ/cc

JWL Fit results:
E0   =      -11.532 kJ/cc
A    =     1225.94 GPa, B    =  12.46 GPa,  C  =     1.55 GPa
R[1] =        4.77,     R[2] =   1.08,   omega =     0.39
RMS fitting error =   1.01 %
```

A.2 COMP 1

A.2.1 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     Mol.   TMD
                                 formation    wt.    (g/cc)
                                 (cal/mol)
GAP        4.00  11.07   5.78    33939    99.09     1.29 C3H5N3O1
HMX       96.00  88.93  94.22    17866   296.17     1.91 C4H8N8O8
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)
GAP        4.00  11.07   5.78    33939    99.09     1.29 C3H5N3O1
HMX       96.00  88.93  94.22    17866   296.17     1.91 C4H8N8O8

Density = 1.8696 g/cc  Mixture TMD = 1.8696 g/cc % TMD = 100.0000

The C-J condition:
The pressure          =          36.36 GPa
The volume            =          0.413 cc/g
The density           =          2.423 g/cc
The energy            =          4.15 kJ/cc explosive
The temperature       =          4013 K
The shock velocity    =          9.227 mm/us
The particle velocity =          2.108 mm/us
The speed of sound    =          7.119 mm/us
Gamma                 =          3.378

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    -1.33
   2.20    -7.46     154      117      100       82      171
   4.10    -8.88     153      115      100       84      161
   6.50    -9.44     152      114      100       85      155
  10.00    -9.80     150      113      100       85      149
  20.00   -10.20     148      111      100       86      142
  40.00   -10.48     147      110      100       86      136
  80.00   -10.70     145      110      100       87      130
 160.00   -10.87

Freezing occurred at T =     1800.0 K and relative V =   2.093
The mechanical energy of detonation =    -10.992 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.992 kJ/cc

JWL Fit results:
E0   =     -11.397 kJ/cc
A    =    1392.07 GPa, B    =    13.06 GPa,  C     =     1.51 GPa
R[1] =         4.97,   R[2] =     1.08,      omega =     0.39
RMS fitting error =   1.33 %
```

A.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)
GAP        4.00  11.07   5.78    33939    99.09     1.29 C3H5N3O1
HMX       96.00  88.93  94.22    17866   296.17     1.91 C4H8N8O8

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)
GAP        4.00  11.07   5.78    33939    99.09     1.29 C3H5N3O1
HMX       96.00  88.93  94.22    17866   296.17     1.91 C4H8N8O8

Density = 1.8696 g/cc  Mixture TMD = 1.8696 g/cc % TMD = 100.0000

The C-J condition:
The pressure          =          37.18 GPa
The volume            =          0.406 cc/g
The density           =          2.464 g/cc
The energy            =          4.49 kJ/cc explosive
The temperature       =          4075 K
The shock velocity    =          9.080 mm/us
The particle velocity =          2.190 mm/us
The speed of sound    =          6.889 mm/us
Gamma                 =          3.145

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    -1.34
   2.20    -7.23     149      114       97       80      166
   4.10    -8.61     148      112       97       82      156
   6.50    -9.16     147      110       97       82      150
  10.00    -9.51     146      109       97       83      145
  20.00    -9.92     144      108       97       84      138
  40.00   -10.22     143      108       97       84      132
  80.00   -10.44     142      107       97       85      127
 160.00   -10.61

Freezing occurred at T =     1800.0 K and relative V =   2.104
The mechanical energy of detonation =    -10.752 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.752 kJ/cc

JWL Fit results:
E0   =      -11.098 kJ/cc
A    =     1113.04 GPa, B    =   11.76 GPa,  C     =     1.78 GPa
R[1] =        4.75,     R[2] =    1.12,      omega =     0.42
RMS fitting error =   0.74 %
```

A.3 COMP 2

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     Mol.   TMD
                                 formation     wt.    (g/cc)
                                 (cal/mol)
BAMO        4.00   6.84   5.75   100382   168.16     1.30 C5H8N6O1
HMX        96.00  93.16  94.25    17866   296.17     1.91 C4H8N8O8

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)
BAMO        4.00   6.84   5.75   100382   168.16     1.30 C5H8N6O1
HMX        96.00  93.16  94.25    17866   296.17     1.91 C4H8N8O8

Density  =  1.8702 g/cc   Mixture TMD =  1.8702 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          36.40 GPa
The volume            =          0.413 cc/g
The density           =          2.424 g/cc
The energy            =          4.16 kJ/cc explosive
The temperature       =          4021 K
The shock velocity    =          9.230 mm/us
The particle velocity =          2.109 mm/us
The speed of sound    =          7.121 mm/us
Gamma                 =          3.377

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    -1.33
   2.20    -7.47     154      118      100       83      171
   4.10    -8.90     153      115      100       84      161
   6.50    -9.45     152      114      100       85      155
  10.00    -9.81     150      113      100       85      150
  20.00   -10.21     149      111      100       86      142
  40.00   -10.50     147      111      100       86      136
  80.00   -10.71     145      110      100       87      130
 160.00   -10.88

Freezing occurred at T =     1800.0 K and relative V =   2.098
The mechanical energy of detonation =    -11.007 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -11.007 kJ/cc

JWL Fit results:
E0   =      -11.335 kJ/cc
A    =      1439.27 GPa, B    =     13.81 GPa,  C     =     1.80 GPa
R[1] =         5.05,     R[2] =      1.14,      omega =     0.43
RMS fitting error =   1.09 %
```

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)
BAMO        4.00   6.84   5.75   100382   168.16     1.30 C5H8N6O1
HMX        96.00  93.16  94.25    17866   296.17     1.91 C4H8N8O8

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)
BAMO        4.00   6.84   5.75   100382   168.16     1.30 C5H8N6O1
HMX        96.00  93.16  94.25    17866   296.17     1.91 C4H8N8O8

Density  =  1.8702 g/cc   Mixture TMD =  1.8702 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          37.28 GPa
The volume            =          0.406 cc/g
The density           =          2.465 g/cc
The energy            =          4.50 kJ/cc explosive
The temperature       =          4080 K
The shock velocity    =          9.088 mm/us
The particle velocity =          2.194 mm/us
The speed of sound    =          6.894 mm/us
Gamma                 =          3.143

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    -1.34
   2.20    -7.25     149      114       97       80      166
   4.10    -8.63     148      112       97       82      156
   6.50    -9.18     147      111       97       82      150
  10.00    -9.53     146      110       97       83      145
  20.00    -9.94     145      109       98       84      139
  40.00   -10.23     143      108       98       84      132
  80.00   -10.46     142      107       98       85      127
 160.00   -10.63

Freezing occurred at T =     1800.0 K and relative V =   2.107
The mechanical energy of detonation =    -10.770 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.770 kJ/cc

JWL Fit results:
E0   =       -11.117 kJ/cc
A    =      1113.31 GPa, B    =    11.78 GPa,  C     =   1.78 GPa
R[1] =         4.75,     R[2] =     1.12,      omega =   0.42
RMS fitting error =   0.74 %
```

A.4 COMP 3

A.4.1 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     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
BAMO        1.00   1.65   1.44   100382   168.16     1.30 C5H8N6O1
GAP         3.00   8.40   4.34    33939    99.09     1.29 C3H5N3O1
HMX        96.00  89.95  94.22    17866   296.17     1.91 C4H8N8O8

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)
BAMO        1.00   1.65   1.44   100382   168.16     1.30 C5H8N6O1
GAP         3.00   8.40   4.34    33939    99.09     1.29 C3H5N3O1
HMX        96.00  89.95  94.22    17866   296.17     1.91 C4H8N8O8

Density  =  1.8697 g/cc   Mixture TMD =  1.8697 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          36.37 GPa
The volume            =          0.413 cc/g
The density           =          2.423 g/cc
The energy            =           4.15 kJ/cc explosive
The temperature       =           4015 K
The shock velocity    =          9.228 mm/us
The particle velocity =          2.108 mm/us
The speed of sound    =          7.120 mm/us
Gamma                 =          3.377

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    -1.33
   2.20    -7.46     154      118      100       82      171
   4.10    -8.89     153      115      100       84      161
   6.50    -9.44     152      114      100       85      155
  10.00    -9.80     150      113      100       85      149
  20.00   -10.20     149      111      100       86      142
  40.00   -10.49     147      110      100       86      136
  80.00   -10.70     145      110      100       87      130
 160.00   -10.87

Freezing occurred at T =     1800.0 K and relative V =   2.094
The mechanical energy of detonation =    -10.996 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.996 kJ/cc

JWL Fit results:
E0   =       -11.323 kJ/cc
A    =      1441.15 GPa, B    =     13.83 GPa,  C     =         1.80 GPa
R[1] =         5.05,     R[2] =      1.14,      omega =         0.43
RMS fitting error =   1.09 %
```

A.4.2 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)
GAP         3.00   8.40   4.34    33939    99.09     1.29 C3H5N3O1
BAMO        1.00   1.65   1.44   100382   168.16     1.30 C5H8N6O1
HMX        96.00  89.95  94.22    17866   296.17     1.91 C4H8N8O8

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)
GAP         3.00   8.40   4.34    33939    99.09     1.29 C3H5N3O1
BAMO        1.00   1.65   1.44   100382   168.16     1.30 C5H8N6O1
HMX        96.00  89.95  94.22    17866   296.17     1.91 C4H8N8O8

Density  =  1.8697 g/cc   Mixture TMD =  1.8697 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          37.21 GPa
The volume            =          0.406 cc/g
The density           =          2.464 g/cc
The energy            =           4.49 kJ/cc explosive
The temperature       =           4076 K
The shock velocity    =          9.082 mm/us
The particle velocity =          2.191 mm/us
The speed of sound    =          6.890 mm/us
Gamma                 =          3.144

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    -1.34
   2.20    -7.23     149      114       97       80      166
   4.10    -8.61     148      112       97       82      156
   6.50    -9.16     147      110       97       82      150
  10.00    -9.52     146      110       97       83      145
  20.00    -9.93     145      108       97       84      138
  40.00   -10.22     143      108       98       84      132
  80.00   -10.44     142      107       98       85      127
 160.00   -10.62

Freezing occurred at T =     1800.0 K and relative V =   2.105
The mechanical energy of detonation =    -10.756 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.757 kJ/cc

JWL Fit results:
E0   =       -11.103 kJ/cc
A    =      1113.02 GPa, B    =    11.76 GPa,  C     =    1.78 GPa
R[1] =         4.75,     R[2] =     1.12,      omega =    0.42
RMS fitting error =   0.74 %
```

A.5 COMP 4

A.5.1 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     Mol.    TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
GAP         0.75   2.22   1.07    33939    99.09     1.29 C3H5N3O1
BAMO        0.25   0.44   0.35   100382   168.16     1.30 C5H8N6O1
DOA         3.00   2.37   5.96  -290392   370.56     0.93 C22H42O4
HMX        96.00  94.97  92.62    17866   296.17     1.91 C4H8N8O8
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)
GAP         0.75   2.22   1.07    33939    99.09     1.29 C3H5N3O1
BAMO        0.25   0.44   0.35   100382   168.16     1.30 C5H8N6O1
DOA         3.00   2.37   5.96  -290392   370.56     0.93 C22H42O4
HMX        96.00  94.97  92.62    17866   296.17     1.91 C4H8N8O8

Density  =  1.8379 g/cc   Mixture TMD =  1.8379 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         34.77 GPa
The volume            =         0.419 cc/g
The density           =         2.385 g/cc
The energy            =          3.99 kJ/cc explosive
The temperature       =          3918 K
The shock velocity    =         9.079 mm/us
The particle velocity =         2.084 mm/us
The speed of sound    =         6.995 mm/us
Gamma                 =         3.357

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    -1.27
   2.20    -7.14     147      112       96       79      164
   4.10    -8.52     147      110       96       81      154
   6.50    -9.06     145      109       96       81      148
  10.00    -9.41     144      108       96       82      143
  20.00    -9.81     143      107       96       83      137
  40.00   -10.10     141      106       96       83      131
  80.00   -10.31     140      106       96       84      125
 160.00   -10.48

Freezing occurred at T =     1800.0 K and relative V =   2.055
The mechanical energy of detonation =    -10.628 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.628 kJ/cc

JWL Fit results:
E0   =      -10.955 kJ/cc
A    =      1340.66 GPa, B    =    12.98 GPa,  C     =     1.73 GPa
R[1] =         5.02,     R[2] =     1.13,      omega =     0.42
RMS fitting error =   1.07 %
```

A.5.2 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)
GAP         0.75   2.22   1.07    33939     99.09     1.29 C3H5N3O1
BAMO        0.25   0.44   0.35   100382   168.16     1.30 C5H8N6O1
DOA         3.00   2.37   5.96  -290392   370.56     0.93 C22H42O4
HMX        96.00  94.97  92.62    17866   296.17     1.91 C4H8N8O8
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)
GAP         0.75   2.22   1.07    33939     99.09     1.29 C3H5N3O1
BAMO        0.25   0.44   0.35   100382   168.16     1.30 C5H8N6O1
DOA         3.00   2.37   5.96  -290392   370.56     0.93 C22H42O4
HMX        96.00  94.97  92.62    17866   296.17     1.91 C4H8N8O8

Density  =  1.8379 g/cc   Mixture TMD =  1.8379 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         34.90 GPa
The volume            =         0.412 cc/g
The density           =         2.428 g/cc
The energy            =          4.24 kJ/cc explosive
The temperature       =          3998 K
The shock velocity    =         8.841 mm/us
The particle velocity =         2.148 mm/us
The speed of sound    =         6.693 mm/us
Gamma                 =         3.116


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    -1.27
   2.20    -6.85     141      108       92       76      157
   4.10    -8.19     141      106       92       78      148
   6.50    -8.73     140      105       93       78      143
  10.00    -9.09     139      105       93       79      139
  20.00    -9.50     138      104       93       80      133
  40.00    -9.80     137      103       94       81      127
  80.00   -10.03     136      103       94       81      122
 160.00   -10.20

Freezing occurred at T =     1800.0 K and relative V =   2.101
The mechanical energy of detonation =    -10.375 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.375 kJ/cc

JWL Fit results:
E0   =       -10.798 kJ/cc
A    =      1026.89 GPa, B    =    11.19 GPa,  C     =    1.50 GPa
R[1] =         4.74,     R[2] =     1.07,      omega =    0.38
RMS fitting error =   0.95 %
```

A.6 COMP 5

A.6.1 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     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
GAP         1.00   2.24   1.35    33939    99.09     1.29 C3H5N3O1
DOA         3.00   1.80   5.67  -290392   370.56     0.93 C22H42O4
RDX        96.00  95.96  92.97    16496   222.13     1.81 C3H6N6O6
Product library title: bkws library

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
GAP         1.00   2.24   1.35    33939    99.09     1.29 C3H5N3O1
DOA         3.00   1.80   5.67  -290392   370.56     0.93 C22H42O4
RDX        96.00  95.96  92.97    16496   222.13     1.81 C3H6N6O6

Density  =  1.7491 g/cc   Mixture TMD =  1.7491 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         31.19 GPa
The volume            =         0.438 cc/g
The density           =         2.285 g/cc
The energy            =          3.66 kJ/cc explosive
The temperature       =          4002 K
The shock velocity    =         8.720 mm/us
The particle velocity =         2.045 mm/us
The speed of sound    =         6.675 mm/us
Gamma                 =         3.264

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    -1.17
   2.20    -6.60     136      104       88       73      151
   4.10    -7.94     137      103       90       75      144
   6.50    -8.47     136      102       90       76      139
  10.00    -8.82     135      102       90       77      134
  20.00    -9.22     134      101       90       78      129
  40.00    -9.51     133      100       91       78      123
  80.00    -9.72     132      100       91       79      118
 160.00    -9.89

Freezing occurred at T =     1800.0 K and relative V =   2.171
The mechanical energy of detonation =    -10.056 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.056 kJ/cc

JWL Fit results:
E0   =      -10.373 kJ/cc
A    =      1112.82 GPa, B    =    11.97 GPa,  C     =     1.72 GPa
R[1] =         4.98,     R[2] =     1.12,      omega =     0.42
RMS fitting error =   1.02 %
```

A.6.2 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)
GAP         1.00   2.95   1.42    33939    99.09     1.29 C3H5N3O1
DOA         3.00   2.36   5.96  -290392   370.56     0.93 C22H42O4
HMX        96.00  94.69  92.62    17866   296.17     1.91 C4H8N8O8

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)
GAP         1.00   2.95   1.42    33939    99.09     1.29 C3H5N3O1
DOA         3.00   2.36   5.96  -290392   370.56     0.93 C22H42O4
HMX        96.00  94.69  92.62    17866   296.17     1.91 C4H8N8O8

Density  =  1.8379 g/cc   Mixture TMD =  1.8379 g/cc   % TMD = 100.0000


The C-J condition:
The pressure          =         34.90 GPa
The volume            =         0.412 cc/g
The density           =         2.428 g/cc
The energy            =          4.24 kJ/cc explosive
The temperature       =          3998 K
The shock velocity    =         8.840 mm/us
The particle velocity =         2.148 mm/us
The speed of sound    =         6.693 mm/us
Gamma                 =         3.116


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    -1.27
   2.20    -6.85     141      108       92       76      157
   4.10    -8.19     141      106       92       78      148
   6.50    -8.73     140      105       93       78      143
  10.00    -9.09     139      105       93       79      139
  20.00    -9.50     138      104       93       80      132
  40.00    -9.80     137      103       93       81      127
  80.00   -10.03     136      103       94       81      122
 160.00   -10.20

Freezing occurred at T =     1800.0 K and relative V =   2.101
The mechanical energy of detonation =    -10.374 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.374 kJ/cc

JWL Fit results:
E0   =      -10.721 kJ/cc
A    =      1022.28 GPa, B    =   11.12 GPa,  C     =    1.73 GPa
R[1] =         4.75,     R[2] =    1.11,      omega =    0.41
RMS fitting error =   0.71 %
```

A.7 COMP 6

A.7.1 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     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
BAMO        1.00   1.76   1.41   100382   168.16     1.30 C5H8N6O1
DOA         3.00   2.39   5.96  -290392   370.56     0.93 C22H42O4
HMX        96.00  95.85  92.62    17866   296.17     1.91 C4H8N8O8
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)
BAMO        1.00   1.76   1.41   100382   168.16     1.30 C5H8N6O1
DOA         3.00   2.39   5.96  -290392   370.56     0.93 C22H42O4
HMX        96.00  95.85  92.62    17866   296.17     1.91 C4H8N8O8

Density  =  1.8380 g/cc   Mixture TMD =  1.8380 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         34.78 GPa
The volume            =         0.419 cc/g
The density           =         2.386 g/cc
The energy            =          3.99 kJ/cc explosive
The temperature       =          3919 K
The shock velocity    =         9.080 mm/us
The particle velocity =         2.084 mm/us
The speed of sound    =         6.996 mm/us
Gamma                 =         3.357

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    -1.27
   2.20    -7.14     147      112       96       79      164
   4.10    -8.52     147      110       96       81      154
   6.50    -9.06     146      109       96       81      148
  10.00    -9.42     144      108       96       82      144
  20.00    -9.81     143      107       96       83      137
  40.00   -10.10     141      106       96       83      131
  80.00   -10.32     140      106       96       84      125
 160.00   -10.48

Freezing occurred at T =     1800.0 K and relative V =   2.056
The mechanical energy of detonation =    -10.631 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.631 kJ/cc

JWL Fit results:
E0   =      -11.037 kJ/cc
A    =      1295.63 GPa, B    =     12.25 GPa,  C     =     1.46 GPa
R[1] =         4.94,     R[2] =      1.07,      omega =     0.38
RMS fitting error =   1.30 %
```

A.7.2 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)
BAMO        1.00   1.76   1.41   100382   168.16     1.30 C5H8N6O1
DOA         3.00   2.39   5.96  -290392   370.56     0.93 C22H42O4
HMX        96.00  95.85  92.62    17866   296.17     1.91 C4H8N8O8

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)
BAMO        1.00   1.76   1.41   100382   168.16     1.30 C5H8N6O1
DOA         3.00   2.39   5.96  -290392   370.56     0.93 C22H42O4
HMX        96.00  95.85  92.62    17866   296.17     1.91 C4H8N8O8

Density  =  1.8380 g/cc   Mixture TMD =  1.8380 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          34.92 GPa
The volume            =          0.412 cc/g
The density           =          2.428 g/cc
The energy            =           4.24 kJ/cc explosive
The temperature       =           3999 K
The shock velocity    =          8.842 mm/us
The particle velocity =          2.149 mm/us
The speed of sound    =          6.694 mm/us
Gamma                 =          3.115


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    -1.27
   2.20    -6.85     141      108       92       76      157
   4.10    -8.20     141      106       93       78      148
   6.50    -8.74     140      105       93       79      143
  10.00    -9.09     139      105       93       79      139
  20.00    -9.50     138      104       93       80      133
  40.00    -9.80     137      103       94       81      127
  80.00   -10.03     136      103       94       81      122
 160.00   -10.21

Freezing occurred at T =     1800.0 K and relative V =   2.102
The mechanical energy of detonation =    -10.378 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.378 kJ/cc

JWL Fit results:
E0   =      -10.801 kJ/cc
A    =      1026.98 GPa, B    =    11.20 GPa,  C     =    1.50 GPa
R[1] =         4.74,     R[2] =     1.07,      omega =    0.38
RMS fitting error =   0.95 %
```

A.8 COMP 7

A.8.1 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   Mol.     TMD
                             formation   wt.    (g/cc)
                             (cal/mol)
HYTEMP  1.00   1.57   1.83  -205067   188.60     1.00 C10H15.46O3.307
DOA     3.00   2.40   5.94  -290392   370.56     0.93 C22H42O4
HMX    96.00  96.03  92.23    17866   296.17     1.91 C4H8N8O8

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)
HYTEMP   1.00   1.57   1.83  -205067   188.60    1.00 C10H15.46O3.307
DOA      3.00   2.40   5.94  -290392   370.56    0.93 C22H42O4
HMX     96.00  96.03  92.23    17866   296.17    1.91 C4H8N8O8

Density = 1.8303 g/cc  Mixture TMD = 1.8303 g/cc % TMD = 100.0000

The C-J condition:
The pressure          =         34.32 GPa
The volume            =         0.421 cc/g
The density           =         2.376 g/cc
The energy            =          3.94 kJ/cc explosive
The temperature       =          3892 K
The shock velocity    =         9.033 mm/us
The particle velocity =         2.076 mm/us
The speed of sound    =         6.958 mm/us
Gamma                 =         3.352

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    -1.26
   2.20    -7.05     145      111       94       78      162
   4.10    -8.41     145      109       95       80      152
   6.50    -8.95     144      108       95       80      146
  10.00    -9.30     143      107       95       81      142
  20.00    -9.70     141      106       95       82      135
  40.00    -9.98     140      105       95       82      129
  80.00   -10.20     138      104       95       83      124
 160.00   -10.36

Freezing occurred at T =     1800.0 K and relative V =   2.042
The mechanical energy of detonation =    -10.514 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.514 kJ/cc

JWL Fit results:
E0   =     -10.920 kJ/cc
A    =    1274.89 GPa, B  =   12.10 GPa,  C     =     1.45 GPa
R[1] =       4.94,   R[2] =    1.07,      omega =     0.38
RMS fitting error = 1.29 %
```

A.8.2 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 formation (cal/mol)	Mol. wt.	TMD (g/cc)	
HYTEMP	1.00	1.57	1.83	-205067	188.60	1.00	$C_{10}H_{15.46}O_{3.307}$
DOA	3.00	2.40	5.94	-290392	370.56	0.93	$C_{22}H_{42}O_4$
HMX	96.00	96.03	92.23	17866	296.17	1.91	$C_4H_8N_8O_8$

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)	Mol. wt.	TMD (g/cc)	
HYTEMP	1.00	1.57	1.83	-205067	188.60	1.00	$C_{10}H_{15.46}O_{3.307}$
DOA	3.00	2.40	5.94	-290392	370.56	0.93	$C_{22}H_{42}O_4$
HMX	96.00	96.03	92.23	17866	296.17	1.91	$C_4H_8N_8O_8$

Density = 1.8303 g/cc Mixture TMD = 1.8303 g/cc % TMD = 100.0000

The C-J condition:

The pressure	=	34.29 GPa
The volume	=	0.414 cc/g
The density	=	2.418 g/cc
The energy	=	4.17 kJ/cc explosive
The temperature	=	3975 K
The shock velocity	=	8.778 mm/us
The particle velocity	=	2.134 mm/us
The speed of sound	=	6.645 mm/us
Gamma	=	3.114

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	-1.24					
2.20	-6.74	139	106	90	75	155
4.10	-8.07	139	105	91	76	146
6.50	-8.61	138	104	91	77	141
10.00	-8.97	138	103	92	78	137
20.00	-9.38	136	102	92	79	131
40.00	-9.67	135	102	92	80	125
80.00	-9.90	134	101	92	80	120
160.00	-10.08					

Freezing occurred at T = 1800.0 K and relative V = 2.095
The mechanical energy of detonation = -10.257 kJ/cc
The thermal energy of detonation = -0.000 kJ/cc
The total energy of detonation = -10.257 kJ/cc

JWL Fit results:
E0 = -10.680 kJ/cc
A = 1008.60 GPa, B = 11.02 GPa, C = 1.48 GPa
R[1] = 4.75, R[2] = 1.07, omega = 0.37
RMS fitting error = 0.94 %

Appendix B Cheetah summary printout 92 wt. % HMX

B.1 COMP 8

B.1.1 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     Mol.    TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
GAP         8.00  20.63  11.36    33939    99.09     1.29 C3H5N3O1
HMX        92.00  79.37  88.64    17866   296.17     1.91 C4H8N8O8

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)
GAP         8.00  20.63  11.36    33939    99.09     1.29 C3H5N3O1
HMX        92.00  79.37  88.64    17866   296.17     1.91 C4H8N8O8

Density  =  1.8355 g/cc   Mixture TMD =  1.8355 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          34.67 GPa
The volume            =          0.419 cc/g
The density           =          2.384 g/cc
The energy            =           3.99 kJ/cc explosive
The temperature       =           3967 K
The shock velocity    =          9.061 mm/us
The particle velocity =          2.084 mm/us
The speed of sound    =          6.977 mm/us
Gamma                 =          3.347

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    -1.27
   2.20    -7.14     147      112       96       79      164
   4.10    -8.52     147      110       96       81      154
   6.50    -9.07     146      109       96       82      148
  10.00    -9.42     145      108       96       82      144
  20.00    -9.83     143      107       96       83      137
  40.00   -10.11     141      106       96       83      131
  80.00   -10.33     140      106       96       84      125
 160.00   -10.50

Freezing occurred at T =     1800.0 K and relative V =   2.091
The mechanical energy of detonation =    -10.645 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.645 kJ/cc

JWL Fit results:
E0   =       -10.971 kJ/cc
A    =      1328.95 GPa, B    =     13.02 GPa,  C     =    1.75 GPa
R[1] =         5.02,     R[2] =      1.13,      omega =    0.43
RMS fitting error =   1.06 %
```

B.1.2 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)
GAP         8.00  20.63  11.36    33939    99.09     1.29 C3H5N3O1
HMX        92.00  79.37  88.64    17866   296.17     1.91 C4H8N8O8

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)
GAP         8.00  20.63  11.36    33939    99.09     1.29 C3H5N3O1
HMX        92.00  79.37  88.64    17866   296.17     1.91 C4H8N8O8

Density  =  1.8355 g/cc   Mixture TMD =  1.8355 g/cc   % TMD = 100.0000


The C-J condition:
The pressure          =         35.11 GPa
The volume            =         0.412 cc/g
The density           =         2.425 g/cc
The energy            =          4.27 kJ/cc explosive
The temperature       =          4034 K
The shock velocity    =         8.871 mm/us
The particle velocity =         2.156 mm/us
The speed of sound    =         6.715 mm/us
Gamma                 =         3.114


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    -1.27
   2.20    -6.89     142      108       92       76      158
   4.10    -8.24     142      107       93       78      149
   6.50    -8.78     141      106       93       79      144
  10.00    -9.13     140      105       93       80      139
  20.00    -9.54     139      104       94       80      133
  40.00    -9.84     138      104       94       81      127
  80.00   -10.07     137      103       94       82      122
 160.00   -10.24

Freezing occurred at T =     1800.0 K and relative V =   2.120
The mechanical energy of detonation =    -10.408 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.408 kJ/cc

JWL Fit results:
E0   =       -10.753 kJ/cc
A    =      1025.55 GPa, B    =     11.19 GPa,  C     =         1.74 GPa
R[1] =         4.74,     R[2] =      1.11,      omega =         0.41
RMS fitting error =   0.71 %
```

B.2 COMP 9

B.2.1 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     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
BAMO        8.00  13.28  11.30   100382   168.16     1.30 C5H8N6O1
HMX        92.00  86.72  88.70    17866   296.17     1.91 C4H8N8O8

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)
BAMO        8.00  13.28  11.30   100382   168.16     1.30 C5H8N6O1
HMX        92.00  86.72  88.70    17866   296.17     1.91 C4H8N8O8

Density  =  1.8366 g/cc   Mixture TMD =  1.8366 g/cc   % TMD = 100.0000


The C-J condition:
The pressure          =         34.75 GPa
The volume            =         0.419 cc/g
The density           =         2.386 g/cc
The energy            =          4.00 kJ/cc explosive
The temperature       =          3982 K
The shock velocity    =         9.067 mm/us
The particle velocity =         2.087 mm/us
The speed of sound    =         6.981 mm/us
Gamma                 =         3.346

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    -1.27
   2.20    -7.16     148      113       96       79      164
   4.10    -8.55     147      111       96       81      155
   6.50    -9.09     146      110       97       82      149
  10.00    -9.45     145      109       97       82      144
  20.00    -9.85     143      108       97       83      137
  40.00   -10.14     142      107       97       83      131
  80.00   -10.36     141      106       97       84      126
 160.00   -10.53

Freezing occurred at T =     1800.0 K and relative V =   2.102
The mechanical energy of detonation =    -10.674 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.674 kJ/cc

JWL Fit results:
E0   =       -11.000 kJ/cc
A    =      1331.27 GPa, B    =     13.06 GPa,  C     =         1.76 GPa
R[1] =         5.02,     R[2] =      1.13,      omega =         0.43
RMS fitting error =   1.06 %
```

B.2.2 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)
BAMO        8.00  13.28  11.30   100382   168.16     1.30 C5H8N6O1
HMX        92.00  86.72  88.70    17866   296.17     1.91 C4H8N8O8

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)
BAMO        8.00  13.28  11.30   100382   168.16     1.30 C5H8N6O1
HMX        92.00  86.72  88.70    17866   296.17     1.91 C4H8N8O8

Density  =  1.8366 g/cc   Mixture TMD =  1.8366 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          35.30 GPa
The volume            =          0.412 cc/g
The density           =          2.427 g/cc
The energy            =           4.29 kJ/cc explosive
The temperature       =           4045 K
The shock velocity    =          8.888 mm/us
The particle velocity =          2.162 mm/us
The speed of sound    =          6.725 mm/us
Gamma                 =          3.110

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    -1.28
   2.20    -6.92     143      109       93       76      159
   4.10    -8.27     142      107       93       78      150
   6.50    -8.81     141      106       94       79      144
  10.00    -9.17     141      106       94       80      140
  20.00    -9.58     139      105       94       81      134
  40.00    -9.88     138      104       94       81      128
  80.00   -10.10     137      103       94       82      123
 160.00   -10.28

Freezing occurred at T =     1800.0 K and relative V =   2.127
The mechanical energy of detonation =    -10.444 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.445 kJ/cc

JWL Fit results:
E0   =       -10.863 kJ/cc
A    =      1030.96 GPa, B    =        11.30 GPa,  C   =       1.51 GPa
R[1] =         4.74,     R[2] =         1.07,    omega =       0.38
RMS fitting error =   0.94 %
```

B.3 COMP 10

B.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)	
GAP	6.00	15.81	8.52	33939	99.09	1.29	$C_3H_5N_3O_1$
BAMO	2.00	3.10	2.82	100382	168.16	1.30	$C_5H_8N_6O_1$
HMX	92.00	81.09	88.66	17866	296.17	1.91	$C_4H_8N_8O_8$

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)	
GAP	6.00	15.81	8.52	33939	99.09	1.29	$C_3H_5N_3O_1$
BAMO	2.00	3.10	2.82	100382	168.16	1.30	$C_5H_8N_6O_1$
HMX	92.00	81.09	88.66	17866	296.17	1.91	$C_4H_8N_8O_8$

Density = 1.8358 g/cc Mixture TMD = 1.8358 g/cc % TMD = 100.0000

The C-J condition:

The pressure	=	34.69 GPa
The volume	=	0.419 cc/g
The density	=	2.384 g/cc
The energy	=	3.99 kJ/cc explosive
The temperature	=	3971 K
The shock velocity	=	9.063 mm/us
The particle velocity	=	2.085 mm/us
The speed of sound	=	6.978 mm/us
Gamma	=	3.347

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	-1.27					
2.20	-7.15	147	113	96	79	164
4.10	-8.53	147	110	96	81	155
6.50	-9.08	146	109	96	82	149
10.00	-9.43	145	109	96	82	144
20.00	-9.83	143	107	96	83	137
40.00	-10.12	142	107	97	83	131
80.00	-10.34	140	106	97	84	125
160.00	-10.51					

Freezing occurred at T = 1800.0 K and relative V = 2.094
The mechanical energy of detonation = -10.653 kJ/cc
The thermal energy of detonation = -0.000 kJ/cc
The total energy of detonation = -10.653 kJ/cc

JWL Fit results:
E0 = -10.978 kJ/cc
A = 1330.40 GPa, B = 13.04 GPa, C = 1.75 GPa
R[1] = 5.02, R[2] = 1.13, omega = 0.43
RMS fitting error = 1.06 %

B.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)
GAP         6.00  15.81   8.52    33939    99.09     1.29 C3H5N3O1
BAMO        2.00   3.10   2.82   100382   168.16     1.30 C5H8N6O1
HMX        92.00  81.09  88.66    17866   296.17     1.91 C4H8N8O8

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)
GAP         6.00  15.81   8.52    33939    99.09     1.29 C3H5N3O1
BAMO        2.00   3.10   2.82   100382   168.16     1.30 C5H8N6O1
HMX        92.00  81.09  88.66    17866   296.17     1.91 C4H8N8O8

Density  =  1.8358 g/cc   Mixture TMD =  1.8358 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          35.16 GPa
The volume            =          0.412 cc/g
The density           =          2.425 g/cc
The energy            =           4.27 kJ/cc explosive
The temperature       =           4037 K
The shock velocity    =          8.875 mm/us
The particle velocity =          2.158 mm/us
The speed of sound    =          6.718 mm/us
Gamma                 =          3.113

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    -1.28
   2.20    -6.90     142      109       92       76      158
   4.10    -8.25     142      107       93       78      149
   6.50    -8.79     141      106       93       79      144
  10.00    -9.14     140      105       93       80      139
  20.00    -9.55     139      104       94       80      133
  40.00    -9.85     138      104       94       81      127
  80.00   -10.08     137      103       94       82      122
 160.00   -10.25

Freezing occurred at T =     1800.0 K and relative V =   2.122
The mechanical energy of detonation =    -10.417 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.417 kJ/cc

JWL Fit results:
E0   =       -10.762 kJ/cc
A    =      1025.86 GPa, B    =     11.20 GPa,  C     =      1.74 GPa
R[1] =         4.74,     R[2] =      1.11,      omega =      0.41
RMS fitting error =   0.71 %
```

B.4 COMP 11

B.4.1 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     Mol.   TMD
                                  formation    wt.    (g/cc)
                                  (cal/mol)
HMX        92.00  90.06  85.74     17866   296.17     1.91 C4H8N8O8
DOA         6.00   4.69  11.52   -290392   370.56     0.93 C22H42O4
GAP         1.50   4.39   2.06     33939    99.09     1.29 C3H5N3O1
BAMO        0.50   0.86   0.68    100382   168.16     1.30 C5H8N6O1

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)
HMX        92.00  90.06  85.74     17866   296.17     1.91 C4H8N8O8
DOA         6.00   4.69  11.52   -290392   370.56     0.93 C22H42O4
GAP         1.50   4.39   2.06     33939    99.09     1.29 C3H5N3O1
BAMO        0.50   0.86   0.68    100382   168.16     1.30 C5H8N6O1

Density  =  1.7754 g/cc   Mixture TMD =  1.7754 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         31.77 GPa
The volume            =         0.433 cc/g
The density           =         2.312 g/cc
The energy            =          3.69 kJ/cc explosive
The temperature       =          3780 K
The shock velocity    =         8.784 mm/us
The particle velocity =         2.037 mm/us
The speed of sound    =         6.746 mm/us
Gamma                 =         3.311

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    -1.17
   2.20    -6.55     135      103       88       72      150
   4.10    -7.84     135      102       89       74      142
   6.50    -8.36     134      101       89       75      137
  10.00    -8.70     133      100       89       76      133
  20.00    -9.10     132       99       89       77      127
  40.00    -9.38     131       99       90       77      121
  80.00    -9.60     130       98       90       78      117
 160.00    -9.77

Freezing occurred at T =     1800.0 K and relative V =   2.009
The mechanical energy of detonation =     -9.958 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.958 kJ/cc

JWL Fit results:
E0   =      -10.284 kJ/cc
A    =      1168.53 GPa, B    =     11.61 GPa,  C     =     1.63 GPa
R[1] =         4.98,     R[2] =      1.12,      omega =     0.41
RMS fitting error =   1.01 %
```

B.4.2 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)
GAP         1.50   4.39   2.06     33939    99.09     1.29 C3H5N3O1
BAMO        0.50   0.86   0.68    100382   168.16     1.30 C5H8N6O1
DOA         6.00   4.69  11.52   -290392   370.56     0.93 C22H42O4
HMX        92.00  90.06  85.74     17866   296.17     1.91 C4H8N8O8

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)
GAP         1.50   4.39   2.06     33939    99.09     1.29 C3H5N3O1
BAMO        0.50   0.86   0.68    100382   168.16     1.30 C5H8N6O1
DOA         6.00   4.69  11.52   -290392   370.56     0.93 C22H42O4
HMX        92.00  90.06  85.74     17866   296.17     1.91 C4H8N8O8

Density  =  1.7754 g/cc   Mixture TMD =  1.7754 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          30.89 GPa
The volume            =          0.425 cc/g
The density           =          2.352 g/cc
The energy            =           3.78 kJ/cc explosive
The temperature       =           3877 K
The shock velocity    =          8.426 mm/us
The particle velocity =          2.065 mm/us
The speed of sound    =          6.362 mm/us
Gamma                 =          3.081

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    -1.13
   2.20    -6.19     128       97       83       68      142
   4.10    -7.47     128       97       84       71      135
   6.50    -7.99     128       96       85       72      131
  10.00    -8.34     128       96       85       73      127
  20.00    -8.75     127       96       86       74      122
  40.00    -9.06     127       95       86       75      117
  80.00    -9.29     126       95       87       75      113
 160.00    -9.48

Freezing occurred at T =     1800.0 K and relative V =   2.104
The mechanical energy of detonation =     -9.701 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.701 kJ/cc

JWL Fit results:
E0   =       -10.049 kJ/cc
A    =       890.68 GPa, B    =   10.13 GPa,  C     =      1.65 GPa
R[1] =         4.76,     R[2] =    1.10,      omega =      0.39
RMS fitting error =   0.67 %
```

B.5 COMP 12

B.5.1 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     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
GAP         2.00   5.82   2.75    33939    99.09     1.29 C3H5N3O1
DOA         6.00   4.67  11.52  -290392   370.56     0.93 C22H42O4
HMX        92.00  89.52  85.74    17866   296.17     1.91 C4H8N8O8

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)
GAP         2.00   5.82   2.75    33939    99.09     1.29 C3H5N3O1
DOA         6.00   4.67  11.52  -290392   370.56     0.93 C22H42O4
HMX        92.00  89.52  85.74    17866   296.17     1.91 C4H8N8O8

Density  =  1.7753 g/cc   Mixture TMD =  1.7753 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         31.77 GPa
The volume            =         0.433 cc/g
The density           =         2.311 g/cc
The energy            =          3.68 kJ/cc explosive
The temperature       =          3779 K
The shock velocity    =         8.783 mm/us
The particle velocity =         2.037 mm/us
The speed of sound    =         6.746 mm/us
Gamma                 =         3.311

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    -1.17
   2.20    -6.55     135      103       88       72      150
   4.10    -7.84     135      102       88       74      142
   6.50    -8.36     134      101       89       75      137
  10.00    -8.70     133      100       89       76      133
  20.00    -9.10     132       99       89       77      127
  40.00    -9.38     131       99       90       77      121
  80.00    -9.60     130       98       90       78      116
 160.00    -9.77

Freezing occurred at T =     1800.0 K and relative V =   2.009
The mechanical energy of detonation =     -9.957 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.957 kJ/cc

JWL Fit results:
E0   =       -10.286 kJ/cc
A    =      1166.39 GPa, B    =    11.58 GPa,  C     =     1.62 GPa
R[1] =         4.97,     R[2] =     1.12,      omega =     0.40
RMS fitting error =   1.01 %
```

B.5.2 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)
GAP         2.00   5.82   2.75    33939    99.09     1.29 C3H5N3O1
DOA         6.00   4.67  11.52  -290392   370.56     0.93 C22H42O4
HMX        92.00  89.52  85.74    17866   296.17     1.91 C4H8N8O8

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)
GAP         2.00   5.82   2.75    33939    99.09     1.29 C3H5N3O1
DOA         6.00   4.67  11.52  -290392   370.56     0.93 C22H42O4
HMX        92.00  89.52  85.74    17866   296.17     1.91 C4H8N8O8

Density  =  1.7753 g/cc   Mixture TMD =  1.7753 g/cc   % TMD = 100.0000


The C-J condition:
The pressure          =          30.88 GPa
The volume            =          0.425 cc/g
The density           =          2.351 g/cc
The energy            =           3.78 kJ/cc explosive
The temperature       =           3877 K
The shock velocity    =          8.425 mm/us
The particle velocity =          2.064 mm/us
The speed of sound    =          6.361 mm/us
Gamma                 =          3.081

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    -1.13
   2.20    -6.19     128       97       83       68      142
   4.10    -7.46     128       97       84       71      135
   6.50    -7.99     128       96       85       72      131
  10.00    -8.34     128       96       85       73      127
  20.00    -8.75     127       96       86       74      122
  40.00    -9.06     127       95       86       75      117
  80.00    -9.29     126       95       87       75      113
 160.00    -9.47

Freezing occurred at T =     1800.0 K and relative V =   2.103
The mechanical energy of detonation =     -9.699 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.699 kJ/cc

JWL Fit results:
E0   =       -10.126 kJ/cc
A    =       895.03 GPa, B    =    10.20 GPa,  C     =         1.44 GPa
R[1] =         4.76,     R[2] =     1.07,      omega =         0.36
RMS fitting error =   0.91 %
```

B.6 COMP 13

B.6.1 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     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
BAMO        2.00   3.51   2.73   100382   168.16     1.30 C5H8N6O1
DOA         6.00   4.78  11.52  -290392   370.56     0.93 C22H42O4
HMX        92.00  91.71  85.75    17866   296.17     1.91 C4H8N8O8

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)
BAMO        2.00   3.51   2.73   100382   168.16     1.30 C5H8N6O1
DOA         6.00   4.78  11.52  -290392   370.56     0.93 C22H42O4
HMX        92.00  91.71  85.75    17866   296.17     1.91 C4H8N8O8

Density  =  1.7756 g/cc   Mixture TMD =  1.7756 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          31.78 GPa
The volume            =          0.433 cc/g
The density           =          2.312 g/cc
The energy            =           3.69 kJ/cc explosive
The temperature       =           3782 K
The shock velocity    =          8.785 mm/us
The particle velocity =          2.038 mm/us
The speed of sound    =          6.747 mm/us
Gamma                 =          3.311

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    -1.17
   2.20    -6.55     135      103       88       72      150
   4.10    -7.84     135      102       89       74      142
   6.50    -8.37     134      101       89       75      137
  10.00    -8.71     134      100       89       76      133
  20.00    -9.10     132       99       89       77      127
  40.00    -9.39     131       99       90       77      121
  80.00    -9.61     130       98       90       78      117
 160.00    -9.78

Freezing occurred at T =     1800.0 K and relative V =   2.011
The mechanical energy of detonation =     -9.963 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.963 kJ/cc

JWL Fit results:
E0   =       -10.371 kJ/cc
A    =      1128.27 GPa, B    =    10.94 GPa,  C     =         1.39 GPa
R[1] =         4.90,     R[2] =     1.07,      omega =         0.37
RMS fitting error =   1.23 %
```

B.6.2 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)
BAMO        2.00   3.51   2.73   100382   168.16     1.30 C5H8N6O1
DOA         6.00   4.78  11.52  -290392   370.56     0.93 C22H42O4
HMX        92.00  91.71  85.75    17866   296.17     1.91 C4H8N8O8

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)
BAMO        2.00   3.51   2.73   100382   168.16     1.30 C5H8N6O1
DOA         6.00   4.78  11.52  -290392   370.56     0.93 C22H42O4
HMX        92.00  91.71  85.75    17866   296.17     1.91 C4H8N8O8

Density  =  1.7756 g/cc   Mixture TMD =  1.7756 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          30.92 GPa
The volume            =          0.425 cc/g
The density           =          2.352 g/cc
The energy            =           3.79 kJ/cc explosive
The temperature       =           3879 K
The shock velocity    =          8.429 mm/us
The particle velocity =          2.066 mm/us
The speed of sound    =          6.363 mm/us
Gamma                 =          3.080


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    -1.13
   2.20    -6.19     128       98       83       68      142
   4.10    -7.47     129       97       84       71      135
   6.50    -8.00     128       96       85       72      131
  10.00    -8.35     128       96       85       73      127
  20.00    -8.76     128       96       86       74      122
  40.00    -9.06     127       95       86       75      117
  80.00    -9.30     126       95       87       75      113
 160.00    -9.48

Freezing occurred at T =     1800.0 K and relative V =   2.105
The mechanical energy of detonation =     -9.707 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.707 kJ/cc

JWL Fit results:
E0   =      -10.135 kJ/cc
A    =       895.44 GPa, B    =    10.22 GPa,  C     =    1.44 GPa
R[1] =         4.76,     R[2] =     1.07,      omega =    0.36
RMS fitting error =   0.91 %
```

B.7 COMP 14

B.7.1 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     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
HYTEMP      2.00   3.14   3.52  -205067   188.60     1.00 C10H15.46O3.307
DOA         6.00   4.80  11.42  -290392   370.56     0.93 C22H42O4
HMX        92.00  92.06  85.05    17866   296.17     1.91 C4H8N8O8

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)
HYTEMP      2.00   3.14   3.52  -205067   188.60     1.00 C10H15.46O3.307
DOA         6.00   4.80  11.42  -290392   370.56     0.93 C22H42O4
HMX        92.00  92.06  85.05    17866   296.17     1.91 C4H8N8O8

Density  =  1.7612 g/cc   Mixture TMD =  1.7612 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         30.96 GPa
The volume            =         0.436 cc/g
The density           =         2.294 g/cc
The energy            =          3.60 kJ/cc explosive
The temperature       =          3729 K
The shock velocity    =         8.698 mm/us
The particle velocity =         2.021 mm/us
The speed of sound    =         6.677 mm/us
Gamma                 =         3.303

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    -1.14
   2.20    -6.38     132      100       85       70      146
   4.10    -7.64     132       99       86       72      138
   6.50    -8.16     131       98       87       73      133
  10.00    -8.49     130       98       87       74      129
  20.00    -8.88     129       97       87       75      124
  40.00    -9.16     128       96       87       75      119
  80.00    -9.38     127       96       88       76      114
 160.00    -9.55

Freezing occurred at T =     1800.0 K and relative V =   1.981
The mechanical energy of detonation =     -9.747 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.747 kJ/cc

JWL Fit results:
E0   =       -10.072 kJ/cc
A    =      1128.74 GPa, B    =    11.24 GPa,  C     =         1.59 GPa
R[1] =         4.97,     R[2] =     1.12,      omega =         0.40
RMS fitting error =   0.99 %
```

B.7.2 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)
HYTEMP      2.00   3.14   3.52  -205067   188.60     1.00 C10H15.46O3.307
DOA         6.00   4.80  11.42  -290392   370.56     0.93 C22H42O4
HMX        92.00  92.06  85.05    17866   296.17     1.91 C4H8N8O8

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)
HYTEMP      2.00    3.14   3.52  -205067   188.60     1.00 C10H15.46O3.307
DOA 4.00    4.80  11.42  -290392   370.56     0.93 C22H42O4
HMX        92.00  92.06  85.05    17866   296.17     1.91 C4H8N8O8

Density  =  1.7612 g/cc   Mixture TMD =  1.7612 g/cc   % TMD = 100.0000


The C-J condition:
The pressure          =         29.79 GPa
The volume            =         0.429 cc/g
The density           =         2.332 g/cc
The energy            =          3.65 kJ/cc explosive
The temperature       =          3829 K
The shock velocity    =         8.311 mm/us
The particle velocity =         2.035 mm/us
The speed of sound    =         6.276 mm/us
Gamma                 =         3.084


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    -1.09
   2.20    -6.00     124       94       80       66      138
   4.10    -7.25     125       94       82       69      131
   6.50    -7.77     125       94       82       70      127
  10.00    -8.12     124       93       83       71      124
  20.00    -8.53     124       93       84       72      119
  40.00    -8.83     123       93       84       73      114
  80.00    -9.06     123       93       85       73      110
 160.00    -9.25

Freezing occurred at T =     1800.0 K and relative V =   2.086
The mechanical energy of detonation =     -9.483 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.483 kJ/cc

JWL Fit results:
E0   =       -9.834 kJ/cc
A    =      865.25 GPa, B    =      9.82 GPa,     C     =         1.61
GPa
R[1] =         4.77,     R[2] =        1.10,      omega =         0.39
RMS fitting error =   0.67 %
```

Appendix C Cheetah summary printout 96 wt. % RDX

C.1 RDX

C.1.1 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     Mol.    TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
RDX       100.00 100.00 100.00    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.    TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
RDX       100.00 100.00 100.00    16496   222.13     1.81 C3H6N6O6

Density  =  1.8060 g/cc   Mixture TMD =  1.8060 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          33.78 GPa
The volume            =          0.426 cc/g
The density           =          2.348 g/cc
The energy            =           3.90 kJ/cc explosive
The temperature       =           4154 K
The shock velocity    =          9.000 mm/us
The particle velocity =          2.078 mm/us
The speed of sound    =          6.922 mm/us
Gamma                 =          3.331

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    -1.26
   2.20    -7.16     148      113       96       79      164
   4.10    -8.58     148      111       97       81      155
   6.50    -9.14     147      110       97       82      150
  10.00    -9.50     146      109       97       83      145
  20.00    -9.90     144      108       97       83      138
  40.00   -10.19     143      107       97       84      132
  80.00   -10.40     141      106       97       84      126
 160.00   -10.57

Freezing occurred at T =     1800.0 K and relative V =   2.225
The mechanical energy of detonation =    -10.695 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.695 kJ/cc

JWL Fit results:
E0   =       -11.012 kJ/cc
A    =      1308.06 GPa, B    =    13.56 GPa,  C     =         1.84 GPa
R[1] =         5.06,     R[2] =     1.14,      omega =         0.44
RMS fitting error =   1.10 %
```

C.1.2 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)
RDX       100.00 100.00 100.00    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                 formation     wt.    (g/cc)
                                 (cal/mol)
RDX       100.00 100.00 100.00    16496   222.13     1.81 C3H6N6O6


Density  =  1.8060 g/cc   Mixture TMD =  1.8060 g/cc   % TMD = 100.0000


The C-J condition:
The pressure          =         34.74 GPa
The volume            =         0.421 cc/g
The density           =         2.378 g/cc
The energy            =          4.18 kJ/cc explosive
The temperature       =          4209 K
The shock velocity    =         8.942 mm/us
The particle velocity =         2.151 mm/us
The speed of sound    =         6.791 mm/us
Gamma                 =         3.157


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    -1.27
   2.20    -6.95     143      110       93       77      159
   4.10    -8.32     143      108       94       79      151
   6.50    -8.87     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   -10.31

Freezing occurred at T =     1800.0 K and relative V =   2.214
The mechanical energy of detonation =    -10.434 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.434 kJ/cc

JWL Fit results:
E0   =       -10.769 kJ/cc
A    =      1062.22 GPa, B    =     11.43 GPa,  C     =      1.81 GPa
R[1] =         4.79,     R[2] =      1.11,      omega =      0.43
RMS fitting error =   0.79 %
```

C.2 COMP 15

C.2.1 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     Mol.   TMD
                               formation     wt.    (g/cc)
                               (cal/mol)
GAP         4.00   8.54   5.50    33939    99.09     1.29 C3H5N3O1
RDX        96.00  91.46  94.50    16496   222.13     1.81 C3H6N6O6

Product library title: bkws library

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                               formation     wt.    (g/cc)
                               (cal/mol)
GAP         4.00   8.54   5.50    33939    99.09     1.29 C3H5N3O1
RDX        96.00  91.46  94.50    16496   222.13     1.81 C3H6N6O6

Density  =  1.7778 g/cc   Mixture TMD =  1.7778 g/cc   % TMD = 100.0000


The C-J condition:
The pressure          =         32.55 GPa
The volume            =         0.431 cc/g
The density           =         2.320 g/cc
The energy            =          3.80 kJ/cc explosive
The temperature       =          4103 K
The shock velocity    =         8.853 mm/us
The particle velocity =         2.068 mm/us
The speed of sound    =         6.785 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    -1.22
   2.20    -6.89     142      108       92       76      158
   4.10    -8.27     142      107       93       78      150
   6.50    -8.82     142      106       94       79      144
  10.00    -9.17     141      106       94       80      140
  20.00    -9.58     139      105       94       81      134
  40.00    -9.86     138      104       94       81      128
  80.00   -10.08     137      103       94       82      122
 160.00   -10.25

Freezing occurred at T =     1800.0 K and relative V =   2.215
The mechanical energy of detonation =    -10.391 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.391 kJ/cc

JWL Fit results:
E0   =       -10.706 kJ/cc
A    =      1185.57 GPa, B    =     12.69 GPa,  C     =         1.79 GPa
R[1] =         5.00,     R[2] =      1.13,      omega =         0.43
RMS fitting error =   1.05 %
```

C.2.2 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)
GAP         4.00   8.54   5.50    33939    99.09     1.29 C3H5N3O1
RDX        96.00  91.46  94.50    16496   222.13     1.81 C3H6N6O6

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


The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                 formation     wt.    (g/cc)
                                 (cal/mol)
GAP         4.00   8.54   5.50    33939    99.09     1.29 C3H5N3O1
RDX        96.00  91.46  94.50    16496   222.13     1.81 C3H6N6O6

Density  =  1.7778 g/cc   Mixture TMD =  1.7778 g/cc   % TMD = 100.0000


The C-J condition:
The pressure          =         33.03 GPa
The volume            =         0.426 cc/g
The density           =         2.347 g/cc
The energy            =          4.00 kJ/cc explosive
The temperature       =          4160 K
The shock velocity    =         8.755 mm/us
The particle velocity =         2.122 mm/us
The speed of sound    =         6.633 mm/us
Gamma                 =         3.125


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    -1.22
   2.20    -6.66     137      105       89       74      153
   4.10    -8.00     138      104       90       76      145
   6.50    -8.54     137      103       91       77      140
  10.00    -8.89     136      102       91       77      136
  20.00    -9.30     135      102       91       78      130
  40.00    -9.59     134      101       92       79      124
  80.00    -9.81     133      100       92       79      119
 160.00    -9.99

Freezing occurred at T =     1800.0 K and relative V =   2.223
The mechanical energy of detonation =    -10.134 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.134 kJ/cc

JWL Fit results:
E0   =       -10.468 kJ/cc
A    =       981.18 GPa, B    =     10.84 GPa,  C     =      1.78 GPa
R[1] =         4.77,     R[2] =      1.11,      omega =      0.42
RMS fitting error =   0.75 %
```

C.3 COMP 16

C.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     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
BAMO        4.00   5.22   5.47   100382   168.16     1.30 C5H8N6O1
RDX        96.00  94.78  94.53    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
BAMO        4.00   5.22   5.47   100382   168.16     1.30 C5H8N6O1
RDX        96.00  94.78  94.53    16496   222.13     1.81 C3H6N6O6

Density  =  1.7783 g/cc   Mixture TMD =  1.7783 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          32.59 GPa
The volume            =          0.431 cc/g
The density           =          2.321 g/cc
The energy            =           3.81 kJ/cc explosive
The temperature       =           4111 K
The shock velocity    =          8.856 mm/us
The particle velocity =          2.069 mm/us
The speed of sound    =          6.787 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    -1.22
   2.20    -6.90     142      109       92       76      158
   4.10    -8.28     143      107       93       78      150
   6.50    -8.83     142      106       94       79      145
  10.00    -9.19     141      106       94       80      140
  20.00    -9.59     140      105       94       81      134
  40.00    -9.88     138      104       94       81      128
  80.00   -10.09     137      103       94       82      122
 160.00   -10.26

Freezing occurred at T =     1800.0 K and relative V =   2.221
The mechanical energy of detonation =    -10.404 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.404 kJ/cc

JWL Fit results:
E0   =       -10.720 kJ/cc
A    =      1184.85 GPa, B    =     12.68 GPa , C     =    1.79 GPa
R[1] =         5.00,     R[2] =      1.13,      omega =    0.43
RMS fitting error =   1.05 %
```

C.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)
BAMO        4.00   5.22   5.47   100382   168.16     1.30 C5H8N6O1
RDX        96.00  94.78  94.53    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                 formation     wt.    (g/cc)
                                 (cal/mol)
BAMO        4.00   5.22   5.47   100382   168.16     1.30 C5H8N6O1
RDX        96.00  94.78  94.53    16496   222.13     1.81 C3H6N6O6

Density  =  1.7783 g/cc   Mixture TMD =  1.7783 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          33.12 GPa
The volume            =          0.426 cc/g
The density           =          2.348 g/cc
The energy            =           4.02 kJ/cc explosive
The temperature       =           4165 K
The shock velocity    =          8.764 mm/us
The particle velocity =          2.125 mm/us
The speed of sound    =          6.639 mm/us
Gamma                 =          3.124


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    -1.22
   2.20    -6.67     138      105       89       74      153
   4.10    -8.01     138      104       90       76      145
   6.50    -8.56     137      103       91       77      140
  10.00    -8.91     137      103       91       78      136
  20.00    -9.32     136      102       91       78      130
  40.00    -9.61     134      101       92       79      124
  80.00    -9.83     133      101       92       80      119
 160.00   -10.00

Freezing occurred at T =     1800.0 K and relative V =   2.227
The mechanical energy of detonation =    -10.151 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.151 kJ/cc

JWL Fit results:
E0   =       -10.485 kJ/cc
A    =       981.99 GPa, B    =   10.87 GPa,  C     =         1.78 GPa
R[1] =         4.77,     R[2]      1.11,      omega =         0.42
RMS fitting error =   0.75 %
```

C.4 COMP 17

C.4.1 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     Mol.   TMD
                                 formation     wt.    (g/cc)
                                 (cal/mol)
GAP         3.00   6.46   4.13    33939    99.09     1.29 C3H5N3O1
BAMO        1.00   1.27   1.37   100382   168.16     1.30 C5H8N6O1
RDX        96.00  92.27  94.51    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                 formation     wt.    (g/cc)
                                 (cal/mol)
GAP         3.00   6.46   4.13    33939    99.09     1.29 C3H5N3O1
BAMO        1.00   1.27   1.37   100382   168.16     1.30 C5H8N6O1
RDX        96.00  92.27  94.51    16496   222.13     1.81 C3H6N6O6

Density  =  1.7779 g/cc   Mixture TMD =  1.7779 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         32.56 GPa
The volume            =         0.431 cc/g
The density           =         2.320 g/cc
The energy            =          3.80 kJ/cc explosive
The temperature       =          4105 K
The shock velocity    =         8.854 mm/us
The particle velocity =         2.069 mm/us
The speed of sound    =         6.785 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    -1.22
   2.20    -6.89     142      109       92       76      158
   4.10    -8.27     142      107       93       78      150
   6.50    -8.82     142      106       94       79      144
  10.00    -9.18     141      106       94       80      140
  20.00    -9.58     139      105       94       81      134
  40.00    -9.87     138      104       94       81      128
  80.00   -10.08     137      103       94       82      122
 160.00   -10.25

Freezing occurred at T =     1800.0 K and relative V =   2.216
The mechanical energy of detonation =    -10.394 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.394 kJ/cc

JWL Fit results:
E0   =       -10.710 kJ/cc
A    =      1185.08 GPa, B    =     12.68 GPa,  C     =         1.79 GPa
R[1] =         5.00,     R[2] =      1.13,      omega =         0.43
RMS fitting error =   1.05 %
```

C.4.2 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)
GAP         3.00   6.46   4.13    33939    99.09     1.29 C3H5N3O1
BAMO        1.00   1.27   1.37   100382   168.16     1.30 C5H8N6O1
RDX        96.00  92.27  94.51    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                 formation     wt.    (g/cc)
                                 (cal/mol)
GAP         3.00   6.46   4.13    33939    99.09     1.29 C3H5N3O1
BAMO        1.00   1.27   1.37   100382   168.16     1.30 C5H8N6O1
RDX        96.00  92.27  94.51    16496   222.13     1.81 C3H6N6O6

Density  =  1.7779 g/cc   Mixture TMD =  1.7779 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          33.06 GPa
The volume            =          0.426 cc/g
The density           =          2.347 g/cc
The energy            =           4.01 kJ/cc explosive
The temperature       =           4161 K
The shock velocity    =          8.757 mm/us
The particle velocity =          2.123 mm/us
The speed of sound    =          6.634 mm/us
Gamma                 =          3.125

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    -1.22
   2.20    -6.66     137      105       89       74      153
   4.10    -8.00     138      104       90       76      145
   6.50    -8.54     137      103       91       77      140
  10.00    -8.90     136      102       91       78      136
  20.00    -9.30     135      102       91       78      130
  40.00    -9.60     134      101       92       79      124
  80.00    -9.82     133      100       92       80      119
 160.00    -9.99

Freezing occurred at T =     1800.0 K and relative V =   2.224
The mechanical energy of detonation =    -10.138 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.138 kJ/cc

JWL Fit results:
E0   =       -10.541 kJ/cc
A    =       983.64 GPa, B    =     10.89 GPa,  C     =      1.54 GPa
R[1] =         4.76,     R[2] =      1.07,      omega =      0.39
RMS fitting error =   0.98 %
```

C.5 COMP 18

C.5.1 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     Mol.   TMD
                                  formation    wt.    (g/cc)
                                  (cal/mol)
GAP         0.75   1.68   1.01     33939     99.09     1.29 C3H5N3O1
BAMO        0.25   0.33   0.34    100382    168.16     1.30 C5H8N6O1
DOA         3.00   1.80   5.67   -290392    370.56     0.93 C22H42O4
RDX        96.00  96.18  92.98     16496    222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                  formation    wt.    (g/cc)
                                  (cal/mol)
GAP         0.75   1.68   1.01     33939     99.09     1.29 C3H5N3O1
BAMO        0.25   0.33   0.34    100382    168.16     1.30 C5H8N6O1
DOA         3.00   1.80   5.67   -290392    370.56     0.93 C22H42O4
RDX        96.00  96.18  92.98     16496    222.13     1.81 C3H6N6O6

Density  =  1.7491 g/cc   Mixture TMD =  1.7491 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         31.19 GPa
The volume            =         0.438 cc/g
The density           =         2.285 g/cc
The energy            =          3.66 kJ/cc explosive
The temperature       =          4002 K
The shock velocity    =         8.720 mm/us
The particle velocity =         2.045 mm/us
The speed of sound    =         6.675 mm/us
Gamma                 =         3.264

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    -1.17
   2.20    -6.60     136      104       88       73      151
   4.10    -7.94     137      103       90       75      144
   6.50    -8.47     136      102       90       76      139
  10.00    -8.82     135      102       90       77      134
  20.00    -9.22     134      101       90       78      129
  40.00    -9.51     133      100       91       78      123
  80.00    -9.72     132      100       91       79      118
 160.00    -9.89

Freezing occurred at T =     1800.0 K and relative V =   2.172
The mechanical energy of detonation =    -10.057 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.057 kJ/cc

JWL Fit results:
E0   =       -10.450 kJ/cc
A    =      1077.69 GPa, B    =     11.37 GPa,  C     =         1.47 GPa
R[1] =         4.90,     R[2] =      1.07,      omega =         0.38
RMS fitting error =   1.25 %
```

C.5.2 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)
GAP         0.75   1.68   1.01    33939    99.09     1.29 C3H5N3O1
BAMO        0.25   0.33   0.34   100382   168.16     1.30 C5H8N6O1
DOA         3.00   1.80   5.67  -290392   370.56     0.93 C22H42O4
RDX        96.00  96.18  92.98    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
GAP         0.75   1.68   1.01    33939    99.09     1.29 C3H5N3O1
BAMO        0.25   0.33   0.34   100382   168.16     1.30 C5H8N6O1
DOA         3.00   1.80   5.67  -290392   370.56     0.93 C22H42O4
RDX        96.00  96.18  92.98    16496   222.13     1.81 C3H6N6O6

Density  =  1.7491 g/cc   Mixture TMD =  1.7491 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         31.05 GPa
The volume            =         0.432 cc/g
The density           =         2.313 g/cc
The energy            =          3.78 kJ/cc explosive
The temperature       =          4075 K
The shock velocity    =         8.534 mm/us
The particle velocity =         2.080 mm/us
The speed of sound    =         6.454 mm/us
Gamma                 =         3.102


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    -1.15
   2.20    -6.32     130      100       85       70      145
   4.10    -7.62     131       99       86       72      138
   6.50    -8.16     131       98       87       73      133
  10.00    -8.51     131       98       87       74      130
  20.00    -8.92     130       97       88       75      124
  40.00    -9.21     129       97       88       76      119
  80.00    -9.44     128       97       88       76      115
 160.00    -9.61

Freezing occurred at T =     1800.0 K and relative V =   2.214
The mechanical energy of detonation =     -9.790 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.790 kJ/cc

JWL Fit results:
E0   =       -10.196 kJ/cc
A    =       911.92 GPa, B    =     10.34 GPa,  C     =      1.50 GPa
R[1] =         4.76,     R[2] =      1.06,      omega =      0.38
RMS fitting error =   0.96 %
```

C.6 COMP 19

C.6.1 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     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
GAP         1.00   2.24   1.35    33939    99.09     1.29 C3H5N3O1
DOA         3.00   1.80   5.67  -290392   370.56     0.93 C22H42O4
RDX        96.00  95.96  92.97    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
GAP         1.00   2.24   1.35    33939    99.09     1.29 C3H5N3O1
DOA         3.00   1.80   5.67  -290392   370.56     0.93 C22H42O4
RDX        96.00  95.96  92.97    16496   222.13     1.81 C3H6N6O6

Density  =  1.7491 g/cc   Mixture TMD =  1.7491 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         31.19 GPa
The volume            =         0.438 cc/g
The density           =         2.285 g/cc
The energy            =          3.66 kJ/cc explosive
The temperature       =          4002 K
The shock velocity    =         8.720 mm/us
The particle velocity =         2.045 mm/us
The speed of sound    =         6.675 mm/us
Gamma                 =         3.264

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    -1.17
   2.20    -6.60     136      104       88       73      151
   4.10    -7.94     137      103       90       75      144
   6.50    -8.47     136      102       90       76      139
  10.00    -8.82     135      102       90       77      134
  20.00    -9.22     134      101       90       78      129
  40.00    -9.51     133      100       91       78      123
  80.00    -9.72     132      100       91       79      118
 160.00    -9.89

Freezing occurred at T =     1800.0 K and relative V =   2.171
The mechanical energy of detonation =    -10.056 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.056 kJ/cc

JWL Fit results:
E0   =       -10.373 kJ/cc
A    =      1112.82 GPa, B    =     11.97 GPa,  C     =    1.72 GPa
R[1] =         4.98,     R[2] =      1.12,      omega =    0.42
RMS fitting error =   1.02 %
```

C.6.2 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)
GAP         1.00   2.24   1.35    33939    99.09     1.29 C3H5N3O1
DOA         3.00   1.80   5.67  -290392   370.56     0.93 C22H42O4
RDX        96.00  95.96  92.97    16496   222.13     1.81 C3H6N6O6

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


The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
GAP         1.00   2.24   1.35    33939    99.09     1.29 C3H5N3O1
DOA         3.00   1.80   5.67  -290392   370.56     0.93 C22H42O4
RDX        96.00  95.96  92.97    16496   222.13     1.81 C3H6N6O6

Density  =  1.7491 g/cc   Mixture TMD =  1.7491 g/cc   % TMD = 100.0000


The C-J condition:
The pressure          =          31.05 GPa
The volume            =          0.432 cc/g
The density           =          2.313 g/cc
The energy            =           3.78 kJ/cc explosive
The temperature       =           4074 K
The shock velocity    =          8.533 mm/us
The particle velocity =          2.080 mm/us
The speed of sound    =          6.453 mm/us
Gamma                 =          3.103

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    -1.15
   2.20    -6.32     130       99       85       70      145
   4.10    -7.62     131       99       86       72      138
   6.50    -8.16     131       98       87       73      133
  10.00    -8.51     130       98       87       74      130
  20.00    -8.92     130       97       87       75      124
  40.00    -9.21     129       97       88       76      119
  80.00    -9.44     128       97       88       76      115
 160.00    -9.61

Freezing occurred at T =     1800.0 K and relative V =   2.214
The mechanical energy of detonation =     -9.789 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.789 kJ/cc

JWL Fit results:
E0   =       -10.195 kJ/cc
A    =       911.91 GPa, B    =     10.35 GPa,  C     =    1.50 GPa
R[1] =         4.76,     R[2] =      1.06,      omega =    0.38
RMS fitting error =   0.96 %
```

C.7 COMP 20

C.7.1 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     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
BAMO        1.00   1.33   1.35   100382   168.16     1.30 C5H8N6O1
DOA         3.00   1.81   5.67  -290392   370.56     0.93 C22H42O4
RDX        96.00  96.85  92.98    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
BAMO        1.00   1.33   1.35   100382   168.16     1.30 C5H8N6O1
DOA         3.00   1.81   5.67  -290392   370.56     0.93 C22H42O4
RDX        96.00  96.85  92.98    16496   222.13     1.81 C3H6N6O6

Density  =  1.7492 g/cc   Mixture TMD =  1.7492 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         31.20 GPa
The volume            =         0.438 cc/g
The density           =         2.285 g/cc
The energy            =          3.66 kJ/cc explosive
The temperature       =          4004 K
The shock velocity    =         8.721 mm/us
The particle velocity =         2.045 mm/us
The speed of sound    =         6.676 mm/us
Gamma                 =         3.264

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    -1.17
   2.20    -6.60     136      104       88       73      151
   4.10    -7.94     137      103       90       75      144
   6.50    -8.47     136      102       90       76      139
  10.00    -8.82     135      102       90       77      135
  20.00    -9.22     134      101       91       78      129
  40.00    -9.51     133      100       91       78      123
  80.00    -9.73     132      100       91       79      118
 160.00    -9.90

Freezing occurred at T =     1800.0 K and relative V =   2.173
The mechanical energy of detonation =    -10.060 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.060 kJ/cc

JWL Fit results:
E0   =       -10.376 kJ/cc
A    =      1113.38 GPa, B    =    11.98 GPa,  C     =         1.72 GPa
R[1] =         4.98,     R[2] =     1.12,      omega =         0.42
RMS fitting error =   1.02 %
```

C.7.2 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)
BAMO        1.00   1.33   1.35   100382   168.16     1.30 C5H8N6O1
DOA         3.00   1.81   5.67  -290392   370.56     0.93 C22H42O4
RDX        96.00  96.85  92.98    16496   222.13     1.81 C3H6N6O6
Product library title: bkwc
Reactant library title: # Version 2.0 by P. Clark Souers

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
BAMO        1.00   1.33   1.35   100382   168.16     1.30 C5H8N6O1
DOA         3.00   1.81   5.67  -290392   370.56     0.93 C22H42O4
RDX        96.00  96.85  92.98    16496   222.13     1.81 C3H6N6O6

Density  =  1.7492 g/cc   Mixture TMD =  1.7492 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          31.07 GPa
The volume            =          0.432 cc/g
The density           =          2.313 g/cc
The energy            =           3.79 kJ/cc explosive
The temperature       =           4076 K
The shock velocity    =          8.535 mm/us
The particle velocity =          2.081 mm/us
The speed of sound    =          6.455 mm/us
Gamma                 =          3.102

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    -1.15
   2.20    -6.32     130      100       85       70      145
   4.10    -7.63     131       99       86       72      138
   6.50    -8.16     131       98       87       73      134
  10.00    -8.51     131       98       87       74      130
  20.00    -8.92     130       97       88       75      124
  40.00    -9.22     129       97       88       76      119
  80.00    -9.44     128       97       88       76      115
 160.00    -9.62

Freezing occurred at T =     1800.0 K and relative V =   2.215
The mechanical energy of detonation =     -9.793 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.793 kJ/cc

JWL Fit results:
E0   =       -10.199 kJ/cc
A    =       912.18 GPa, B    =    10.35 GPa,  C     =         1.50 GPa
R[1] =         4.76,     R[2] =     1.06,      omega =         0.38
RMS fitting error =   0.96 %
```

C.8 COMP 21

C.8.1 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)	
HYTEMP	1.00	1.19	1.74	-205067	188.60	1.00	$C_{10}H_{15.46}O_{3.307}$
DOA	3.00	1.82	5.65	-290392	370.56	0.93	$C_{22}H_{42}O_4$
RDX	96.00	96.99	92.61	16496	222.13	1.81	$C_3H_6N_6O_6$

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)	
HYTEMP	1.00	1.19	1.74	-205067	188.60	1.00	$C_{10}H_{15.46}O_{3.307}$
DOA	3.00	1.82	5.65	-290392	370.56	0.93	$C_{22}H_{42}O_4$
RDX	96.00	96.99	92.61	16496	222.13	1.81	$C_3H_6N_6O_6$

Density = 1.7422 g/cc Mixture TMD = 1.7422 g/cc % TMD = 100.0000

The C-J condition:

The pressure	=	30.80 GPa
The volume	=	0.439 cc/g
The density	=	2.276 g/cc
The energy	=	3.61 kJ/cc explosive
The temperature	=	3975 K
The shock velocity	=	8.679 mm/us
The particle velocity	=	2.037 mm/us
The speed of sound	=	6.642 mm/us
Gamma	=	3.261

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	-1.16					
2.20	-6.52	134	103	87	72	149
4.10	-7.84	135	102	88	74	142
6.50	-8.37	134	101	89	75	137
10.00	-8.72	134	100	89	76	133
20.00	-9.11	133	99	89	77	127
40.00	-9.40	131	99	90	77	122
80.00	-9.62	130	98	90	78	117
160.00	-9.78					

Freezing occurred at T = 1800.0 K and relative V = 2.157
The mechanical energy of detonation = -9.952 kJ/cc
The thermal energy of detonation = -0.000 kJ/cc
The total energy of detonation = -9.952 kJ/cc

JWL Fit results:
E0 = -10.268 kJ/cc
A = 1095.33 GPa, B = 11.79 GPa, C = 1.70 GPa
R[1] = 4.98, R[2] = 1.12, omega = 0.42
RMS fitting error = 1.01 %

C.8.2 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 formation (cal/mol)	Mol. wt.	TMD (g/cc)	
HYTEMP	1.00	1.19	1.74	-205067	188.60	1.00	$C_{10}H_{15.46}O_{3.307}$
DOA	3.00	1.82	5.65	-290392	370.56	0.93	$C_{22}H_{42}O_4$
RDX	96.00	96.99	92.61	16496	222.13	1.81	$C_3H_6N_6O_6$

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)	
HYTEMP	1.00	1.19	1.74	-205067	188.60	1.00	$C_{10}H_{15.46}O_{3.307}$
DOA	3.00	1.82	5.65	-290392	370.56	0.93	$C_{22}H_{42}O_4$
RDX	96.00	96.99	92.61	16496	222.13	1.81	$C_3H_6N_6O_6$

Density = 1.7422 g/cc Mixture TMD = 1.7422 g/cc % TMD = 100.0000

The C-J condition:

The pressure	=	30.52 GPa
The volume	=	0.434 cc/g
The density	=	2.304 g/cc
The energy	=	3.72 kJ/cc explosive
The temperature	=	4049 K
The shock velocity	=	8.475 mm/us
The particle velocity	=	2.067 mm/us
The speed of sound	=	6.409 mm/us
Gamma	=	3.101

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	-6.22	128	98	83	69	143
4.10	-7.51	129	97	85	71	136
6.50	-8.04	129	97	85	72	132
10.00	-8.39	129	97	86	73	128
20.00	-8.80	128	96	86	74	123
40.00	-9.10	127	96	87	75	118
80.00	-9.32	127	95	87	75	113
160.00	-9.50					

Freezing occurred at T = 1800.0 K and relative V = 2.206
The mechanical energy of detonation = -9.681 kJ/cc
The thermal energy of detonation = -0.000 kJ/cc
The total energy of detonation = -9.681 kJ/cc

JWL Fit results:
E0 = -10.088 kJ/cc
A = 896.66 GPa, B = 10.19 GPa, C = 1.49 GPa
R[1] = 4.77, R[2] = 1.06, omega = 0.38
RMS fitting error = 0.95 %

Appendix D Cheetah summary printout 92 wt. % RDX

D.1 COMP 22

D.1.1 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     Mol.    TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
GAP         8.00  16.31  10.83    33939    99.09     1.29 C3H5N3O1
RDX        92.00  83.69  89.17    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.    TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
GAP         8.00  16.31  10.83    33939    99.09     1.29 C3H5N3O1
RDX        92.00  83.69  89.17    16496   222.13     1.81 C3H6N6O6

Density  =  1.7504 g/cc   Mixture TMD =  1.7504 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         31.24 GPa
The volume            =         0.437 cc/g
The density           =         2.287 g/cc
The energy            =          3.67 kJ/cc explosive
The temperature       =          4049 K
The shock velocity    =         8.720 mm/us
The particle velocity =         2.047 mm/us
The speed of sound    =         6.673 mm/us
Gamma                 =         3.260

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    -1.17
   2.20    -6.62     137      104       89       73      152
   4.10    -7.97     137      103       90       75      144
   6.50    -8.51     137      102       90       76      139
  10.00    -8.86     136      102       91       77      135
  20.00    -9.26     135      101       91       78      129
  40.00    -9.55     134      100       91       79      123
  80.00    -9.76     132      100       91       79      118
 160.00    -9.93

Freezing occurred at T =     1800.0 K and relative V =   2.204
The mechanical energy of detonation =    -10.096 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.096 kJ/cc

JWL Fit results:
E0   =       -10.411 kJ/cc
A    =      1113.03 GPa, B    =    12.05 GPa,  C     =         1.74 GPa
R[1] =         4.98,     R[2] =     1.12,      omega =         0.42
RMS fitting error =   1.02 %
```

D.1.2 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)
GAP         8.00  16.31  10.83    33939    99.09     1.29 C3H5N3O1
RDX        92.00  83.69  89.17    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                              formation     wt.    (g/cc)
                              (cal/mol)
GAP         8.00  16.31  10.83    33939    99.09     1.29 C3H5N3O1
RDX        92.00  83.69  89.17    16496   222.13     1.81 C3H6N6O6

Density  =  1.7504 g/cc   Mixture TMD =  1.7504 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          31.39 GPa
The volume            =          0.432 cc/g
The density           =          2.315 g/cc
The energy            =           3.83 kJ/cc explosive
The temperature       =           4109 K
The shock velocity    =          8.576 mm/us
The particle velocity =          2.091 mm/us
The speed of sound    =          6.485 mm/us
Gamma                 =          3.101

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    -1.16
   2.20    -6.38     131      100       85       70      146
   4.10    -7.69     132      100       87       73      139
   6.50    -8.22     132       99       87       74      135
  10.00    -8.57     131       99       88       75      131
  20.00    -8.98     131       98       88       76      125
  40.00    -9.28     130       98       89       76      120
  80.00    -9.50     129       97       89       77      115
 160.00    -9.67

Freezing occurred at T =     1800.0 K and relative V =   2.231
The mechanical energy of detonation =     -9.846 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.846 kJ/cc

JWL Fit results:
E0   =       -10.179 kJ/cc
A    =       915.84 GPa, B    =     10.37 GPa,  C     =     1.74 GPa
R[1] =         4.76,     R[2] =      1.10,      omega =     0.42
RMS fitting error =   0.73 %
```

D.2 COMP 23

D.2.1 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     Mol.   TMD
                               formation     wt.    (g/cc)
                               (cal/mol)
BAMO        8.00  10.30  10.78   100382   168.16     1.30 C5H8N6O1
RDX        92.00  89.70  89.22    16496   222.13     1.81 C3H6N6O6

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


The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                               formation     wt.    (g/cc)
                               (cal/mol)
BAMO        8.00  10.30  10.78   100382   168.16     1.30 C5H8N6O1
RDX        92.00  89.70  89.22    16496   222.13     1.81 C3H6N6O6

Density  =  1.7515 g/cc   Mixture TMD =  1.7515 g/cc   % TMD = 100.0000


The C-J condition:
The pressure          =         31.31 GPa
The volume            =         0.437 cc/g
The density           =         2.289 g/cc
The energy            =          3.68 kJ/cc explosive
The temperature       =          4064 K
The shock velocity    =         8.725 mm/us
The particle velocity =         2.049 mm/us
The speed of sound    =         6.676 mm/us
Gamma                 =         3.259

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    -1.18
   2.20    -6.64     137      105       89       73      152
   4.10    -7.99     137      103       90       76      145
   6.50    -8.53     137      103       91       77      140
  10.00    -8.88     136      102       91       77      135
  20.00    -9.28     135      101       91       78      129
  40.00    -9.57     134      101       91       79      124
  80.00    -9.79     133      100       91       79      119
 160.00    -9.96

Freezing occurred at T =     1800.0 K and relative V =   2.216
The mechanical energy of detonation =    -10.123 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.123 kJ/cc

JWL Fit results:
E0   =      -10.438 kJ/cc
A    =      1113.73 GPa, B    =     12.07 GPa,  C     =         1.75 GPa
R[1] =         4.98,     R[2] =      1.12,      omega =         0.42
RMS fitting error =   1.02 %
```

D.2.2 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 formation (cal/mol)	Mol. wt.	TMD (g/cc)	
BAMO	8.00	10.30	10.78	100382	168.16	1.30	$C_5H_8N_6O_1$
RDX	92.00	89.70	89.22	16496	222.13	1.81	$C_3H_6N_6O_6$

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)	Mol. wt.	TMD (g/cc)	
BAMO	8.00	10.30	10.78	100382	168.16	1.30	$C_5H_8N_6O_1$
RDX	92.00	89.70	89.22	16496	222.13	1.81	$C_3H_6N_6O_6$

Density = 1.7515 g/cc Mixture TMD = 1.7515 g/cc % TMD = 100.0000

The C-J condition:

The pressure	=	31.55 GPa
The volume	=	0.432 cc/g
The density	=	2.317 g/cc
The energy	=	3.85 kJ/cc explosive
The temperature	=	4121 K
The shock velocity	=	8.593 mm/us
The particle velocity	=	2.097 mm/us
The speed of sound	=	6.496 mm/us
Gamma	=	3.098

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	-1.17					
2.20	-6.40	132	101	86	71	147
4.10	-7.72	133	100	87	73	140
6.50	-8.25	132	99	88	74	135
10.00	-8.61	132	99	88	75	131
20.00	-9.01	131	98	88	76	126
40.00	-9.31	130	98	89	77	120
80.00	-9.53	129	98	89	77	116
160.00	-9.71					

Freezing occurred at T = 1800.0 K and relative V = 2.239
The mechanical energy of detonation = -9.880 kJ/cc
The thermal energy of detonation = -0.000 kJ/cc
The total energy of detonation = -9.880 kJ/cc

JWL Fit results:
E0 = -10.213 kJ/cc
A = 918.07 GPa, B = 10.43 GPa, C = 1.74 GPa
R[1] = 4.76, R[2] = 1.11, omega = 0.42
RMS fitting error = 0.73 %

D.3 COMP 24

D.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     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
GAP         6.00  12.44   8.12    33939    99.09     1.29 C3H5N3O1
BAMO        2.00   2.44   2.69   100382   168.16     1.30 C5H8N6O1
RDX        92.00  85.11  89.18    16496   222.13     1.81 C3H6N6O6
Product library title: bkws library

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
GAP         6.00  12.44   8.12    33939    99.09     1.29 C3H5N3O1
BAMO        2.00   2.44   2.69   100382   168.16     1.30 c5h8n6o1
RDX        92.00  85.11  89.18    16496   222.13     1.81 C3H6N6O6

Density  =  1.7507 g/cc   Mixture TMD =  1.7507 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         31.26 GPa
The volume            =         0.437 cc/g
The density           =         2.288 g/cc
The energy            =          3.67 kJ/cc explosive
The temperature       =          4052 K
The shock velocity    =         8.721 mm/us
The particle velocity =         2.047 mm/us
The speed of sound    =         6.674 mm/us
Gamma                 =         3.259

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    -1.17
   2.20    -6.63     137      104       89       73      152
   4.10    -7.97     137      103       90       75      144
   6.50    -8.51     137      103       90       76      139
  10.00    -8.86     136      102       91       77      135
  20.00    -9.26     135      101       91       78      129
  40.00    -9.55     134      101       91       79      124
  80.00    -9.77     133      100       91       79      119
 160.00    -9.94

Freezing occurred at T =     1800.0 K and relative V =   2.207
The mechanical energy of detonation =    -10.103 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.103 kJ/cc

JWL Fit results:
E0   =       -10.494 kJ/cc
A    =      1075.92 GPa, B    =    11.42 GPa,  C     =         1.48 GPa
R[1] =         4.90,     R[2] =     1.07,      omega =         0.38
RMS fitting error =   1.25 %
```

D.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)
GAP         6.00  12.44   8.12    33939    99.09     1.29 C3H5N3O1
BAMO        2.00   2.44   2.69   100382   168.16     1.30 C5H8N6O1
RDX        92.00  85.11  89.18    16496   222.13     1.81 C3H6N6O6

Product library title: bkwc

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                 formation     wt.    (g/cc)
                                 (cal/mol)
GAP         6.00  12.44   8.12    33939    99.09     1.29 C3H5N3O1
BAMO        2.00   2.44   2.69   100382   168.16     1.30 C5H8N6O1
RDX        92.00  85.11  89.18    16496   222.13     1.81 C3H6N6O6

Density  =  1.7507 g/cc   Mixture TMD =  1.7507 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         31.43 GPa
The volume            =         0.432 cc/g
The density           =         2.315 g/cc
The energy            =          3.83 kJ/cc explosive
The temperature       =          4112 K
The shock velocity    =         8.581 mm/us
The particle velocity =         2.092 mm/us
The speed of sound    =         6.488 mm/us
Gamma                 =         3.101

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    -1.16
   2.20    -6.38     132      101       85       71      146
   4.10    -7.70     132      100       87       73      139
   6.50    -8.23     132       99       87       74      135
  10.00    -8.58     132       99       88       75      131
  20.00    -8.99     131       98       88       76      125
  40.00    -9.28     130       98       89       76      120
  80.00    -9.51     129       97       89       77      115
 160.00    -9.68

Freezing occurred at T =     1800.0 K and relative V =   2.233
The mechanical energy of detonation =     -9.854 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.854 kJ/cc

JWL Fit results:
E0   =       -10.258 kJ/cc
A    =       919.87 GPa, B    =     10.45 GPa,  C     =         1.51 GPa
R[1] =         4.76,     R[2] =      1.07,      omega =         0.38
RMS fitting error =   0.96 %
```

D.4 COMP 25

D.4.1 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     Mol.    TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
GAP         1.50   3.38   1.97    33939     99.09     1.29 C3H5N3O1
BAMO        0.50   0.66   0.65   100382   168.16     1.30 C5H8N6O1
DOA         6.00   3.61  11.00  -290392   370.56     0.93 C22H42O4
RDX        92.00  92.35  86.38    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.    TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
GAP         1.50   3.38   1.97    33939     99.09     1.29 C3H5N3O1
BAMO        0.50   0.66   0.65   100382   168.16     1.30 C5H8N6O1
DOA         6.00   3.61  11.00  -290392   370.56     0.93 C22H42O4
RDX        92.00  92.35  86.38    16496   222.13     1.81 C3H6N6O6

Density  =  1.6957 g/cc   Mixture TMD =  1.6957 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         28.73 GPa
The volume            =         0.450 cc/g
The density           =         2.220 g/cc
The energy            =          3.39 kJ/cc explosive
The temperature       =          3852 K
The shock velocity    =         8.467 mm/us
The particle velocity =         2.001 mm/us
The speed of sound    =         6.467 mm/us
Gamma                 =         3.232

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    -1.08
   2.20    -6.08     125       96       81       67      140
   4.10    -7.34     126       95       83       70      133
   6.50    -7.85     126       95       83       71      129
  10.00    -8.19     126       94       84       71      125
  20.00    -8.59     125       94       84       72      120
  40.00    -8.87     124       93       85       73      115
  80.00    -9.09     123       93       85       74      110
 160.00    -9.26

Freezing occurred at T =     1800.0 K and relative V =   2.113
The mechanical energy of detonation =     -9.464 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.464 kJ/cc

JWL Fit results:
E0   =        -9.781 kJ/cc
A    =       987.87 GPa, B    =     10.73 GPa,  C     =         1.62 GPa
R[1] =         4.94,     R[2] =      1.11,      omega =         0.40
RMS fitting error =   0.97 %
```

D.4.2 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)
DOA         6.00   3.61  11.00  -290392   370.56     0.93 C22H42O4
RDX        92.00  92.35  86.38    16496   222.13     1.81 C3H6N6O6
BAMO        0.50   0.66   0.65   100382   168.16     1.30 C5H8N6O1
GAP         1.50   3.38   1.97    33939    99.09     1.29 C3H5N3O1

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)
DOA         6.00   3.61  11.00  -290392   370.56     0.93 C22H42O4
RDX        92.00  92.35  86.38    16496   222.13     1.81 C3H6N6O6
BAMO        0.50   0.66   0.65   100382   168.16     1.30 C5H8N6O1
GAP         1.50   3.38   1.97    33939    99.09     1.29 C3H5N3O1

Density  =  1.6957 g/cc   Mixture TMD =  1.6957 g/cc   % TMD = 100.0000


The C-J condition:
The pressure          =         27.69 GPa
The volume            =         0.445 cc/g
The density           =         2.247 g/cc
The energy            =          3.40 kJ/cc explosive
The temperature       =          3939 K
The shock velocity    =         8.158 mm/us
The particle velocity =         2.001 mm/us
The speed of sound    =         6.156 mm/us
Gamma                 =         3.076

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    -1.03
   2.20    -5.75     119       91       77       64      132
   4.10    -6.99     120       91       79       66      127
   6.50    -7.51     120       90       80       67      123
  10.00    -7.85     120       90       80       68      120
  20.00    -8.26     120       90       81       70      115
  40.00    -8.56     120       90       82       70      111
  80.00    -8.79     119       90       82       71      107
 160.00    -8.97

Freezing occurred at T =     1800.0 K and relative V =   2.201
The mechanical energy of detonation =     -9.197 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.197 kJ/cc

JWL Fit results:
E0   =       -9.535 kJ/cc
A    =       803.50 GPa, B    =     9.42 GPa,  C     =         1.64 GPa
R[1] =         4.79,     R[2] =     1.10,      omega =         0.39
RMS fitting error =   0.70 %
```

D.5 COMP 26

D.5.1 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     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
GAP         2.00   4.48   2.62    33939    99.09     1.29 C3H5N3O1
DOA         6.00   3.59  11.00  -290392   370.56     0.93 C22H42O4
RDX        92.00  91.93  86.38    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
GAP         2.00   4.48   2.62    33939    99.09     1.29 C3H5N3O1
DOA         6.00   3.59  11.00  -290392   370.56     0.93 C22H42O4
RDX        92.00  91.93  86.38    16496   222.13     1.81 C3H6N6O6

Density  =  1.6956 g/cc   Mixture TMD =  1.6956 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         28.72 GPa
The volume            =         0.450 cc/g
The density           =         2.220 g/cc
The energy            =          3.39 kJ/cc explosive
The temperature       =          3851 K
The shock velocity    =         8.467 mm/us
The particle velocity =         2.000 mm/us
The speed of sound    =         6.467 mm/us
Gamma                 =         3.233


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    -1.08
   2.20    -6.08     125       96       81       67      140
   4.10    -7.34     126       95       83       69      133
   6.50    -7.85     126       95       83       71      129
  10.00    -8.19     126       94       84       71      125
  20.00    -8.58     125       94       84       72      120
  40.00    -8.87     124       93       85       73      115
  80.00    -9.09     123       93       85       74      110
 160.00    -9.26

Freezing occurred at T =     1800.0 K and relative V =   2.112
The mechanical energy of detonation =     -9.462 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.462 kJ/cc

JWL Fit results:
E0   =        -9.779 kJ/cc
A    =       988.42 GPa, B    =   10.74 GPa,  C     =    1.62 GPa
R[1] =         4.94,     R[2] =    1.11,      omega =    0.40
RMS fitting error =   0.97 %
```

D.5.2 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)
GAP         2.00   4.48   2.62    33939    99.09     1.29 C3H5N3O1
DOA         6.00   3.59  11.00  -290392   370.56     0.93 C22H42O4
RDX        92.00  91.93  86.38    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
GAP         2.00   4.48   2.62    33939    99.09     1.29 C3H5N3O1
DOA         6.00   3.59  11.00  -290392   370.56     0.93 C22H42O4
RDX        92.00  91.93  86.38    16496   222.13     1.81 C3H6N6O6

Density  =  1.6956 g/cc   Mixture TMD =  1.6956 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         27.68 GPa
The volume            =         0.445 cc/g
The density           =         2.247 g/cc
The energy            =          3.40 kJ/cc explosive
The temperature       =          3938 K
The shock velocity    =         8.157 mm/us
The particle velocity =         2.001 mm/us
The speed of sound    =         6.155 mm/us
Gamma                 =         3.076


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    -1.03
   2.20    -5.75     118       90       77       63      132
   4.10    -6.99     120       90       79       66      127
   6.50    -7.50     120       90       80       67      123
  10.00    -7.85     120       90       80       68      120
  20.00    -8.26     120       90       81       70      115
  40.00    -8.56     120       90       82       70      111
  80.00    -8.79     119       90       82       71      107
 160.00    -8.97

Freezing occurred at T =     1800.0 K and relative V =   2.201
The mechanical energy of detonation =     -9.195 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.195 kJ/cc

JWL Fit results:
E0   =        -9.607 kJ/cc
A    =       807.45 GPa, B    =     9.50 GPa,  C     =    1.44 GPa
R[1] =         4.78,     R[2] =     1.06,      omega =    0.36
RMS fitting error =   0.93 %
```

D.6 COMP 27

D.6.1 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     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
BAMO        2.00   2.69   2.61   100382   168.16     1.30 C5H8N6O1
DOA         6.00   3.66  11.00  -290392   370.56     0.93 C22H42O4
RDX        92.00  93.65  86.39    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
BAMO        2.00   2.69   2.61   100382   168.16     1.30 C5H8N6O1
DOA         6.00   3.66  11.00  -290392   370.56     0.93 C22H42O4
RDX        92.00  93.65  86.39    16496   222.13     1.81 C3H6N6O6

Density  =  1.6959 g/cc   Mixture TMD =  1.6959 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         28.74 GPa
The volume            =         0.450 cc/g
The density           =         2.221 g/cc
The energy            =          3.39 kJ/cc explosive
The temperature       =          3855 K
The shock velocity    =         8.468 mm/us
The particle velocity =         2.001 mm/us
The speed of sound    =         6.468 mm/us
Gamma                 =         3.232

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    -1.08
   2.20    -6.09     125       96       81       67      140
   4.10    -7.34     126       95       83       70      133
   6.50    -7.86     126       95       83       71      129
  10.00    -8.20     126       94       84       71      125
  20.00    -8.59     125       94       84       72      120
  40.00    -8.88     124       93       85       73      115
  80.00    -9.10     123       93       85       74      110
 160.00    -9.27

Freezing occurred at T =     1800.0 K and relative V =   2.115
The mechanical energy of detonation =     -9.469 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.469 kJ/cc

JWL Fit results:
E0   =        -9.865 kJ/cc
A    =       958.68 GPa, B    =    10.23 GPa,  C     =     1.39 GPa
R[1] =         4.87,     R[2] =     1.06,      omega =     0.36
RMS fitting error =   1.20 %
```

D.6.2 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)
BAMO        2.00   2.69   2.61   100382   168.16     1.30 C5H8N6O1
DOA         6.00   3.66  11.00  -290392   370.56     0.93 C22H42O4
RDX        92.00  93.65  86.39    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.    TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
BAMO        2.00   2.69   2.61   100382   168.16     1.30 C5H8N6O1
DOA         6.00   3.66  11.00  -290392   370.56     0.93 C22H42O4
RDX        92.00  93.65  86.39    16496   222.13     1.81 C3H6N6O6

Density  =  1.6959 g/cc   Mixture TMD =  1.6959 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          27.71 GPa
The volume            =          0.445 cc/g
The density           =          2.247 g/cc
The energy            =           3.40 kJ/cc explosive
The temperature       =           3941 K
The shock velocity    =          8.160 mm/us
The particle velocity =          2.002 mm/us
The speed of sound    =          6.158 mm/us
Gamma                 =          3.075

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    -1.03
   2.20    -5.75     119       91       77       64      132
   4.10    -6.99     120       91       79       66      127
   6.50    -7.51     121       90       80       67      123
  10.00    -7.86     121       90       80       68      120
  20.00    -8.27     120       90       81       70      115
  40.00    -8.56     120       90       82       70      111
  80.00    -8.80     119       90       82       71      107
 160.00    -8.98

Freezing occurred at T =     1800.0 K and relative V =   2.203
The mechanical energy of detonation =     -9.203 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.203 kJ/cc

JWL Fit results:
E0   =        -9.540 kJ/cc
A    =       803.92 GPa, B    =      9.43 GPa,  C     =         1.64 GPa
R[1] =         4.79,     R[2] =      1.10,      omega =         0.39
RMS fitting error =   0.70 %
```

D.7 COMP 28

D.7.1 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)	
HYTEMP	2.00	2.40	3.37	-205067	188.60	1.00	$C_{10}H_{15.46}O_{3.307}$
DOA	6.00	3.67	10.91	-290392	370.56	0.93	$C_{22}H_{42}O_4$
RDX	92.00	93.92	85.72	16496	222.13	1.81	$C_3H_6N_6O_6$

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)	
HYTEMP	2.00	2.40	3.37	-205067	188.60	1.00	$C_{10}H_{15.46}O_{3.307}$
DOA	6.00	3.67	10.91	-290392	370.56	0.93	$C_{22}H_{42}O_4$
RDX	92.00	93.92	85.72	16496	222.13	1.81	$C_3H_6N_6O_6$

Density = 1.6827 g/cc Mixture TMD = 1.6827 g/cc % TMD = 100.0000

The C-J condition:

The pressure	=	28.01 GPa
The volume	=	0.454 cc/g
The density	=	2.204 g/cc
The energy	=	3.31 kJ/cc explosive
The temperature	=	3799 K
The shock velocity	=	8.389 mm/us
The particle velocity	=	1.985 mm/us
The speed of sound	=	6.404 mm/us
Gamma	=	3.227

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	-1.05					
2.20	-5.93	122	93	79	66	136
4.10	-7.16	123	93	81	68	130
6.50	-7.66	123	92	81	69	125
10.00	-8.00	123	92	82	70	122
20.00	-8.39	122	92	82	71	117
40.00	-8.67	121	91	83	71	112
80.00	-8.89	121	91	83	72	108
160.00	-9.06					

Freezing occurred at T = 1800.0 K and relative V = 2.082
The mechanical energy of detonation = -9.268 kJ/cc
The thermal energy of detonation = -0.000 kJ/cc
The total energy of detonation = -9.268 kJ/cc

JWL Fit results:
E0 = -9.584 kJ/cc
A = 957.39 GPa, B = 10.39 GPa, C = 1.58 GPa
R[1] = 4.93, R[2] = 1.11, omega = 0.40
RMS fitting error = 0.96 %

D.7.2 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)
HYTEMP      2.00   2.40   3.37  -205067   188.60     1.00 C10H15.46O3.307
DOA         6.00   3.67  10.91  -290392   370.56     0.93 C22H42O4
RDX        92.00  93.92  85.72    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
HYTEMP      2.00   2.40   3.37  -205067   188.60     1.00 C10H15.46O3.307
DOA         6.00   3.67  10.91  -290392   370.56     0.93 C22H42O4
RDX        92.00  93.92  85.72    16496   222.13     1.81 C3H6N6O6

Density  =  1.6827 g/cc   Mixture TMD =  1.6827 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          26.72 GPa
The volume            =          0.449 cc/g
The density           =          2.229 g/cc
The energy            =           3.28 kJ/cc explosive
The temperature       =           3887 K
The shock velocity    =          8.048 mm/us
The particle velocity =          1.973 mm/us
The speed of sound    =          6.074 mm/us
Gamma                 =          3.078

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    -1.00
   2.20    -5.57     115       88       75       62      128
   4.10    -6.79     117       88       77       64      123
   6.50    -7.30     117       88       77       66      119
  10.00    -7.64     117       88       78       67      116
  20.00    -8.05     117       88       79       68      112
  40.00    -8.35     117       88       80       69      108
  80.00    -8.58     116       88       80       69      104
 160.00    -8.76

Freezing occurred at T =     1800.0 K and relative V =   2.180
The mechanical energy of detonation =     -8.995 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -8.995 kJ/cc

JWL Fit results:
E0   =        -9.335 kJ/cc
A    =       780.66 GPa, B    =    9.14 GPa,  C     =         1.61 GPa
R[1] =         4.80,     R[2] =    1.10,      omega =         0.39
RMS fitting error =   0.70 %
```

Appendix E Cheetah summary printout 87 wt. % HMX

E.1 COMP 29

E.1.1 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     Mol.    TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
HMX        87.00  71.72  76.45    17866    296.17     1.91 C4H8N8O8
DOA         7.00   4.61  12.67  -290392    370.56     0.93 C22H42O4
HTPB        5.00  22.57   9.30     1195     54.09     0.90 C4H6
IPDI        1.00   1.10   1.58   -88910    222.28     1.06 C12H18N2O2
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)
HMX        87.00  71.72  76.45    17866    296.17     1.91 C4H8N8O8
DOA         7.00   4.61  12.67  -290392    370.56     0.93 C22H42O4
HTPB        5.00  22.57   9.30     1195     54.09     0.90 C4H6
IPDI        1.00   1.10   1.58   -88910    222.28     1.06 C12H18N2O2

Density  =  1.6740 g/cc   Mixture TMD =  1.6740 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          27.15 GPa
The volume            =          0.457 cc/g
The density           =          2.190 g/cc
The energy            =           3.20 kJ/cc explosive
The temperature       =           3547 K
The shock velocity    =          8.294 mm/us
The particle velocity =          1.955 mm/us
The speed of sound    =          6.338 mm/us
Gamma                 =          3.242

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    -1.01
   2.20    -5.61     116       88       75       62      129
   4.10    -6.77     117       88       76       64      123
   6.50    -7.26     117       87       77       65      119
  10.00    -7.58     116       87       78       66      116
  20.00    -7.97     116       87       78       67      111
  40.00    -8.26     115       87       79       68      107
  80.00    -8.48     115       87       79       69      103
 160.00    -8.66

Freezing occurred at T =     1800.0 K and relative V =   1.936
The mechanical energy of detonation =     -8.940 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -8.940 kJ/cc

JWL Fit results:
E0   =        -9.264 kJ/cc
A    =       923.94 GPa, B    =      9.41 GPa,  C     =         1.45 GPa
R[1] =         4.90,     R[2] =      1.10,      omega =         0.37
RMS fitting error =   0.90 %
```

E.1.2 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 formation (cal/mol)	Mol. wt.	TMD (g/cc)	
HTPB	5.00	22.57	9.30	1195	54.09	0.90	C_4H_6
IPDI	1.00	1.10	1.58	-88910	222.28	1.06	$C_{12}H_{18}N_2O_2$
HMX	87.00	71.72	76.45	17866	296.17	1.91	$C_4H_8N_8O_8$
DOA	7.00	4.61	12.67	-290392	370.56	0.93	$C_{22}H_{42}O_4$

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)	Mol. wt.	TMD (g/cc)	
HTPB	5.00	22.57	9.30	1195	54.09	0.90	C_4H_6
IPDI	1.00	1.10	1.58	-88910	222.28	1.06	$C_{12}H_{18}N_2O_2$
HMX	87.00	71.72	76.45	17866	296.17	1.91	$C_4H_8N_8O_8$
DOA	7.00	4.61	12.67	-290392	370.56	0.93	$C_{22}H_{42}O_4$

Density = 1.6740 g/cc Mixture TMD = 1.6740 g/cc % TMD = 100.0000

The C-J condition:

The pressure	=	24.53 GPa
The volume	=	0.450 cc/g
The density	=	2.221 g/cc
The energy	=	3.02 kJ/cc explosive
The temperature	=	3664 K
The shock velocity	=	7.714 mm/us
The particle velocity	=	1.900 mm/us
The speed of sound	=	5.813 mm/us
Gamma	=	3.060

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	-0.91					
2.20	-5.17	107	81	69	57	119
4.10	-6.33	109	82	71	60	115
6.50	-6.83	110	82	73	61	112
10.00	-7.18	110	83	73	63	109
20.00	-7.59	110	83	74	64	106
40.00	-7.90	110	83	75	65	102
80.00	-8.14	111	83	76	66	99
160.00	-8.34					

Freezing occurred at T = 1800.0 K and relative V = 2.103
The mechanical energy of detonation = -8.683 kJ/cc
The thermal energy of detonation = -0.000 kJ/cc
The total energy of detonation = -8.683 kJ/cc

JWL Fit results:
E0 = -9.035 kJ/cc
A = 723.04 GPa, B = 8.72 GPa, C = 1.50 GPa
R[1] = 4.83, R[2] = 1.10, omega = 0.36
RMS fitting error = 0.67 %

E.2 COMP 30

E.2.1 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     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
HMX        87.00  83.66  78.62     17866   296.17     1.91 C4H8N8O8
DOA         7.00   5.38  13.03   -290392   370.56     0.93 C22H42O4
pNIMMO      5.00   9.68   6.72     73853   147.13     1.28 c5h9n1o4
IPDI        1.00   1.28   1.62    -88910   222.28     1.06 C12H18N2O2

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)
HMX        87.00  83.66  78.62     17866   296.17     1.91 C4H8N8O8
DOA         7.00   5.38  13.03   -290392   370.56     0.93 C22H42O4
pNIMMO      5.00   9.68   6.72     73853   147.13     1.28 c5h9n1o4
IPDI        1.00   1.28   1.62    -88910   222.28     1.06 C12H18N2O2

Density  =  1.7216 g/cc   Mixture TMD =  1.7216 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         29.84 GPa
The volume            =         0.444 cc/g
The density           =         2.250 g/cc
The energy            =          3.51 kJ/cc explosive
The temperature       =          3748 K
The shock velocity    =         8.588 mm/us
The particle velocity =         2.018 mm/us
The speed of sound    =         6.570 mm/us
Gamma                 =         3.255

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    -6.23     128       98       83       69      143
   4.10    -7.49     129       97       85       71      136
   6.50    -8.01     129       97       85       72      131
  10.00    -8.35     128       96       85       73      127
  20.00    -8.75     127       96       86       74      122
  40.00    -9.05     127       95       86       74      117
  80.00    -9.28     126       95       87       75      113
 160.00    -9.46

Freezing occurred at T =     1800.0 K and relative V =   2.055
The mechanical energy of detonation =     -9.695 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.695 kJ/cc

JWL Fit results:
E0   =       -10.106 kJ/cc
A    =      1002.22 GPa, B    =    10.24 GPa,  C     =         1.36 GPa
R[1] =         4.85,     R[2] =     1.06,      omega =         0.35
RMS fitting error =   1.20 %
```

E.2.2 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 formation (cal/mol)	Mol. wt.	TMD (g/cc)	
pNIMMO	5.00	9.68	6.72	73853	147.13	1.28	$C_5H_9N_1O_4$
IPDI	1.00	1.28	1.62	-88910	222.28	1.06	$C_{12}H_{18}N_2O_2$
HMX	87.00	83.66	78.62	17866	296.17	1.91	$C_4H_8N_8O_8$
DOA	7.00	5.38	13.03	-290392	370.56	0.93	$C_{22}H_{42}O_4$

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)	Mol. wt.	TMD (g/cc)	
pNIMMO	5.00	9.68	6.72	73853	147.13	1.28	$C_5H_9N_1O_4$
IPDI	1.00	1.28	1.62	-88910	222.28	1.06	$C_{12}H_{18}N_2O_2$
HMX	87.00	83.66	78.62	17866	296.17	1.91	$C_4H_8N_8O_8$
DOA	7.00	5.38	13.03	-290392	370.56	0.93	$C_{22}H_{42}O_4$

Density = 1.7216 g/cc Mixture TMD = 1.7216 g/cc % TMD = 100.0000

The C-J condition:

The pressure	=	28.09 GPa
The volume	=	0.437 cc/g
The density	=	2.288 g/cc
The energy	=	3.48 kJ/cc explosive
The temperature	=	3867 K
The shock velocity	=	8.118 mm/us
The particle velocity	=	2.010 mm/us
The speed of sound	=	6.108 mm/us
Gamma	=	3.038

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	-1.04					
2.20	-5.80	120	91	78	64	133
4.10	-7.06	122	92	80	67	128
6.50	-7.59	122	91	81	68	124
10.00	-7.95	122	91	81	69	121
20.00	-8.37	122	91	82	70	117
40.00	-8.69	121	91	83	71	112
80.00	-8.93	121	91	83	72	108
160.00	-9.13					

Freezing occurred at T = 1800.0 K and relative V = 2.193
The mechanical energy of detonation = -9.409 kJ/cc
The thermal energy of detonation = -0.000 kJ/cc
The total energy of detonation = -9.409 kJ/cc

JWL Fit results:
E0 = -9.842 kJ/cc
A = 794.84 GPa, B = 9.67 GPa, C = 1.43 GPa
R[1] = 4.76, R[2] = 1.06, omega = 0.35
RMS fitting error = 0.90 %

E.3 COMP 31

E.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     Mol.    TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
HMX        87.00  79.91  78.68     17866   296.17     1.91 C4H8N8O8
DOA         7.00   5.14  13.04   -290392   370.56     0.93 C22H42O4
GAP         5.00  13.73   6.66     33939    99.09     1.29 C3H5N3O1
IPDI        1.00   1.22   1.63    -88910   222.28     1.06 C12H18N2O2

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)
HMX        87.00  79.91  78.68     17866   296.17     1.91 C4H8N8O8
DOA         7.00   5.14  13.04   -290392   370.56     0.93 C22H42O4
GAP         5.00  13.73   6.66     33939    99.09     1.29 C3H5N3O1
IPDI        1.00   1.22   1.63    -88910   222.28     1.06 C12H18N2O2

Density  =  1.7227 g/cc   Mixture TMD =  1.7227 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          29.30 GPa
The volume            =          0.445 cc/g
The density           =          2.249 g/cc
The energy            =           3.43 kJ/cc explosive
The temperature       =           3671 K
The shock velocity    =          8.528 mm/us
The particle velocity =          1.995 mm/us
The speed of sound    =          6.533 mm/us
Gamma                 =          3.276

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    -1.08
   2.20    -6.05     125       95       81       67      139
   4.10    -7.28     125       94       82       69      132
   6.50    -7.78     125       94       83       70      127
  10.00    -8.11     124       93       83       71      124
  20.00    -8.50     124       93       83       72      119
  40.00    -8.78     123       92       84       72      114
  80.00    -9.00     122       92       84       73      109
 160.00    -9.18

Freezing occurred at T =     1800.0 K and relative V =   1.973
The mechanical energy of detonation =     -9.398 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.398 kJ/cc

JWL Fit results:
E0   =        -9.723 kJ/cc
A    =      1037.40 GPa, B    =     10.47 GPa,  C     =   1.54 GPa
R[1] =         4.94,     R[2] =      1.11,      omega =   0.39
RMS fitting error =   0.95 %
```

E.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)
GAP         5.00  13.73   6.66     33939     99.09     1.29 C3H5N3O1
IPDI        1.00   1.22   1.63    -88910    222.28     1.06 C12H18N2O2
HMX        87.00  79.91  78.68     17866    296.17     1.91 C4H8N8O8
DOA         7.00   5.14  13.04   -290392    370.56     0.93 C22H42O4

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)
GAP         5.00  13.73   6.66     33939     99.09     1.29 C3H5N3O1
IPDI        1.00   1.22   1.63    -88910    222.28     1.06 C12H18N2O2
HMX        87.00  79.91  78.68     17866    296.17     1.91 C4H8N8O8
DOA         7.00   5.14  13.04   -290392    370.56     0.93 C22H42O4

Density  =  1.7227 g/cc   Mixture TMD =  1.7227 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          27.68 GPa
The volume            =          0.438 cc/g
The density           =          2.284 g/cc
The energy            =           3.40 kJ/cc explosive
The temperature       =           3774 K
The shock velocity    =          8.087 mm/us
The particle velocity =          1.986 mm/us
The speed of sound    =          6.101 mm/us
Gamma                 =          3.071

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    -1.02
   2.20    -5.66     117       89       76       63       130
   4.10    -6.88     118       89       78       65       125
   6.50    -7.39     119       89       78       66       121
  10.00    -7.74     119       89       79       67       118
  20.00    -8.15     119       89       80       69       114
  40.00    -8.45     118       89       81       70       109
  80.00    -8.69     118       89       81       70       105
 160.00    -8.88

Freezing occurred at T =     1800.0 K and relative V =   2.098
The mechanical energy of detonation =     -9.148 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.148 kJ/cc

JWL Fit results:
E0   =        -9.497 kJ/cc
A    =       806.40 GPa, B    =    9.40 GPa,  C     =   1.57 GPa
R[1] =         4.79,     R[2] =    1.10,      omega =   0.38
RMS fitting error =   0.66 %
```

E.4 COMP 32

E.4.1 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	87.00	84.69	78.70	17866	296.17	1.91	$C_4H_8N_8O_8$
DOA	7.00	5.45	13.04	-290392	370.56	0.93	$C_{22}H_{42}O_4$
BAMO	5.00	8.57	6.63	100382	168.16	1.30	$C_5H_8N_6O_1$
IPDI	1.00	1.30	1.63	-88910	222.28	1.06	$C_{12}H_{18}N_2O_2$

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	87.00	84.69	78.70	17866	296.17	1.91	$C_4H_8N_8O_8$
DOA	7.00	5.45	13.04	-290392	370.56	0.93	$C_{22}H_{42}O_4$
BAMO	5.00	8.57	6.63	100382	168.16	1.30	$C_5H_8N_6O_1$
IPDI	1.00	1.30	1.63	-88910	222.28	1.06	$C_{12}H_{18}N_2O_2$

Density = 1.7234 g/cc Mixture TMD = 1.7234 g/cc % TMD = 100.0000

The C-J condition:

The pressure	=	29.34 GPa
The volume	=	0.445 cc/g
The density	=	2.250 g/cc
The energy	=	3.43 kJ/cc explosive
The temperature	=	3679 K
The shock velocity	=	8.531 mm/us
The particle velocity	=	1.995 mm/us
The speed of sound	=	6.536 mm/us
Gamma	=	3.275

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	-1.08					
2.20	-6.06	125	95	81	67	139
4.10	-7.29	125	94	82	69	132
6.50	-7.79	125	94	83	70	128
10.00	-8.12	125	93	83	71	124
20.00	-8.51	124	93	84	72	119
40.00	-8.80	123	93	84	72	114
80.00	-9.02	122	92	84	73	109
160.00	-9.19					

Freezing occurred at T = 1800.0 K and relative V = 1.979
The mechanical energy of detonation = -9.414 kJ/cc
The thermal energy of detonation = -0.000 kJ/cc
The total energy of detonation = -9.414 kJ/cc

JWL Fit results:
E0 = -9.825 kJ/cc
A = 1006.54 GPa, B = 9.94 GPa, C = 1.33 GPa
R[1] = 4.87, R[2] = 1.06, omega = 0.35
RMS fitting error = 1.18 %

E.4.2 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 formation (cal/mol)	Mol. wt.	TMD (g/cc)	
BAMO	5.00	8.57	6.63	100382	168.16	1.30	$C_5H_8N_6O_1$
IPDI	1.00	1.30	1.63	-88910	222.28	1.06	$C_{12}H_{18}N_2O_2$
DOA	7.00	5.45	13.04	-290392	370.56	0.93	$C_{22}H_{42}O_4$
HMX	87.00	84.69	78.70	17866	296.17	1.91	$C_4H_8N_8O_8$

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)	Mol. wt.	TMD (g/cc)	
BAMO	5.00	8.57	6.63	100382	168.16	1.30	$C_5H_8N_6O_1$
IPDI	1.00	1.30	1.63	-88910	222.28	1.06	$C_{12}H_{18}N_2O_2$
DOA	7.00	5.45	13.04	-290392	370.56	0.93	$C_{22}H_{42}O_4$
HMX	87.00	84.69	78.70	17866	296.17	1.91	$C_4H_8N_8O_8$

Density = 1.7234 g/cc Mixture TMD = 1.7234 g/cc % TMD = 100.0000

The C-J condition:

The pressure	=	27.77 GPa
The volume	=	0.438 cc/g
The density	=	2.285 g/cc
The energy	=	3.41 kJ/cc explosive
The temperature	=	3781 K
The shock velocity	=	8.097 mm/us
The particle velocity	=	1.990 mm/us
The speed of sound	=	6.107 mm/us
Gamma	=	3.069

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	-1.02					
2.20	-5.68	117	89	76	63	130
4.10	-6.90	119	89	78	65	125
6.50	-7.41	119	89	79	67	121
10.00	-7.76	119	89	79	68	118
20.00	-8.17	119	89	80	69	114
40.00	-8.47	118	89	81	70	110
80.00	-8.71	118	89	81	71	106
160.00	-8.90					

Freezing occurred at T = 1800.0 K and relative V = 2.103
The mechanical energy of detonation = -9.168 kJ/cc
The thermal energy of detonation = -0.000 kJ/cc
The total energy of detonation = -9.168 kJ/cc

JWL Fit results:
E0 = -9.600 kJ/cc
A = 811.64 GPa, B = 9.51 GPa, C = 1.38 GPa
R[1] = 4.79, R[2] = 1.06, omega = 0.34
RMS fitting error = 0.90 %

E.5 COMP 33

E.5.1 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     Mol.    TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
HMX        87.00  73.20  81.48     17866   296.17     1.91 C4H8N8O8
IPDI        2.00   2.24   3.37    -88910   222.28     1.06 C12H18N2O2
GAP         8.00  20.12  11.04     33939    99.09     1.29 C3H5N3O1
BAMO        3.00   4.45   4.12    100382   168.16     1.30 C5H8N6O1

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)
HMX        87.00  73.20  81.48     17866   296.17     1.91 C4H8N8O8
IPDI        2.00   2.24   3.37    -88910   222.28     1.06 C12H18N2O2
GAP         8.00  20.12  11.04     33939    99.09     1.29 C3H5N3O1
BAMO        3.00   4.45   4.12    100382   168.16     1.30 C5H8N6O1

Density  =  1.7841 g/cc   Mixture TMD =  1.7841 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         32.09 GPa
The volume            =         0.430 cc/g
The density           =         2.324 g/cc
The energy            =          3.73 kJ/cc explosive
The temperature       =          3871 K
The shock velocity    =         8.802 mm/us
The particle velocity =         2.044 mm/us
The speed of sound    =         6.758 mm/us
Gamma                 =         3.307

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    -1.18
   2.20    -6.64     137      104       89       73      152
   4.10    -7.95     137      103       90       75      144
   6.50    -8.48     136      102       90       76      139
  10.00    -8.83     135      102       90       77      135
  20.00    -9.22     134      101       91       78      129
  40.00    -9.51     133      100       91       78      123
  80.00    -9.73     132      100       91       79      118
 160.00    -9.90

Freezing occurred at T =     1800.0 K and relative V =   2.071
The mechanical energy of detonation =    -10.087 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =    -10.087 kJ/cc

JWL Fit results:
E0   =       -10.410 kJ/cc
A    =      1178.61 GPa, B    =    11.81 GPa,  C     =    1.66 GPa
R[1] =         4.98,     R[2] =     1.12,      omega =    0.41
RMS fitting error =   1.01 %
```

E.5.2 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        87.00  73.20  81.48    17866   296.17     1.91 C4H8N8O8
IPDI        2.00   2.24   3.37   -88910   222.28     1.06 C12H18N2O2
GAP         8.00  20.12  11.04    33939    99.09     1.29 C3H5N3O1
BAMO        3.00   4.45   4.12   100382   168.16     1.30 C5H8N6O1

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        87.00  73.20  81.48    17866   296.17     1.91 C4H8N8O8
IPDI        2.00   2.24   3.37   -88910   222.28     1.06 C12H18N2O2
GAP         8.00  20.12  11.04    33939    99.09     1.29 C3H5N3O1
BAMO        3.00   4.45   4.12   100382   168.16     1.30 C5H8N6O1

Density  =  1.7841 g/cc   Mixture TMD =  1.7841 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         31.85 GPa
The volume            =         0.423 cc/g
The density           =         2.363 g/cc
The energy            =          3.90 kJ/cc explosive
The temperature       =          3947 K
The shock velocity    =         8.534 mm/us
The particle velocity =         2.092 mm/us
The speed of sound    =         6.442 mm/us
Gamma                 =         3.080

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    -1.16
   2.20    -6.35     131      100       85       70      146
   4.10    -7.64     131       99       86       72      138
   6.50    -8.17     131       98       87       73      134
  10.00    -8.52     131       98       87       74      130
  20.00    -8.93     130       97       88       75      125
  40.00    -9.23     129       97       88       76      119
  80.00    -9.46     128       97       88       77      115
 160.00    -9.64

Freezing occurred at T =     1800.0 K and relative V =   2.132
The mechanical energy of detonation =     -9.854 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.854 kJ/cc

JWL Fit results:
E0   =       -10.198 kJ/cc
A    =       911.74 GPa, B    =   10.36 GPa,  C     =   1.67 GPa
R[1] =         4.74,     R[2] =    1.11,      omega =   0.40
RMS fitting error =   0.67 %
```

Appendix F Cheetah summary printout 87 wt. % RDX

F.1 COMP 34

F.1.1 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     Mol.    TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
HTPB        5.00  18.22   8.93     1195    54.09     0.90 C4H6
IPDI        1.00   0.89   1.52   -88910   222.28     1.06 C12H18N2O2
DOA         7.00   3.72  12.16  -290392   370.56     0.93 C22H42O4
RDX        87.00  77.18  77.40    16496   222.13     1.81 C3H6N6O6
Product library title: bkws library
Reactant library title: # Version 2.0 by P. Clark Souers

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.    TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
HTPB        5.00  18.22   8.93     1195    54.09     0.90 C4H6
IPDI        1.00   0.89   1.52   -88910   222.28     1.06 C12H18N2O2
DOA         7.00   3.72  12.16  -290392   370.56     0.93 C22H42O4
RDX        87.00  77.18  77.40    16496   222.13     1.81 C3H6N6O6

Density  =  1.6067 g/cc   Mixture TMD =  1.6067 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         24.77 GPa
The volume            =         0.474 cc/g
The density           =         2.111 g/cc
The energy            =          2.96 kJ/cc explosive
The temperature       =          3603 K
The shock velocity    =         8.033 mm/us
The particle velocity =         1.919 mm/us
The speed of sound    =         6.114 mm/us
Gamma                 =         3.185

Cylinder runs:             % of standards
  V/V0     Energy    TATB     PETN      HMX    CL-20   TRITON
 (rel.)   (kJ/cc)  1.83g/cc 1.76g/cc 1.89g/cc 2.04g/cc 1.70g/cc
   1.00    -0.93
   2.20    -5.25     108       83       70       58      120
   4.10    -6.38     110       83       72       60      116
   6.50    -6.86     110       83       73       62      112
  10.00    -7.18     110       83       73       63      109
  20.00    -7.57     110       83       74       64      106
  40.00    -7.85     110       83       75       65      102
  80.00    -8.08     110       83       75       65       98
 160.00    -8.26

Freezing occurred at T =     1800.0 K and relative V =   2.023
The mechanical energy of detonation =     -8.545 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -8.545 kJ/cc
JWL Fit results:
E0   =        -8.954 kJ/cc
A    =       785.19 GPa, B    =  8.43 GPa,  C     =     1.25 GPa
R[1] =         4.82,     R[2] =  1.04,      omega =     0.33
RMS fitting error =   1.10 %
```

F.1.2 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)
HTPB        5.00  18.22   8.93     1195    54.09     0.90 C4H6
IPDI        1.00   0.89   1.52   -88910   222.28     1.06 C12H18N2O2
DOA         7.00   3.72  12.16  -290392   370.56     0.93 C22H42O4
RDX        87.00  77.18  77.40    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
HTPB        5.00  18.22   8.93     1195    54.09     0.90 C4H6
IPDI        1.00   0.89   1.52   -88910   222.28     1.06 C12H18N2O2
DOA         7.00   3.72  12.16  -290392   370.56     0.93 C22H42O4
RDX        87.00  77.18  77.40    16496   222.13     1.81 C3H6N6O6

Density  =  1.6067 g/cc   Mixture TMD =  1.6067 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         22.22 GPa
The volume            =         0.469 cc/g
The density           =         2.132 g/cc
The energy            =          2.74 kJ/cc explosive
The temperature       =          3708 K
The shock velocity    =         7.491 mm/us
The particle velocity =         1.846 mm/us
The speed of sound    =         5.644 mm/us
Gamma                 =         3.057

Cylinder runs:             % of standards
  V/V0     Energy    TATB     PETN      HMX    CL-20   TRITON
 (rel.)   (kJ/cc)  1.83g/cc 1.76g/cc 1.89g/cc 2.04g/cc 1.70g/cc
   1.00    -0.84
   2.20    -4.85     100       76       65       54      111
   4.10    -5.98     103       77       68       57      108
   6.50    -6.47     104       78       69       58      106
  10.00    -6.81     104       78       70       59      104
  20.00    -7.21     105       79       71       61      101
  40.00    -7.52     105       79       72       62       97
  80.00    -7.76     105       79       72       63       94
 160.00    -7.96

Freezing occurred at T =     1800.0 K and relative V =   2.178
The mechanical energy of detonation =     -8.287 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -8.287 kJ/cc

JWL Fit results:
E0   =        -8.632 kJ/cc
A    =       659.38 GPa, B    =     8.19 GPa,  C     =         1.48 GPa
R[1] =         4.86,     R[2] =     1.09,      omega =         0.36
RMS fitting error =   0.71 %
```

F.2 COMP 35

F.2.1 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     Mol.    TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
pNIMMO      5.00   7.57   6.45     73853   147.13     1.28 C5H9N1O4
IPDI        1.00   1.00   1.56    -88910   222.28     1.06 C12H18N2O2
DOA         7.00   4.21  12.49   -290392   370.56     0.93 C22H42O4
RDX        87.00  87.22  79.51     16496   222.13     1.81 C3H6N6O6

Product library title: bkws library
Reactant library title: # Version 2.0 by P. Clark Souers
The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.    TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
pNIMMO      5.00   7.57   6.45     73853   147.13     1.28 C5H9N1O4
IPDI        1.00   1.00   1.56    -88910   222.28     1.06 C12H18N2O2
DOA         7.00   4.21  12.49   -290392   370.56     0.93 C22H42O4
RDX        87.00  87.22  79.51     16496   222.13     1.81 C3H6N6O6

Density  =  1.6504 g/cc   Mixture TMD =  1.6504 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          27.21 GPa
The volume            =          0.461 cc/g
The density           =          2.168 g/cc
The energy            =           3.25 kJ/cc explosive
The temperature       =           3811 K
The shock velocity    =          8.309 mm/us
The particle velocity =          1.984 mm/us
The speed of sound    =          6.325 mm/us
Gamma                 =          3.188

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    -1.03
   2.20    -5.82     120       92       78       64      134
   4.10    -7.05     121       91       80       67      128
   6.50    -7.56     121       91       80       68      124
  10.00    -7.90     121       91       81       69      120
  20.00    -8.30     121       91       81       70      116
  40.00    -8.59     120       90       82       71      111
  80.00    -8.82     120       90       82       71      107
 160.00    -9.00

Freezing occurred at T =     1800.0 K and relative V =   2.150
The mechanical energy of detonation =     -9.249 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.249 kJ/cc

JWL Fit results:
E0   =        -9.564 kJ/cc
A    =       894.33 GPa, B    =    10.12 GPa,  C     =   1.58 GPa
R[1] =         4.90,     R[2] =     1.11,      omega =   0.39
RMS fitting error =   0.94 %
```

F.2.2 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)
pNIMMO      5.00   7.57   6.45    73853   147.13     1.28 C5H9N1O4
IPDI        1.00   1.00   1.56   -88910   222.28     1.06 C12H18N2O2
DOA         7.00   4.21  12.49  -290392   370.56     0.93 C22H42O4
RDX        87.00  87.22  79.51    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                             formation     wt.    (g/cc)
                             (cal/mol)
pNIMMO      5.00   7.57   6.45    73853   147.13     1.28 C5H9N1O4
IPDI        1.00   1.00   1.56   -88910   222.28     1.06 C12H18N2O2
DOA         7.00   4.21  12.49  -290392   370.56     0.93 C22H42O4
RDX        87.00  87.22  79.51    16496   222.13     1.81 C3H6N6O6

Density  =  1.6504 g/cc   Mixture TMD =  1.6504 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         25.42 GPa
The volume            =         0.456 cc/g
The density           =         2.194 g/cc
The energy            =          3.15 kJ/cc explosive
The temperature       =          3917 K
The shock velocity    =         7.883 mm/us
The particle velocity =         1.954 mm/us
The speed of sound    =         5.929 mm/us
Gamma                 =         3.035


Cylinder runs:             % of standards
  V/V0     Energy    TATB     PETN      HMX    CL-20   TRITON
 (rel.)   (kJ/cc)  1.83g/cc 1.76g/cc 1.89g/cc 2.04g/cc 1.70g/cc
   1.00    -0.96
   2.20    -5.43     112       86       73       60       125
   4.10    -6.66     115       86       75       63       121
   6.50    -7.17     115       86       76       64       117
  10.00    -7.52     115       87       77       66       115
  20.00    -7.94     116       87       78       67       111
  40.00    -8.25     115       87       79       68       107
  80.00    -8.49     115       87       79       69       103
 160.00    -8.68

Freezing occurred at T =     1800.0 K and relative V =   2.279
The mechanical energy of detonation =     -8.960 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -8.960 kJ/cc

JWL Fit results:
E0   =        -9.299 kJ/cc
A    =       719.64 GPa, B   = 8.98 GPa,   C      = 1.62 GPa
R[1] =         4.79,    R[2] = 1.09,       omega  = 0.38
RMS fitting error =   0.69 %
```

F.3 COMP 36

F.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     Mol.    TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
GAP         5.00  10.84   6.39    33939    99.09     1.29 C3H5N3O1
IPDI        1.00   0.97   1.56   -88910   222.28     1.06 C12H18N2O2
DOA         7.00   4.06  12.50  -290392   370.56     0.93 C22H42O4
RDX        87.00  84.14  79.56    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.    TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
GAP         5.00  10.84   6.39    33939    99.09     1.29 C3H5N3O1
IPDI        1.00   0.97   1.56   -88910   222.28     1.06 C12H18N2O2
DOA         7.00   4.06  12.50  -290392   370.56     0.93 C22H42O4
RDX        87.00  84.14  79.56    16496   222.13     1.81 C3H6N6O6

Density  =  1.6515 g/cc   Mixture TMD =  1.6515 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         26.70 GPa
The volume            =         0.462 cc/g
The density           =         2.166 g/cc
The energy            =          3.17 kJ/cc explosive
The temperature       =          3733 K
The shock velocity    =         8.249 mm/us
The particle velocity =         1.960 mm/us
The speed of sound    =         6.290 mm/us
Gamma                 =         3.210

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    -1.01
   2.20    -5.66     117       89       76       63      130
   4.10    -6.85     118       89       77       65      124
   6.50    -7.34     118       88       78       66      120
  10.00    -7.67     118       88       78       67      117
  20.00    -8.06     117       88       79       68      112
  40.00    -8.34     117       88       80       69      108
  80.00    -8.56     116       88       80       69      104
 160.00    -8.74

Freezing occurred at T =     1800.0 K and relative V =   2.065
The mechanical energy of detonation =     -8.971 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -8.971 kJ/cc

JWL Fit results:
E0   =        -9.288 kJ/cc
A    =       895.52 GPa, B    =    9.76 GPa,  C     =    1.53 GPa
R[1] =         4.92,     R[2] =    1.11,      omega =    0.39
RMS fitting error =   0.92 %
```

F.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)
GAP         5.00  10.84   6.39    33939    99.09     1.29 C3H5N3O1
IPDI        1.00   0.97   1.56   -88910   222.28     1.06 C12H18N2O2
DOA         7.00   4.06  12.50  -290392   370.56     0.93 C22H42O4
RDX        87.00  84.14  79.56    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.    TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
GAP         5.00  10.84   6.39    33939    99.09     1.29 C3H5N3O1
IPDI        1.00   0.97   1.56   -88910   222.28     1.06 C12H18N2O2
DOA         7.00   4.06  12.50  -290392   370.56     0.93 C22H42O4
RDX        87.00  84.14  79.56    16496   222.13     1.81 C3H6N6O6

Density  =  1.6515 g/cc   Mixture TMD =  1.6515 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         25.01 GPa
The volume            =         0.457 cc/g
The density           =         2.190 g/cc
The energy            =          3.07 kJ/cc explosive
The temperature       =          3825 K
The shock velocity    =         7.849 mm/us
The particle velocity =         1.929 mm/us
The speed of sound    =         5.920 mm/us
Gamma                 =         3.068

Cylinder runs:             % of standards
  V/V0     Energy    TATB     PETN      HMX    CL-20   TRITON
 (rel.)   (kJ/cc)  1.83g/cc 1.76g/cc 1.89g/cc 2.04g/cc 1.70g/cc
   1.00    -0.94
   2.20    -5.30     109       83       71       59      121
   4.10    -6.48     112       84       73       61      117
   6.50    -6.98     112       84       74       63      114
  10.00    -7.32     112       84       75       64      112
  20.00    -7.73     112       84       76       65      108
  40.00    -8.03     112       85       77       66      104
  80.00    -8.26     112       85       77       67      100
 160.00    -8.45

Freezing occurred at T =     1800.0 K and relative V =   2.182
The mechanical energy of detonation =     -8.715 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -8.715 kJ/cc

JWL Fit results:
E0   =        -9.055 kJ/cc
A    =       733.44 GPa, B    =   8.78 GPa,  C     =   1.56 GPa
R[1] =         4.82,     R[2] =   1.10,      omega =    0.38
RMS fitting error =   0.69 %
```

F.4 COMP 37

F.4.1 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     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
BAMO        5.00   6.68   6.35   100382   168.16     1.30 C5H8N6O1
IPDI        1.00   1.01   1.56   -88910   222.28     1.06 C12H18N2O2
DOA         7.00   4.25  12.50  -290392   370.56     0.93 C22H42O4
RDX        87.00  88.06  79.59    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
BAMO        5.00   6.68   6.35   100382   168.16     1.30 C5H8N6O1
IPDI        1.00   1.01   1.56   -88910   222.28     1.06 C12H18N2O2
DOA         7.00   4.25  12.50  -290392   370.56     0.93 C22H42O4
RDX        87.00  88.06  79.59    16496   222.13     1.81 C3H6N6O6

Density  =  1.6521 g/cc   Mixture TMD =  1.6521 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         26.73 GPa
The volume            =         0.462 cc/g
The density           =         2.167 g/cc
The energy            =          3.17 kJ/cc explosive
The temperature       =          3741 K
The shock velocity    =         8.253 mm/us
The particle velocity =         1.960 mm/us
The speed of sound    =         6.292 mm/us
Gamma                 =         3.210

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    -1.01
   2.20    -5.67     117       89       76       63      130
   4.10    -6.86     118       89       77       65      124
   6.50    -7.35     118       89       78       66      120
  10.00    -7.68     118       88       79       67      117
  20.00    -8.07     117       88       79       68      113
  40.00    -8.36     117       88       80       69      108
  80.00    -8.58     116       88       80       69      104
 160.00    -8.75

Freezing occurred at T =     1800.0 K and relative V =   2.072
The mechanical energy of detonation =     -8.986 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -8.986 kJ/cc

JWL Fit results:
E0   =        -9.303 kJ/cc
A    =       896.73 GPa, B    =    9.77 GPa,  C     =     1.53 GPa
R[1] =         4.92,     R[2] =    1.11,      omega =     0.39
RMS fitting error =   0.92 %
```

F.4.2 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)
BAMO        5.00   6.68   6.35   100382   168.16     1.30 C5H8N6O1
IPDI        1.00   1.01   1.56   -88910   222.28     1.06 C12H18N2O2
DOA         7.00   4.25  12.50  -290392   370.56     0.93 C22H42O4
RDX        87.00  88.06  79.59    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
BAMO        5.00   6.68   6.35   100382   168.16     1.30 C5H8N6O1
IPDI        1.00   1.01   1.56   -88910   222.28     1.06 C12H18N2O2
DOA         7.00   4.25  12.50  -290392   370.56     0.93 C22H42O4
RDX        87.00  88.06  79.59    16496   222.13     1.81 C3H6N6O6

Density  =  1.6521 g/cc   Mixture TMD =  1.6521 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =          25.09 GPa
The volume            =          0.456 cc/g
The density           =          2.191 g/cc
The energy            =           3.08 kJ/cc explosive
The temperature       =           3832 K
The shock velocity    =          7.859 mm/us
The particle velocity =          1.932 mm/us
The speed of sound    =          5.926 mm/us
Gamma                 =          3.067

Cylinder runs:              % of standards
  V/V0     Energy    TATB     PETN      HMX    CL-20   TRITON
 (rel.)   (kJ/cc)  1.83g/cc 1.76g/cc 1.89g/cc 2.04g/cc 1.70g/cc
   1.00    -0.94
   2.20    -5.31     110       84       71       59      122
   4.10    -6.50     112       84       73       62      118
   6.50    -7.00     112       84       74       63      115
  10.00    -7.34     113       84       75       64      112
  20.00    -7.75     113       85       76       65      108
  40.00    -8.05     113       85       77       66      104
  80.00    -8.28     112       85       77       67      101
 160.00    -8.47

Freezing occurred at T =     1800.0 K and relative V =   2.188
The mechanical energy of detonation =     -8.734 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -8.734 kJ/cc

JWL Fit results:
E0   =        -9.074 kJ/cc
A    =       734.63 GPa, B    =      8.81 GPa,  C     =         1.57 GPa
R[1] =         4.82,     R[2] =      1.10,      omega =         0.38
RMS fitting error =   0.69 %
```

F.5 COMP 38

F.5.1 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     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
BAMO        3.00   3.57   3.94   100382   168.16     1.30 C5H8N6O1
GAP         8.00  16.17  10.57    33939    99.09     1.29 C3H5N3O1
IPDI        2.00   1.80   3.22   -88910   222.28     1.06 C12H18N2O2
RDX        87.00  78.45  82.27    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                  formation     wt.    (g/cc)
                                  (cal/mol)
BAMO        3.00   3.57   3.94   100382   168.16     1.30 C5H8N6O1
GAP         8.00  16.17  10.57    33939    99.09     1.29 C3H5N3O1
IPDI        2.00   1.80   3.22   -88910   222.28     1.06 C12H18N2O2
RDX        87.00  78.45  82.27    16496   222.13     1.81 C3H6N6O6

Density  =  1.7078 g/cc   Mixture TMD =  1.7078 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         29.16 GPa
The volume            =         0.447 cc/g
The density           =         2.236 g/cc
The energy            =          3.44 kJ/cc explosive
The temperature       =          3941 K
The shock velocity    =         8.501 mm/us
The particle velocity =         2.008 mm/us
The speed of sound    =         6.492 mm/us
Gamma                 =         3.233

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    -1.10
   2.20    -6.19     128       97       83       68      142
   4.10    -7.47     129       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       73      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 =   2.172
The mechanical energy of detonation =     -9.608 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.608 kJ/cc

JWL Fit results:
E0   =         -9.923 kJ/cc
A    =      1004.18 GPa, B    =     10.95 GPa,  C     =    1.65 GPa
R[1] =         4.94,     R[2] =      1.12,      omega =    0.41
RMS fitting error =   0.97 %
```

F.5.2 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)
BAMO        3.00   3.57   3.94   100382   168.16     1.30 C5H8N6O1
GAP         8.00  16.17  10.57    33939    99.09     1.29 C3H5N3O1
IPDI        2.00   1.80   3.22   -88910   222.28     1.06 C12H18N2O2
RDX        87.00  78.45  82.27    16496   222.13     1.81 C3H6N6O6

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

The composition:
Name      % wt.   % mol  % vol    Heat of     Mol.   TMD
                                 formation     wt.    (g/cc)
                                 (cal/mol)
BAMO        3.00   3.57   3.94   100382   168.16     1.30 C5H8N6O1
GAP         8.00  16.17  10.57    33939    99.09     1.29 C3H5N3O1
IPDI        2.00   1.80   3.22   -88910   222.28     1.06 C12H18N2O2
RDX        87.00  78.45  82.27    16496   222.13     1.81 C3H6N6O6

Density  =  1.7078 g/cc   Mixture TMD =  1.7078 g/cc   % TMD = 100.0000

The C-J condition:
The pressure          =         28.70 GPa
The volume            =         0.442 cc/g
The density           =         2.263 g/cc
The energy            =          3.52 kJ/cc explosive
The temperature       =          4008 K
The shock velocity    =         8.275 mm/us
The particle velocity =         2.031 mm/us
The speed of sound    =         6.245 mm/us
Gamma                 =         3.075

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    -1.07
   2.20    -5.91     122       93       79       65      136
   4.10    -7.17     123       93       81       68      130
   6.50    -7.69     123       93       82       69      126
  10.00    -8.04     123       93       82       70      123
  20.00    -8.45     123       92       83       71      118
  40.00    -8.75     122       92       83       72      113
  80.00    -8.98     122       92       84       73      109
 160.00    -9.16

Freezing occurred at T =     1800.0 K and relative V =   2.230
The mechanical energy of detonation =     -9.366 kJ/cc
The thermal energy of detonation    =     -0.000 kJ/cc
The total energy of detonation      =     -9.366 kJ/cc

JWL Fit results:
E0   =        -9.700 kJ/cc
A    =       826.95 GPa, B    =  9.67 GPa,  C     =    1.66 GPa
R[1] =         4.77,     R[2]    1.10,      omega =    0.40
RMS fitting error =   0.70 %
```