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HEXANITROSTILBENE AT VARIOUS CHARGE DENSITIES

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ABSTRACT

We have attempted here to provide an extensive description of the detonation behavior for the unique and useful high explosive hexanitrostilbene (HNS). To accomplish this we have compiled and evaluated the necessary experimental results measured by detonation of the pure material at charge densities of 1.00, 1.20, 1.40, 1.60, and 1.65 ($\text{g/cm}^3 = \text{Mg/m}^3$). Estimates of the equation of state of the detonation products were made for each charge density. To confirm these estimates we carried out two-dimensional hydrodynamic (HEMP code) calculations to simulate the cylinder test experiments for two charge densities of 1.2 and 1.6 Mg/m^3 . Detailed comparisons of the calculational and experimental results were made for these two tests.

Interpolation and extrapolation of the equation of state parameters provided final estimates for the other charge densities. The results are summarized in five sets of Chapman-Jouguet parameters and JWL equation of state coefficients.

INTRODUCTION

Because hexanitrostilbene (HNS) is chemically stable at elevated temperature and possesses relatively high shock sensitivity, it has become an important explosive material especially in initiator and booster applications. It is important in many of these applications to have an accurate estimate of its performance (i.e., the duration and magnitude of the impulse delivered by the detonation of the charge). Considerable experimental work^{1,2,3} on HNS has been performed in order to provide this information.

We have evaluated these data and summarized the explosive performance in a set of equation of state coefficients.⁴ This equation of state, used in hydrodynamic calculations, predicts the behavior of HNS at various charge densities for almost any charge geometry. The description presented applies directly to charge sizes sufficiently large to ignore edge effects on the detonation wave.

The conditions for direct applicability are

$$1 - \frac{D}{D_{\infty}} < \delta$$

where $\delta = 0.01$ is sufficiently small for most applications.* In most applications the error introduced in ignoring edge effects is negligible. For precise predictions in situations where this criterion is not met provision must be made in the hydrodynamic model to account for the reaction zone behavior.

EXPERIMENTAL RESULTS

The experimental and calculational methods used to determine the equation of state have been described by Lee, et al,⁴ and much of the experimental data on HNS has been described previously.^{2,3} The discussion here will be primarily directed toward the estimation of the C-J pressures and detonation energies.

On the basis of P_{CJ} measurements on TNT we have reason to question Slape's² P_{CJ} results on HNS. The chemical energy and chemical composition of HNS and TNT are very similar. We have chosen to adjust the pressures for HNS upward to fall within the generally accepted range of values for TNT.

For similar materials such as HNS and TNT a good estimate of the ratio of their C-J pressures can be obtained from the quantity $K = \rho_0 D^2$. The values obtained for TNT are $D = 6.93 \text{ mm}/\mu\text{s}$ at $\rho_0 = 1.63 \text{ Mg}/\text{m}^3$ and for HNS $D = 7.03 \text{ mm}/\mu\text{s}$ at $\rho_0 = 1.65 \text{ Mg}/\text{m}^3$ giving a ratio of 1.04 for $K(\text{HNS})/K(\text{TNT})$. The average Chapman-Jouguet pressure for TNT computed from a list (see Table 4) of reported values adjusted to a density of 1.63 is 207 kbar (20.7 GPa). The resulting estimate of C-J pressure for HNS at $\rho_0 = 1.65$ is 215 kbar 21.5 GPa.

The pressures estimated for densities of 1.6, 1.4, 1.2, and 1.0 Mg/m^3 were obtained from a C-J pressure curve (determined by fitting the reported TNT C-J pressure values and maintaining the same shape as the more precise P_{CJ} versus density dependence for HMX). The results are shown in Figure 1.

For HNS the calculated heat of detonation ΔH_d based on H_2O as a gaseous detonation product is 5.69 MJ/kg. The value calculated for $\Delta H_d(\text{TNT})_{\text{calc}}$

* D_{∞} is the detonation velocity for infinite charge size.

is 5.40 MJ/kg. Since an experimental value (detonation calorimetry) is not available for HNS we have adjusted the experimental value for TNT⁵ ($\Delta H_d(\text{TNT})_{\text{exp}} = 4.27$) by the factor $\Delta H_d(\text{HNS})_{\text{calc}}/\Delta H_d(\text{TNT})_{\text{calc}}$ to provide an estimate for the experimental value for HNS, giving $\Delta H_d(\text{HNS})_{\text{exp}} = 4.5$ MJ/kg. In addition we have made a correction corresponding to the difference in results found in calorimetry experiments between high density and low density high explosive charges.⁶ The heat of detonation at a density of 1.00 Mg/m³ is thereby reduced 10 percent. The value at a density of 1.65 Mg/m³ is as calculated above. The values at intermediate densities were interpolated.

RESULTS

The Chapman-Jouguet parameters and the JWL coefficients are listed in Table 1. The results of the experiments and the hydrodynamic calculation for the cylinder test are given in Table 2. Values for pressure volume and energy for isentropic expansion of the detonation products are listed in Table 3. Equation of state descriptions for intermediate densities can be obtained by interpolation between the values for the JWL coefficients R_1 , R_2 , and W^* , and calculation of the necessary values for A, B, and C to satisfy the appropriate Chapman-Jouguet conditions.⁴ We have been successful in using the JWL equation of state in fitting the behavior of a large variety of explosives. The form of the JWL equation is:

$$P = A \left(1 - \frac{\omega}{R_1 V} \right) e^{-R_1 V} + B \left(1 - \frac{\omega}{R_2 V} \right) e^{-R_2 V} + \frac{\omega E}{V},$$

where A, B, R_1 , R_2 , and ω are constants, and V is the relative volume v/v_0 . The equation for P as a function of V at constant entropy is :

$$P_s = A e^{-R_1 V} + B e^{-R_2 V} + C V^{-(\omega+1)}$$

and the energy equation is:

$$E_s = \frac{A e^{-R_1 V}}{R_1} + \frac{B e^{-R_2 V}}{R_2} + \frac{C}{\omega V^{\omega}}.$$

* ω and W are equivalent.

Table 1. JWL Coefficients

A	1.627	2.631	3.665	4.606	4.631
B	0.1082	0.07224	0.06750	0.07262	0.08873
C	0.006580	0.00945	0.01163	0.01338	0.01349
R ₁	5.4	5.0	4.8	4.60	4.55
R ₂	1.8	1.5	1.40	1.30	1.35
W	0.25	0.30	0.32	0.35	0.35
C-J PARAMETERS					
*P _{CJ}	0.075	0.105	.145	0.200	0.215 Mbar
Density	1.00	1.20	1.40	1.60	1.65 Mg/m ³
D	5.10	5.74	6.34	6.95	7.03 mm/μs
*E _o	0.041	0.050	.060	0.071	0.0745 Mbcc/cc
Γ	2.468	2.765	2.881	2.864	2.804

*Systeme International Equivalence

1.0 Mb = 100 GPa
 1.0 Kb = 100 MPa
 1.0 Mbcc = 10⁻⁴ GPa · m³ = 10⁻⁴ GJ = 100 MJ
 1.0 Mbcc/cc = 100 GPa · Mg/m³ = 100 GPa

Table 2.1 Calculated and Experimental Cylinder Test Results
HNS Density = 1.60 Mg/m³

R-RO cm	TEXP μ s	TCALC	DT	VEXP cm/ μ s	VCALC	DV
0.00	0.00			0.0000		
0.05	0.79	1.0068	-0.2168	0.0579	0.0588	-0.0009
0.10	1.65	1.7154	-0.0554	0.	0.0817	0.
0.15	2.30	2.3111	-0.0111	0.	0.0871	0.
0.20	2.80	2.8545	-0.0545	0.	0.0967	0.
0.25	3.31	3.3587	-0.0487	0.	0.1002	0.
0.30	3.88	3.8473	0.0327	0.	0.1061	0.
0.35	4.39	4.3094	0.0806	0.	0.1092	0.
0.40	4.76	4.7641	-0.0041	0.1122	0.1115	0.0007
0.50	5.64	5.6334	0.0066	0.1169	0.1165	0.0004
0.60	6.47	6.4716	-0.0016	0.1207	0.1213	-0.0006
0.70	7.30	7.2869	0.0131	0.1239	0.1250	-0.0011
0.80	8.10	8.0833	0.0167	0.1266	0.1271	-0.0005
0.90	8.88	8.8642	0.0158	0.1289	0.1288	0.0001
1.00	9.65	9.6330	0.0170	0.1309	0.1306	0.0003
1.10	10.41	10.3921	0.0179	0.1377	0.1324	0.0003
1.20	11.16	11.1432	0.0168	0.1342	0.1340	0.0002
1.30	11.90	11.8871	0.0129	0.1355	0.1352	0.0003
1.40	12.63	12.6245	0.0055	0.1367	0.1362	0.0005
1.50	13.36	13.3562	0.0038	0.1377	0.1371	0.0006
1.60	14.08	14.0828	-0.0028	0.1387	0.1380	0.0007
1.70	14.81	14.8048	0.0052	0.1395	0.1388	0.0007
1.80	15.51	15.5226	-0.0126	0.1402	0.1396	0.0006
1.90	16.23	16.2366	-0.0066	0.1408	0.1404	0.0004
2.00	16.94	16.9470	-0.0070	0.1414	0.1411	0.0003
2.20	18.35	18.3581	-0.0081	0.1423	0.1423	-0.0000
2.40	19.76	19.7579	0.0021	0.1431	0.1434	-0.0003
2.60	0.	21.1476	0.	0.	0.1444	0.
2.80	0.	22.5285	0.	0.	0.1453	0.
3.00	0.	23.9017	0.	0.	0.1460	0.
3.20	0.	0.	0.	0.	0.	0.

Table 2.2

HNS Density = 1.2 Mg/m³

R-R0 cm	TEXP μ s	TCALC	DT	VEXP cm/ μ s	VCALC	DV
0.00				0.0000		
0.05	1.31	1.2956	0.0144	0.0383	0.0468	-0.0085
0.10	2.26	2.2227	0.0373	0.	0.0592	0.
0.15	3.02	3.0024	0.0176	0.	0.0683	0.
0.20	3.72	3.7077	0.0123	0.	0.0737	0.
0.25	4.37	4.3595	0.0105	0.	0.0786	0.
0.30	4.98	4.9810	-0.0010	0.	0.0828	0.
0.35	5.56	5.5737	-0.0137	0.	0.0855	0.
0.40	6.15	6.1484	0.0016	0.0891	0.0887	0.0004
0.50	7.24	7.2502	-0.0102	0.0937	0.0932	0.0005
0.60	8.29	8.3071	-0.0171	0.0971	0.0965	0.0006
0.70	9.31	9.3316	-0.0216	0.0997	0.0991	0.0006
0.80	10.30	10.3313	-0.0313	0.1017	0.1012	0.0005
0.90	11.27	11.3116	-0.0416	0.1033	0.1030	0.0003
1.00	12.24	12.2761	-0.0361	0.1046	0.1045	0.0001
1.10	13.19	13.2275	-0.0375	0.1057	0.1058	-0.0001
1.20	14.13	14.1676	-0.0376	0.1067	0.1070	-0.0003
1.30	15.06	15.0978	-0.0378	0.1077	0.1080	-0.0003
1.40	15.99	16.0195	-0.0295	0.1086	0.1090	-0.0004
1.50	16.90	16.9334	-0.0334	0.1094	0.1099	-0.0005
1.60	17.81	17.8403	-0.0303	0.1103	0.1107	-0.0004
1.70	18.72	18.7408	-0.0208	0.1111	0.1114	-0.0003
1.80	19.61	19.6355	-0.0255	0.1115	0.1121	-0.0002
1.90	20.51	20.5249	-0.0149	0.1125	0.1128	-0.0003
2.00	21.39	21.4094	-0.0194	0.1131	0.1134	-0.0003
2.20	23.15	23.1649	-0.0149	0.1141	0.1145	-0.0004
2.40	24.90	0.	0.	0.1150	0.	0.
2.60	0.	0.	0.	0.	0.	0.
2.80	0.	0.	0.	0.	0.	0.
3.00	0.	0.	0.	0.	0.	0.
3.20	0.	0.	0.	0.	0.	0.

Table 3.1 C-J Isentropic Pressures, Volumes and Energies
HNS Charge Density = 1.65 Mg/m³

V/Vo	* P Mb	* E Mbcc/cc	Γ
0.600	3.684E-01	1.417E-01	2.4235
0.737	2.150E-01	1.028E-01	2.8043
0.800	1.699E-01	9.072E-02	2.9403
1.000	8.543E-02	6.634E-02	3.1830
1.100	6.301E-02	5.900E-02	3.1941
1.200	4.781E-02	5.350E-02	3.1426
1.300	3.731E-02	4.928E-02	3.0457
1.400	2.990E-02	4.594E-02	2.9233
1.500	2.455E-02	4.323E-02	2.7940
1.600	2.058E-02	4.098E-02	2.6723
1.600	1.520E-02	3.745E-02	2.4833
2.000	1.177E-02	3.478E-02	2.3742
2.250	8.936E-03	3.221E-02	2.3185
2.500	7.006E-03	3.023E-02	2.3037
2.750	5.627E-03	2.866E-02	2.2934
3.000	4.613E-03	2.739E-02	2.2694
3.500	3.274E-03	2.545E-02	2.1639
4.000	2.477E-03	2.403E-02	2.0056
5.000	1.640E-03	2.202E-02	1.6921
6.000	1.228E-03	2.061E-02	1.4980
7.000	9.824E-04	1.951E-02	1.4076
8.000	8.164E-04	1.862E-02	1.3710
9.000	6.953E-04	1.787E-02	1.3573
10.000	6.028E-04	1.722E-02	1.3525
12.000	4.712E-04	1.615E-02	1.3503
15.000	3.486E-04	1.494E-02	1.3500

* See footnote, Table 1, page 4.

Table 3.2

HNS Charge Density = 1.60 Mg/m³

V/Vo	* P Mb	* E Mbcc/cc	Γ
0.600	3.515E-01	1.347E-01	2.4654
0.741	2.00E-01	9.688E-02	2.8642
0.800	1.599E-01	8.635E-02	2.9927
1.000	7.947E-02	6.353E-02	3.23000
1.100	5.837E-02	5.671E-02	3.2312
1.200	4.418E-02	5.163E-02	3.1641
1.300	3.444E-02	4.773E-02	3.0480
1.400	2.762E-02	4.464E-02	2.9053
1.500	2.272E-02	4.214E-02	2.7569
1.600	1.910E-02	4.006E-02	2.6188
1.800	1.422E-02	3.677E-02	2.4063
2.000	1.111E-02	3.426E-02	2.2857
2.250	8.524E-03	3.182E-02	2.2257
2.500	6.748E-03	2.993E-02	2.2131
2.750	5.465E-03	2.841E-02	2.2088
3.000	4.512E-03	2.717E-02	2.1937
3.500	3.235E-03	2.526E-02	2.1113
4.000	2.461E-03	2.385E-02	1.9772
5.000	1.633E-03	2.186E-02	1.6943
6.000	1.221E-03	2.045E-02	1.5071
7.000	9.758E-04	1.936E-02	1.4144
8.000	8.103E-04	1.847E-02	1.3747
9.000	6.899E-04	1.772E-02	1.3590
10.000	5.981E-04	1.700E-02	1.3532
12.000	4.675E-04	1.603E-02	1.3504
15.000	3.459E-04	1.482E-02	1.3500

* See footnote, Table 1, page 4.

Table 3.3

HNS Charge Density = 1.4 Mg/m³

V/Vo	* P Mb	* E Mbcc/cc	Γ
0.600	2.577E-01	1.065E-01	2.5111
0.742	1.450E-01	7.868E-02	2.8810
0.800	1.164E-01	7.118E-02	2.9873
1.000	5.844E-02	5.452E-02	3.1385
1.100	4.339E-02	4.948E-02	3.0968
1.200	3.327E-02	4.568E-02	2.9972
1.300	2.631E-02	4.272E-02	2.8642
1.400	2.139E-02	4.035E-02	2.7208
1.500	1.781E-02	3.840E-02	2.5851
1.600	1.513E-02	3.676E-02	2.4684
1.800	1.143E-02	3.413E-02	2.3051
2.000	9.012E-03	3.210E-02	2.2222
2.250	6.955E-03	3.012E-02	2.1830
2.500	5.531E-03	2.857E-02	2.1669
2.750	4.503E-03	2.732E-02	2.1445
3.000	3.742E-03	2.630E-02	2.1062
3.500	2.728E-03	2.470E-02	1.9808
4.000	2.116E-03	2.350E-02	1.8251
5.000	1.451E-03	2.176E-02	1.5605
6.000	1.108E-03	2.050E-02	1.4170
7.000	8.952E-04	1.950E-02	1.3555
8.000	7.483E-04	1.869E-02	1.3322
9.000	6.400E-04	1.795E-02	1.3240
10.000	5.568E-04	1.740E-02	1.3213
12.000	4.376E-04	1.641E-02	1.3201
15.000	3.260E-04	1.528E-02	1.3200

* See footnote, Table 1, page 4.

Table 3.4

HNS Charge Density = 1.2 Mg/m³

V/Vo	* P Mb	* E Mbcc/cc	Γ
0.600	1.787E-01	8.250E-02	2.4802
0.734	1.050E-01	6.394E-02	2.7654
0.800	8.257E-02	5.783E-02	2.8491
1.000	4.330E-02	4.580E-02	2.8892
1.100	3.297E-02	4.202E-02	2.8165
1.200	2.592E-02	3.909E-02	2.7127
1.300	2.095E-02	3.676E-02	2.6003
1.400	1.735E-02	3.486E-02	2.4961
1.500	1.465E-02	3.326E-02	2.4096
1.600	1.257E-02	3.191E-02	2.3442
1.800	9.582E-03	2.971E-02	2.2703
2.000	7.555E-03	2.801E-02	2.2469
2.250	5.800E-03	2.636E-02	2.2431
2.500	4.581E-03	2.507E-02	2.2327
2.750	3.708E-03	2.404E-02	2.1991
3.000	3.069E-03	2.319E-02	2.1403
3.500	2.234E-03	2.189E-02	1.9709
4.000	1.738E-03	2.091E-02	1.7843
5.000	1.206E-03	1.947E-02	1.5054
6.000	9.292E-04	1.841E-02	1.3739
7.000	7.551E-04	1.757E-02	1.3242
8.000	6.336E-04	1.688E-02	1.3075
9.000	5.433E-04	1.630E-02	1.3022
10.000	4.737E-04	1.579E-02	1.3006
12.000	3.737E-04	1.496E-02	1.3000
15.000	2.796E-04	1.398E-02	1.3000

* See footnote, Table 1, page 4.

Table 3.5

HNS Charge Density = 1.0 Mg/m³

V/Vo	* P Mb	* E Mbcc/cc	Γ
0.600	1.129E-01	6.212E-02	2.3175
0.712	7.500E-02	5.181E-02	2.4680
0.800	5.598E-02	4.608E-02	2.5239
1.000	3.182E-02	3.762E-02	2.5178
1.100	2.507E-02	3.479E-02	2.4865
1.200	2.022E-02	3.254E-02	2.4575
1.300	1.662E-02	3.071E-02	2.4387
1.400	1.388E-02	2.919E-02	2.4324
1.500	1.173E-02	2.791E-02	2.4374
1.600	1.002E-02	2.683E-02	2.4506
1.800	7.492E-03	2.509E-02	2.4863
2.000	5.757E-03	2.378E-02	2.5122
2.250	4.282E-03	2.254E-02	2.5049
2.500	3.298E-03	2.160E-02	2.4433
2.750	2.625E-03	2.086E-02	2.3335
3.000	2.155E-03	2.027E-02	2.1922
3.500	1.573E-02	1.935E-02	1.8881
4.000	1.244E-03	1.865E-02	1.6365
5.000	8.934E-04	1.761E-02	1.3659
6.000	7.029E-04	1.682E-02	1.2000
7.000	5.782E-04	1.618E-02	1.2572
8.000	4.891E-04	1.565E-02	1.2516
9.000	4.221E-04	1.519E-02	1.2504
10.000	3.700E-04	1.480E-02	1.2501
12.000	2.946E-04	1.414E-02	1.2500
15.000	2.229E-04	1.337E-02	1.2500

* See footnote, Table 1, page 4.

Table 4a. C-J Pressure for TNT Density of 1.63 Mg/m³

Density (ρ) Mg/m ³	Pressure kb*	Pressure kb* Adjusted to ρ 1.63	Reference
1.636	188.4	186	W. Deal J. Chem Phys <u>27</u> , 796 (1957)
1.614	189	195	Coleburn & Liddiard J. Chem Phys 1029, <u>44</u> (1966)
1.62	210	213	Ilyukhin, Pakhil et al. Doklady <u>131</u> 793 (1960)
1.622	187.2	190	Coleburn NOLTR 64-58 (1964)
1.62	212	215	Y. Apin & Voskoboynikov Pratl. Mekhan i Tekh. Fig <u>4</u> 54 (1960)
1.632	213		R. Jameson BRL Private Communication
1.630	220		R. Crain Private Communication
1.63	225		R. Craig 10th Comb. Symp. (1965)

Table 4b. Density Dependence

Density (ρ) Mg/m ³	Pressure kb*	Reference
1.44	178	W. Davis, B. Craig & J. Ramsey 4th Det. Symposium
1.08	115	
.95	62.2	Vevetennikov, Dremine, Shvedov Fiz. Goreniya i Vstryva No. 3, 3 (1965)
1.00	76.3	
1.00	78.5	
1.59	179	
1.00	64	Dremine, Zaitzev, Ilyukhin, Pokhil 8th Comb. Symp. 1960, 610 (1962)
1.14	94	
1.30	123	
1.45	162	
1.59	202	

* See footnote, Table 1, page 4.

Figure 1. Detonation Pressures for HNS

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