Fernando G. Bastante [1] , *María Araújo Fernández* [1] , *Eduardo Giráldez* [1] .
CINTECX, GESSMin group, University of Vigo

PREDICTIVE MODEL FOR EXPLOSIVE DETONATION PARAMETERS FROM AN EQUATION OF STATE BASED ON DETONATION VELOCITY. Physical Chemistry Chemical Physics 2022

DEoS DATABASE

Average values	
Q_DEoS (cal/g)	1160
w (m/s per kg/m³)	3.37
Do (m/s)	2215
C (m/s per cal/g)	1.0

$$w = \left(\frac{\partial D}{\partial \rho_o}\right)_Q \qquad C = \left(\frac{\partial D}{\partial Q}\right)_{\rho_o}$$

EXPLOSIVES ***238*** *CHNO Composition (mol/100g)* *Other elements (% weight X)* *hierarchy* *[Cl+F+P+Si] as inerts*

Acronym	Name	ΔH°_{298} (cal/g)	reference	C	H	N	O	X: {Cl+F+P+Si}	Comp.	type (Xiong)	C (s)	H2O (g)	CO2 (g)	N2 (g)	H2 (g)	O2 (g)	Q_DEoS (cal/g)	Q_{KJ} (cal/g)	Phi (KJ)	Do (DEoS)	w (DEoS)	C (DEoS)
abh	azobis(2,2′,4,4′,6,6′-hexanitrobiphenyl)	133	[8]	2.745	0.686	1.601	2.745	0.0	CHNO	3.0	1.544	0.343	1.201	0.801	0.000	0.000	1306	1460	5.28	2368	2.9	0.9
AFX902	AFX902	-299	[c]	1.046	3.745	3.651	1.826	3.3	CHNOX		1.046	1.826	0.000	1.826	0.047	0.000	652	756		1672	3.7	1.3
bchmx	cis-1,3,4,6-tetranitrooctahydroimidazo-[4,5-d]imidazole	192	[3]	1.360	2.040	2.720	2.720	0.0	CHNO	2.0	0.510	1.020	0.850	1.360	0.000	0.000	1530	1581	6.92	2563	3.4	0.8
BCHMX/GAP (84/16)	BCHMX/GAP (84/16)	335	[4]	1.671	2.669	2.706	2.459	0.0	CHNO	3.0	1.109	1.334	0.562	1.353	0.000	0.000	1525	1635	6.79	2558	3.4	0.8
BCHMX/PIB (91/9)	BCHMX/PIB (91/9)	148	[c]	1.827	2.976	2.475	2.525	0.0	CHNO	3.0	1.308	1.488	0.518	1.238	0.000	0.000	1365	1496	6.39	2420	3.4	0.9
BCHMX/SYLGARD (85/15)	BCHMX/SYLGARD (85/15)	-97	[3]	1.549	2.883	2.346	2.502	5.6	CHNOX		1.018	1.442	0.530	1.173	0.000	0.000	1133	1235		2205	3.4	1.0
BCHMX/VITON (95/5)	BCHMX/VITON (95/5)	94	[c]	1.426	2.031	2.584	2.584	3.3	CHNOX		0.641	1.016	0.784	1.292	0.000	0.000	1354	1418		2411	3.4	0.9
BCHMX/VITON (97/3)	BCHMX/VITON (97/3)	133	[c]	1.399	2.035	2.638	2.638	2.0	CHNOX		0.589	1.017	0.810	1.319	0.000	0.000	1424	1483		2473	3.4	0.9
btf	benzotris[1,2,5]oxadiazole-1,4,7-trioxide	551	[47]	2.380	0.000	2.380	2.380	0.0	CNO	3.0	1.190	0.000	1.190	1.190	0.000	0.000	1551	1670	5.84	2580	3.2	0.8
btnen	bis(2,2,2-trinitroethyl) nitramine	-17	[48]	1.031	1.031	2.061	3.607	0.0	CHNO	1.0	0.000	0.515	1.031	1.031	0.000	0.515	1250	1250	6.22	2317	3.2	0.9
BTNEN/BTF (60/40)	BTNEN/BTF (60/40)	210	[c]	1.570	0.618	2.189	3.116	0.0	CHNO	2.0	0.167	0.309	1.404	1.094	0.000	0.000	1692	1709	6.86	2695	3.2	0.8
BTNEN/HMX (30/70)	BTNEN/HMX (30/70)	37	[c]	1.255	2.200	2.509	2.973	0.0	CHNO	2.0	0.318	1.100	0.936	1.255	0.000	0.000	1522	1554	7.01	2556	3.4	0.8
BTNEN/HMX (32/68)	BTNEN/HMX (32/68)	36	[c]	1.248	2.167	2.496	2.991	0.0	CHNO	2.0	0.294	1.083	0.954	1.248	0.000	0.000	1530	1559	7.03	2562	3.4	0.8
BTNEN/RDX (56/44)	BTNEN/RDX (56/44)	20	[c]	1.171	1.766	2.343	3.209	0.0	CHNO	2.0	0.009	0.883	1.163	1.171	0.000	0.000	1623	1624	7.22	2639	3.4	0.8
btneu	bis(trinitroethyl) urea	-199	[48]	1.295	1.554	2.072	3.367	0.0	CHNO	1.0	0.000	0.777	1.295	1.036	0.000	0.000	1468	1468	6.75	2510	3.3	0.9
bttc	bis-(2,2,2-trinitroethyl)-carbonate	-388	[48]	1.288	1.031	1.546	3.865	0.0	CHNO	1.0	0.000	0.515	1.288	0.773	0.000	0.386	1122	1122	5.77	2194	3.1	1.0
cl-20	hexanitrohexaazaisowurtzitane	448	[4]	1.369	1.369	2.739	2.739	0.0	CHNO	2.0	0.342	0.685	1.027	1.369	0.000	0.000	1776	1810	7.31	2761	3.4	0.8
CL20/GAP (84/16)	CL20/GAP (84/16)	320	[4]	1.675	2.092	2.691	2.505	0.0	CHNO	3.0	0.946	1.046	0.729	1.346	0.000	0.000	1516	1611	6.68	2551	3.4	0.8
CL-20/HTPB (91/9)	CL-20/HTPB (91/9)	407	[c]	1.890	2.258	2.500	2.500	0.0	CHNO	3.0	1.205	1.129	0.685	1.250	0.000	0.000	1584	1705	6.68	2608	3.3	0.8
CL-20/HTPB (92/8)	CL-20/HTPB (92/8)	412	[c]	1.832	2.159	2.527	2.526	0.0	CHNO	3.0	1.109	1.080	0.723	1.263	0.000	0.000	1605	1716	6.75	2625	3.3	0.8
CL-20/PIB (91/9)	CL-20/PIB (91/9)	381	[c]	1.835	2.366	2.492	2.542	0.0	CHNO	3.0	1.156	1.183	0.679	1.246	0.000	0.000	1588	1704	6.75	2611	3.3	0.8
CL20/SYLGARD (85/15)	CL20/SYLGARD (85/15)	-46	[3]	1.545	2.298	2.365	2.540	5.4	CHNOX		0.849	1.149	0.696	1.182	0.000	0.000	1187	1272		2257	3.4	1.0
COMP B	COMP B	10	[c]	2.032	2.637	2.177	2.653	0.0	CHNO	3.0	1.364	1.318	0.667	1.089	0.000	0.000	1263	1399	6.00	2328	3.3	0.9
COMP C3	composition c3 (as single)	-14	[8][10]average	1.899	2.829	2.339	2.599	0.0	CHNO	3.0	1.307	1.414	0.592	1.169	0.000	0.000	1230	1361	6.04	2298	3.3	0.9
COMP C4	COMP C4	33	[c]	1.818	3.578	2.458	2.508	0.0	CHNO	3.0	1.459	1.789	0.359	1.229	0.000	0.000	1260	1405	6.26	2325	3.4	0.9
daaf	3,3′-diamino-4,4′-azoxyfurazan	500	[35]	1.886	1.886	3.771	1.414	0.0	CHNO	3.0	1.650	0.943	0.236	1.886	0.000	0.000	1101	1266	5.58	2174	3.4	1.0
DAAF/HMX/VITON (45/50/5)	DAAF/HMX/VITON (45/50/5)	166	[c]	1.658	2.293	3.048	1.987	3.3	CHNOX		1.237	1.146	0.420	1.524	0.000	0.000	1100	1224		2173	3.4	1.0
DAAF/HMX/VITON (60/35/5)	DAAF/HMX/VITON (60/35/5)	232	[c]	1.738	2.170	3.208	1.794	3.3	CHNOX		1.383	1.085	0.354	1.604	0.000	0.000	1054	1193		2127	3.4	1.0
DAAF/HMX/VITON (80/15/5)	DAAF/HMX/VITON (80/15/5)	320	[c]	1.845	2.007	3.422	1.537	3.3	CHNOX		1.578	1.004	0.266	1.711	0.000	0.000	993	1151		2064	3.4	1.0
DAAF/RDX/VITON (60/35/5)	DAAF/RDX/VITON (60/35/5)	234	[c]	1.738	2.170	3.208	1.794	3.3	CHNOX		1.383	1.085	0.354	1.604	0.000	0.000	1056	1195		2129	3.4	1.0
DAAF/RDX/VITON (80/15/5)	DAAF/RDX/VITON (80/15/5)	321	[c]	1.845	2.007	3.422	1.537	3.3	CHNOX		1.578	1.004	0.266	1.711	0.000	0.000	994	1151		2065	3.4	1.0
DAAF/VITON (95/5)	DAAF/VITON (95/5)	386	[c]	1.925	1.885	3.583	1.344	3.3	CHNOX		1.724	0.942	0.201	1.791	0.000	0.000	947	1119		2016	3.4	1.1
datb	1,3-diamino-2,4,6-trinitrobenzene	-120	[8]	2.468	2.056	2.056	2.468	0.0	CHNO	3.0	1.748	1.028	0.720	1.028	0.000	0.000	976	1151	5.02	2047	3.1	1.0
degn	diethyleneglycol dinitrate	-507	[8]	2.040	4.079	1.020	3.569	0.0	CHNO	3.0	1.275	2.040	0.765	0.510	0.000	0.000	1264	1391	6.25	2329	3.3	0.9
dina	di(2-nitroxyethyl)-nitramine	-314	[8]	1.666	3.332	1.666	3.332	0.0	CHNO	3.0	0.833	1.666	0.833	0.833	0.000	0.000	1349	1432	6.55	2406	3.4	0.9
dipam	(2.2′,4,4′,6,6′-hexanitro-[1,1-biphenyl]-3,3′-diamine)	-44	[8]	2.642	1.321	1.761	2.642	0.0	CHNO	3.0	1.651	0.660	0.991	0.881	0.000	0.000	1104	1269	5.08	2177	3.0	1.0
dipetn	dipentaerythritol hexanitrate	-446	[8]	1.907	3.052	1.144	3.624	0.0	CHNO	2.0	0.858	1.526	1.049	0.572	0.000	0.000	1337	1423	6.34	2395	3.2	0.9
dipicrylamine	hexanitrodiphenylamine	23	[48]	2.732	1.138	1.594	2.732	0.0	CHNO	3.0	1.651	0.569	1.081	0.797	0.000	0.000	1204	1369	5.18	2273	2.9	0.9
dmtnb	dinitrophenoxyethylnitrate	-243	[48]	2.929	2.563	1.098	2.929	0.0	CHNO	3.0	2.105	1.281	0.824	0.549	0.000	0.000	1062	1272	5.02	2135	3.0	1.0
dmttp	ethyl picrate	-187	[48]	3.111	2.722	1.167	2.722	0.0	CHNO	3.0	2.430	1.361	0.681	0.583	0.000	0.000	997	1240	4.80	2069	2.9	1.0
dnaf	dinitrodiazenofuroxan	554	[47]	1.388	0.000	2.777	2.777	0.0	CNO	1.0	0.000	0.000	1.388	1.388	0.000	0.000	1860	1860	7.19	2825	3.5	0.8
DNAN/RDX/NTO (40/20/40)	DNAN/RDX/NTO (40/20/40)	-163	[c]	2.298	2.367	2.174	2.472	0.0	CHNO	3.0	1.654	1.183	0.644	1.087	0.000	0.000	962	1127	5.13	2032	3.2	1.1
dnb	dinitrobenzol	-37	[8]	3.569	2.379	1.190	2.379	0.0	CHNO	3.0	2.974	1.190	0.595	0.595	0.000	0.000	913	1210	4.30	1979	2.8	1.1
dndmo	n,n′-dinitro-n,n′- dimethyloxamide	-355	[48]	1.941	2.911	1.941	2.911	0.0	CHNO	3.0	1.213	1.455	0.728	0.970	0.000	0.000	1050	1171	5.62	2123	3.3	1.0
dnff	3,4-bis(4-nitrofurazan-3-yl)furoxan	503	[35]	1.922	0.000	2.563	2.563	0.0	CNO	2.0	0.641	0.000	1.282	1.282	0.000	0.000	1644	1708	6.36	2657	3.3	0.8
dnmt	1-methyl-3,5-dinitro-1,2,4-triazole	253	[35]	1.733	1.733	2.889	2.311	0.0	CHNO	3.0	1.011	0.867	0.722	1.444	0.000	0.000	1332	1433	6.18	2391	3.3	0.9
DNMT/HMX (49.5/50.5)	DNMT/HMX (49.5/50.5)	156	[c]	1.540	2.222	2.794	2.508	0.0	CHNO	3.0	0.842	1.111	0.699	1.397	0.000	0.000	1371	1455	6.48	2425	3.4	0.9
dnp	3,4-dinitropyrazole	182	[35]	1.898	1.265	2.530	2.530	0.0	CHNO	3.0	0.949	0.633	0.949	1.265	0.000	0.000	1345	1440	6.03	2403	3.2	0.9
dnq	dinitroguanidine	0	[47]	0.671	2.013	3.354	2.683	0.0	CHNO	1.0	0.000	1.006	0.671	1.677	0.000	0.168	1213	1213	6.53	2281	3.6	0.9
dntfx	dinitrofuroxanyl	389	[56]	1.538	0.000	2.307	3.076	0.0	CNO	1.0	0.000	0.000	1.538	1.153	0.000	0.000	1835	1835	7.03	2807	3.4	0.8
dp12	dp12	-228	[8]	1.428	2.856	0.952	1.904	36.2	CHNOX		1.190	1.428	0.238	0.476	0.000	0.000	702	821		1735	3.3	1.2
edad	ethylenediamine dinitrate	-837	[48]	1.075	5.373	2.149	3.224	0.0	CHNO	3.0	0.806	2.686	0.269	1.075	0.000	0.000	888	968	5.94	1952	3.7	1.1
EDC-11	EDC-11	18	[c]	1.887	2.546	2.273	2.683	0.0	CHNO	3.0	1.183	1.273	0.705	1.137	0.000	0.000	1298	1416	6.15	2360	3.3	0.9
EDC-24	EDC-24	40	[c]	1.640	3.279	2.566	2.566	0.0	CHNO	3.0	1.176	1.640	0.463	1.283	0.000	0.000	1305	1423	6.43	2367	3.4	0.9
edna	ethylene dinitramine	-165	[8]	1.332	3.997	2.665	2.665	0.0	CHNO	3.0	0.999	1.999	0.333	1.332	0.000	0.000	1204	1304	6.48	2273	3.6	0.9
etdn	ethylene glycol dinitrate	-383	[8]	1.315	2.630	1.315	3.946	0.0	CHNO	1.0	0.000	1.315	1.315	0.658	0.000	0.000	1614	1614	7.29	2632	3.3	0.8
etn	erythritol tetranitrate	-376	[12]	1.324	1.986	1.324	3.972	0.0	CHNO	1.0	0.000	0.993	1.324	0.662	0.000	0.166	1443	1443	6.74	2489	3.2	0.9
explosive d	ammonium picrate	-382	[8]	2.438	2.438	1.625	2.844	0.0	CHNO	3.0	1.625	1.219	0.813	0.813	0.000	0.000	924	1087	4.99	1992	3.1	1.1
fefo	1,1 [methylenebis (oxy)]bis [2-fluoro-2,2-dinitroethane]	-555	[8]	1.562	1.874	1.250	3.124	11.9	CHNOX		0.469	0.937	1.093	0.625	0.000	0.000	969	1015		2039	3.2	1.1
FM1	FM1	-505	[c]	1.907	2.872	1.266	3.164	5.9	CHNOX		1.043	1.436	0.864	0.633	0.000	0.000	1033	1137		2106	3.2	1.0
fox-12	guanylurea dinitramide	-406	[20]	0.956	3.347	3.347	2.391	0.0	CHNO	3.0	0.598	1.674	0.359	1.674	0.000	0.000	838	898	5.56	1897	3.7	1.1
fox-7	diaminodinitroethylene	-216	[35]	1.351	2.701	2.701	2.701	0.0	CHNO	3.0	0.675	1.351	0.675	1.351	0.000	0.000	1132	1200	6.10	2204	3.5	1.0
FOX-7/EVA (95.1/4.9)	FOX-7/EVA (95.1/4.9)	-202	[c]	1.581	3.113	2.569	2.618	0.0	CHNO	3.0	1.050	1.556	0.531	1.284	0.000	0.000	1092	1197	5.94	2164	3.4	1.0
FOX-7/EVA (95/5)	FOX-7/EVA (95/5)	-202	[c]	1.586	3.121	2.566	2.617	0.0	CHNO	3.0	1.058	1.560	0.528	1.283	0.000	0.000	1091	1196	5.93	2164	3.4	1.0
FOX-7/TNT (30/70)	FOX-7/TNT (30/70)	-120	[c]	2.563	2.351	1.735	2.660	0.0	CHNO	3.0	1.821	1.176	0.742	0.867	0.000	0.000	1076	1258	5.23	2149	3.1	1.0
FOX-7/TNT (60/40)	FOX-7/TNT (60/40)	-161	[c]	2.043	2.501	2.149	2.677	0.0	CHNO	3.0	1.330	1.251	0.713	1.075	0.000	0.000	1100	1233	5.61	2173	3.3	1.0
FOX-7/VITON (95/5)	FOX-7/VITON (95/5)	-294	[c]	1.417	2.660	2.566	2.566	3.3	CHNOX		0.799	1.330	0.618	1.283	0.000	0.000	976	1056		2047	3.5	1.0
FOX-7/WAX (98.5/1.5)	FOX-7/WAX (98.5/1.5)	-215	[c]	1.437	2.875	2.661	2.661	0.0	CHNO	3.0	0.826	1.437	0.612	1.330	0.000	0.000	1109	1191	6.02	2181	3.5	1.0
H2O2/H2O (90,5/9,5)	H2O2/H2O (90,5/9,5)	-1573	[c]	0.000	6.376	0.000	5.849	0.0	HO	1.0	0.000	3.188	0.000	0.000	0.000	1.330	270	270	3.49	1076	3.3	2.0
ha	hydrazinium azide	533	[57]	0.000	6.660	6.660	0.000	0.0	HN	4.0	0.000	0.000	0.000	3.330	3.330	0.000	533	533	5.96	1512	5.2	1.4
hac	hydrazoic acid	1497	[57]	0.000	2.324	6.972	0.000	0.0	HN	4.0	0.000	0.000	0.000	3.486	1.162	0.000	1497	1497	8.34	2535	4.4	0.8
HAC/W (60/40)	HAC/W (60/40)	-619	[c]	0.000	5.835	4.183	2.220	0.0	HNO	5.0	0.000	2.220	0.000	2.092	0.697	0.000	665	665	5.77	1689	4.3	1.3
HAC/W (62/38)	HAC/W (62/38)	-513	[c]	0.000	5.660	4.323	2.109	0.0	HNO	5.0	0.000	2.109	0.000	2.161	0.720	0.000	706	706	5.94	1741	4.3	1.2

Fernando G. Bastante [1] , *María Araújo Fernández* [1] , *Eduardo Giráldez* [1] .
CINTECX, GESSMin group, University of Vigo

PREDICTIVE MODEL FOR EXPLOSIVE DETONATION PARAMETERS FROM AN EQUATION OF STATE BASED ON DETONATION VELOCITY. Physical Chemistry Chemical Physics 2022

DEoS DATABASE

	Average values
Q_DEoS (cal/g)	1160
w (m/s per kg/m^3)	3.37
Do (m/s)	2215
C (m/s per cal/g)	1.0

$$w = \left(\frac{\partial D}{\partial \rho_o}\right)_Q \qquad C = \left(\frac{\partial D}{\partial Q}\right)_{\rho_o}$$

EXPLOSIVES ***238*** *CHNO Composition (mol/100g)* *Other elements (% weight X)* *hierarchy* *[Cl+F+P+Si] as inerts*

Acronym	Name	ΔH°_{298} (cal/g)	reference	C	H	N	O	X: {Cl+F+P+Si}	Comp.	type (Xiong)	C (s)	H2O (g)	CO2 (g)	N2 (g)	H2 (g)	O2 (g)	Q_DEoS (cal/g)	Q_{KJ} (cal/g)	Phi (KJ)	Do (DEoS)	w (DEoS)	C (DEoS)
HAC/W (69/31)	HAC/W (69/31)	-164	[c]	0.000	5.080	4.783	1.743	0.0	HNO	5.0	0.000	1.743	0.000	2.391	0.797	0.000	843	843	6.45	1903	4.3	1.1
HAC/W (78/26)	HAC/W (78/26)	354	[c]	0.000	4.220	5.466	1.199	0.0	HNO	5.0	0.000	1.199	0.000	2.733	0.911	0.000	1047	1047	7.12	2120	4.4	1.0
HAC/W (88/12)	HAC/W (88/12)	873	[c]	0.000	3.360	6.149	0.655	0.0	HNO	5.0	0.000	0.655	0.000	3.075	1.025	0.000	1251	1251	7.71	2317	4.4	0.9
HAC/W (93/7)	HAC/W (93/7)	1132	[c]	0.000	2.930	6.491	0.383	0.0	HNO	5.0	0.000	0.383	0.000	3.246	1.082	0.000	1353	1353	7.98	2410	4.4	0.9
HAC/W (98/2)	HAC/W (98/2)	1407	[c]	0.000	2.473	6.854	0.094	0.0	HNO	5.0	0.000	0.094	0.000	3.427	1.142	0.000	1461	1461	8.26	2504	4.4	0.9
hco	1,3,3,5,7,7-hexanitro-1,5-diazacyclooctane	-17	[33]	1.562	2.082	2.082	3.124	0.0	CHNO	2.0	0.521	1.041	1.041	1.041	0.000	0.000	1512	1564	6.77	2547	3.3	0.8
hmx	cyclotetramethylenetetranitramine	61	[8]	1.351	2.701	2.701	2.701	0.0	CHNO	3.0	0.675	1.351	0.675	1.351	0.000	0.000	1409	1476	6.77	2459	3.5	0.9
HMX/EXON (91/9)	HMX/EXON (91/9)	-31	[c]	1.448	2.648	2.446	2.446	6.6	CHNOX		0.887	1.324	0.561	1.223	0.000	0.000	1173	1262		2244	3.4	1.0
HMX/GAP (84/16)	HMX/GAP (84/16)	208	[4]	1.642	2.877	2.714	2.460	0.0	CHNO	3.0	1.132	1.439	0.511	1.357	0.000	0.000	1407	1520	6.59	2457	3.4	0.9
HMX/HN (75/25)	HMX/HN (75/25)	-110	[c]	1.013	3.341	2.815	2.815	0.0	CHNO	2.0	0.441	1.670	0.572	1.407	0.000	0.000	1350	1394	6.94	2407	3.6	0.9
HMX/PIB (91/9)	HMX/PIB (91/9)	28	[c]	1.818	3.578	2.458	2.508	0.0	CHNO	3.0	1.459	1.789	0.359	1.229	0.000	0.000	1254	1400	6.25	2320	3.4	0.9
HMX/SYLGARD (85/15)	HMX/SYLGARD (85/15)	-203	[3]	1.535	3.424	2.325	2.505	5.5	CHNOX		1.138	1.712	0.397	1.163	0.000	0.000	1046	1160		2119	3.5	1.0
HMX/TATB/VITON (10/80/10)	HMX/TATB/VITON (10/80/10)	-286	[c]	2.262	2.317	2.130	2.130	6.6	CHNOX		1.776	1.158	0.486	1.065	0.000	0.000	663	840		1686	3.2	1.3
HMX/TATB/VITON (20/70/10)	HMX/TATB/VITON (20/70/10)	-266	[c]	2.164	2.354	2.167	2.167	6.6	CHNOX		1.669	1.177	0.495	1.084	0.000	0.000	713	880		1750	3.2	1.2
HMX/TATB/VITON (30/60/10)	HMX/TATB/VITON (30/60/10)	-245	[c]	2.067	2.392	2.205	2.205	6.6	CHNOX		1.563	1.196	0.504	1.102	0.000	0.000	764	920		1811	3.2	1.2
HMX/TATB/VITON (40/50/10)	HMX/TATB/VITON (40/50/10)	-225	[c]	1.970	2.430	2.243	2.243	6.6	CHNOX		1.456	1.215	0.514	1.121	0.000	0.000	815	960		1870	3.3	1.1
HMX/TATB/VITON (50/40/10)	HMX/TATB/VITON (50/40/10)	-205	[c]	1.872	2.467	2.280	2.280	6.6	CHNOX		1.349	1.234	0.523	1.140	0.000	0.000	866	1001		1928	3.3	1.1
HMX/TATB/VITON (60/30/10)	HMX/TATB/VITON (60/30/10)	-184	[c]	1.775	2.505	2.318	2.318	6.6	CHNOX		1.242	1.253	0.533	1.159	0.000	0.000	916	1041		1983	3.3	1.1
HMX/TATB/VITON (70/20/10)	HMX/TATB/VITON (70/20/10)	-164	[c]	1.678	2.543	2.356	2.356	6.6	CHNOX		1.135	1.271	0.542	1.178	0.000	0.000	967	1081		2037	3.4	1.1
HMX/TATB/VITON (80/10/10)	HMX/TATB/VITON (80/10/10)	-144	[c]	1.580	2.581	2.393	2.393	6.6	CHNOX		1.029	1.290	0.552	1.197	0.000	0.000	1018	1121		2090	3.4	1.0
HMX/TNT (60/40)	HMX/TNT (60/40)	5	[c]	2.043	2.501	2.149	2.677	0.0	CHNO	3.0	1.330	1.251	0.713	1.075	0.000	0.000	1266	1399	5.98	2331	3.3	0.9
HMX/TNT (70/30)	HMX/TNT (70/30)	19	[c]	1.870	2.551	2.287	2.683	0.0	CHNO	3.0	1.166	1.276	0.704	1.144	0.000	0.000	1302	1418	6.17	2364	3.3	0.9
HMX/TNT (75/25)	HMX/TNT (75/25)	26	[c]	1.783	2.576	2.356	2.686	0.0	CHNO	3.0	1.084	1.288	0.699	1.178	0.000	0.000	1319	1428	6.27	2380	3.3	0.9
HMX/TNT (78/22)	HMX/TNT (78/22)	30	[c]	1.732	2.591	2.398	2.688	0.0	CHNO	3.0	1.035	1.296	0.696	1.199	0.000	0.000	1330	1434	6.33	2389	3.4	0.9
HMX/TNT (80/20)	HMX/TNT (80/20)	33	[c]	1.697	2.601	2.425	2.689	0.0	CHNO	3.0	1.003	1.301	0.694	1.213	0.000	0.000	1337	1438	6.37	2396	3.4	0.9
HMX/TNT (89/11)	HMX/TNT (89/11)	45	[c]	1.541	2.646	2.549	2.695	0.0	CHNO	3.0	0.855	1.323	0.686	1.275	0.000	0.000	1369	1455	6.55	2424	3.4	0.9
HMX/TNT (90/10)	HMX/TNT (90/10)	47	[c]	1.524	2.651	2.563	2.695	0.0	CHNO	3.0	0.839	1.326	0.685	1.282	0.000	0.000	1373	1457	6.57	2428	3.4	0.9
hn	hydrazine nitrate	-621	[8]	0.000	5.260	3.156	3.156	0.0	HNO	1.0	0.000	2.630	0.000	1.578	0.000	0.263	899	899	6.34	1965	3.9	1.1
hnab	2,2',4,4',6,6'-hexanitroazobenzene	150	[8]	2.654	0.885	1.769	2.654	0.0	CHNO	3.0	1.548	0.442	1.106	0.885	0.000	0.000	1291	1446	5.35	2354	3.0	0.9
hnb	hexanitrobenzene	136	[47]	1.724	0.000	1.724	3.447	0.0	CNO	1.0	0.000	0.000	1.724	0.862	0.000	0.000	1758	1758	6.74	2747	3.3	0.8
hnbp	2,2',4,4',6,6'-hexanitrobiphenyl	34	[48]	2.829	0.943	1.414	2.829	0.0	CHNO	3.0	1.650	0.471	1.179	0.707	0.000	0.000	1250	1415	5.17	2317	2.9	0.9
hnetn	hexanitroethane	67	[47]	0.667	0.000	2.000	3.999	0.0	CNO	1.0	0.000	0.000	0.667	1.000	0.000	1.333	694	694	4.56	1725	3.1	1.2
hns	2,2´, 4,4´6,6´-hexanitrostilbene	42	[8]	3.109	1.333	1.333	2.665	0.0	CHNO	3.0	2.110	0.666	0.999	0.666	0.000	0.000	1156	1367	4.88	2227	2.9	1.0
HZ/HN (21/79)	HZ/HN (21/79)	-411	[c]	0.000	6.777	3.804	2.493	0.0	HNO	5.0	0.000	2.493	0.000	1.902	0.895	0.000	1030	1030	7.38	2102	4.4	1.0
HZ/HN (70/30)	HZ/HN (70/30)	77	[c]	0.000	10.316	5.316	0.947	0.0	HNO	5.0	0.000	0.947	0.000	2.658	4.211	0.000	624	624	6.99	1637	5.5	1.3
IMX-104	IMX-104	-175	[c]	2.142	2.188	2.363	2.436	0.0	CHNO	3.0	1.471	1.094	0.671	1.182	0.000	0.000	941	1088	5.14	2010	3.2	1.1
ipn	isopropyl nitrate	-523	[48]	2.855	6.661	0.952	2.855	0.0	CHNO	4.0	2.855	2.855	0.000	0.476	0.476	0.000	842	1127	5.31	1901	3.4	1.1
LLM-105/VITON (95/5)	LLM-105/VITON (95/5)	498	[c]	2.275	0.807	2.856	1.785	3.3	CHNOX		1.585	0.404	0.691	1.428	0.000	0.000	1222	1381		2291	3.1	0.9
LLM-175/VITON (95/5)	LLM-175/VITON (95/5)	498	[c]	2.275	0.807	2.856	1.785	3.3	CHNOX		1.585	0.404	0.691	1.428	0.000	0.000	1222	1381		2291	3.1	0.9
LX-01	LX-01	-265	[c]	1.525	3.727	1.694	3.388	0.0	CHNO	3.0	0.763	1.864	0.762	0.847	0.000	0.000	1453	1529	6.95	2497	3.4	0.9
LX-04	LX-04	-215	[c]	1.549	2.577	2.296	2.296	9.9	CHNOX		1.045	1.288	0.504	1.148	0.000	0.000	899	1003		1964	3.4	1.1
LX-07	LX-07	-123	[c]	1.483	2.618	2.431	2.431	6.6	CHNOX		0.922	1.309	0.561	1.216	0.000	0.000	1069	1161		2142	3.4	1.0
LX-09	LX-09	20	[c]	1.425	2.736	2.592	2.721	0.3	CHNOX		0.749	1.368	0.677	1.296	0.000	0.000	1372	1447		2427	3.5	0.9
LX-10	LX-10	-31	[c]	1.417	2.660	2.566	2.566	3.3	CHNOX		0.799	1.330	0.618	1.283	0.000	0.000	1239	1319		2306	3.5	0.9
LX-11	LX-11	-307	[c]	1.615	2.535	2.161	2.161	13.2	CHNOX		1.168	1.268	0.447	1.081	0.000	0.000	729	846		1769	3.4	1.2
LX-14	LX-14	15	[c]	1.521	2.917	2.588	2.659	0.0	CHNO	3.0	0.921	1.459	0.600	1.294	0.000	0.000	1331	1423	6.51	2390	3.4	0.9
LX-15	LX-15	-30	[c]	3.051	1.290	1.266	2.532	3.8	CHNOX		2.107	0.645	0.943	0.633	0.000	0.000	1019	1230		2091	2.8	1.0
LX-17	LX-17	-237	[c]	2.295	2.186	2.150	2.150	5.7	CHNOX		1.767	1.093	0.528	1.075	0.000	0.000	715	892		1752	3.2	1.2
manitrol	mannitol hexanitrate	-336	[48]	1.327	1.769	1.327	3.981	0.0	CHNO	1.0	0.000	0.885	1.327	0.663	0.000	0.221	1423	1423	6.64	2471	3.2	0.9
md	methylene dinitramine	-102	[8]	0.735	2.940	2.940	2.940	0.0	CHNO	1.0	0.000	1.470	0.735	1.470	0.000	0.000	1439	1439	7.27	2485	3.7	0.9
MEN-II	MEN-II	-747	[c]	2.060	7.055	1.329	3.096	0.0	CHNO	5.0	2.060	3.096	0.000	0.665	0.432	0.000	837	1043	5.74	1895	3.6	1.1
metn	metriol trinitrate	-415	[8]	1.960	3.527	1.176	3.527	0.0	CHNO	3.0	1.078	1.764	0.882	0.588	0.000	0.000	1326	1434	6.35	2386	3.3	0.9
nag	nitroaminoguanidine	45	[48]	0.840	4.199	4.199	1.680	0.0	CHNO	5.0	0.840	1.680	0.000	2.099	0.420	0.000	931	1015	6.19	1999	3.9	1.1
ng	nitroglycerine	-390	[8]	1.321	2.202	1.321	3.963	0.0	CHNO	1.0	0.000	1.101	1.321	0.661	0.000	0.110	1489	1489	6.89	2528	3.3	0.8
nm	nitromethane	-443	[8]	1.638	4.915	1.638	3.277	0.0	CHNO	3.0	1.229	2.457	0.410	0.819	0.000	0.000	1240	1363	6.54	2307	3.5	0.9
nmet	methylnitrate	-479	[48]	1.298	3.894	1.298	3.894	0.0	CHNO	2.0	0.325	1.947	0.974	0.649	0.000	0.000	1530	1562	7.32	2562	3.4	0.8
no	nitric oxide	617	[33]	0.000	0.000	3.333	3.333	0.0	NO	1.0	0.000	0.000	0.000	1.666	0.000	1.666	617	617	4.53	1627	3.1	1.3
nona	2,2',2",4,4',4",6,6',6"-nonanitroterphenyl	43	[48]	2.833	0.787	1.417	2.833	0.0	CHNO	3.0	1.613	0.394	1.220	0.708	0.000	0.000	1257	1418	5.15	2322	2.9	0.9
ng	nitroguanidine	-221	[47]	0.961	3.844	3.844	1.922	0.0	CHNO	5.0	0.961	1.922	0.000	1.922	0.000	0.000	794	890	5.50	1846	3.8	1.2
NQ/ESTANE (95/5)	NQ/ESTANE (95/5)	-257	[c]	1.169	4.026	3.661	1.914	0.0	CHNO	5.0	1.169	1.914	0.000	1.830	0.099	0.000	732	849	5.30	1772	3.7	1.2
NQ/TNT(35/65)	NQ/TNT(35/65)	-128	[c]	2.340	2.776	2.204	2.390	0.0	CHNO	3.0	1.839	1.388	0.501	1.102	0.000	0.000	961	1145	5.17	2031	3.2	1.1
NQ/TNT(50/50)	NQ/TNT(50/50)	-150	[c]	2.021	3.022	2.582	2.282	0.0	CHNO	3.0	1.636	1.511	0.385	1.291	0.000	0.000	923	1086	5.27	1990	3.3	1.1
NQ/TNT(80/20)	NQ/TNT(80/20)	-192	[c]	1.385	3.515	3.339	2.066	0.0	CHNO	3.0	1.231	1.758	0.154	1.670	0.000	0.000	845	968	5.44	1905	3.6	1.1
NQ/TNT(90/10)	NQ/TNT(90/10)	-207	[c]	1.173	3.679	3.591	1.994	0.0	CHNO	3.0	1.096	1.840	0.077	1.796	0.000	0.000	819	929	5.47	1875	3.7	1.1
NQ/TNT(95/5)	NQ/TNT(95/5)	-214	[c]	1.067	3.762	3.717	1.958	0.0	CHNO	3.0	1.028	1.881	0.039	1.859	0.000	0.000	807	909	5.49	1861	3.7	1.2
nto	3-nitro-1,2,4 triazol 5-one	-215	[8]	1.538	1.538	3.075	2.307	0.0	CHNO	3.0	0.769	0.769	0.769	1.538	0.000	0.000	875	952	5.16	1938	3.4	1.1
NTO/RDX/TNT (50/12/38)	NTO/RDX/TNT (50/12/38)	-129	[c]	2.102	1.930	2.364	2.481	0.0	CHNO	3.0	1.344	0.965	0.758	1.182	0.000	0.000	1007	1141	5.27	2079	3.2	1.0
NTO/TNT (30/70)	NTO/TNT (30/70)	-119	[c]	2.619	2.002	1.847	2.541	0.0	CHNO	3.0	1.849	1.001	0.770	0.924	0.000	0.000	999	1183	4.98	2070	3.1	1.0
NTO/TNT (50/50)	NTO/TNT (50/50)	-147	[c]	2.310	1.870	2.198	2.474	0.0	CHNO	3.0	1.540	0.935	0.770	1.099	0.000	0.000	963	1117	5.05	2033	3.2	1.1
NTO/TNT (60/40)	NTO/TNT (60/40)	-161	[c]	2.155	1.803	2.374	2.441	0.0	CHNO	3.0	1.386	0.902	0.770	1.187	0.000	0.000	946	1084	5.08	2015	3.2	1.1
OCTOL	OCTOL	28	[c]	1.761	2.583	2.374	2.687	0.0	CHNO	3.0	1.063	1.291	0.698	1.187	0.000	0.000	1324	1430	6.30	2384	3.3	0.9
ont	octanitroterphenyl	33	[48]	3.049	1.016	1.355	2.711	0.0	CHNO	3.0	1.948	0.508	1.101	0.678	0.000	0.000	1168	1363	4.89	2239	2.8	1.0
PAX-41	PAX-41	-36	[c]	2.114	2.816	2.109	2.639	0.0	CHNO	3.0	1.499	1.408	0.616	1.055	0.000	0.000	1207	1357	5.85	2276	3.3	0.9

Fernando G. Bastante [1] *, María Araújo Fernández* [1] *, Eduardo Giráldez* [1] .
CINTECX, GESSMin group, University of Vigo

PREDICTIVE MODEL FOR EXPLOSIVE DETONATION PARAMETERS FROM AN EQUATION OF STATE BASED ON DETONATION VELOCITY. Physical Chemistry Chemical Physics 2022

DEoS DATABASE

	Average values
Q_DEoS (cal/g)	1160
w (m/s per kg/m³)	3.37
Do (m/s)	2215
C (m/s per cal/g)	1.0

$w = \left(\frac{\partial D}{\partial \rho_o}\right)_Q$

$C = \left(\frac{\partial D}{\partial Q}\right)_{\rho_o}$

EXPLOSIVES ***238*** *CHNO Composition (mol/100g)* *Other elements (% weight X)* *hierarchy* *[Cl+F+P+Si] as inerts*

Acronym	Name	ΔH^o_{298} (cal/g)	reference	C	H	N	O	X: {Cl+F+P+Si}	Comp.	type (Xiong)	C (s)	H2O (g)	CO2 (g)	N2 (g)	H2 (g)	O2 (g)	Q_DEoS (cal/g)	Q_{KJ} (cal/g)	Phi (KJ)	Do (DEoS)	w (DEoS)	C (DEoS)
PBX-9007	PBX-9007	65	[c]	1.970	3.218	2.431	2.440	0.0	CHNO	3.0	1.554	1.609	0.416	1.216	0.000	0.000	1230	1386	6.04	2298	3.4	0.9
PBX-9010	PBX-9010	-80	[c]	1.409	2.480	2.431	2.431	7.6	CHNOX		0.813	1.240	0.596	1.216	0.000	0.000	1115	1197		2188	3.4	1.0
PBX-9011	PBX-9011	-40	[c]	1.729	3.181	2.450	2.607	0.0	CHNO	3.0	1.220	1.590	0.508	1.225	0.000	0.000	1235	1357	6.20	2302	3.4	0.9
PBX-9205	PBX-9205	58	[c]	1.826	3.141	2.485	2.506	0.0	CHNO	3.0	1.359	1.570	0.468	1.243	0.000	0.000	1270	1406	6.21	2334	3.4	0.9
PBX-9404	PBX-9404	8	[c]	1.401	2.745	2.565	2.690	1.4	CHNOX		0.743	1.373	0.659	1.282	0.000	0.000	1346	1420		2404	3.5	0.9
PBX-9407	PBX-9407	8	[c]	1.412	2.668	2.539	2.539	4.2	CHNOX		0.810	1.334	0.603	1.270	0.000	0.000	1265	1346		2330	3.5	0.9
PBX-9408	PBX-9408	12	[c]	1.426	2.781	2.574	2.679	1.2	CHNOX		0.782	1.391	0.644	1.287	0.000	0.000	1344	1422		2401	3.5	0.9
PBX9501	PBX9501	22	[c]	1.467	2.850	2.603	2.690	0.0	CHNO	3.0	0.835	1.425	0.633	1.301	0.000	0.000	1358	1441	6.60	2414	3.5	0.9
PBX9502	PBX9502	-206	[c]	2.305	2.232	2.208	2.208	3.8	CHNOX		1.759	1.116	0.546	1.104	0.000	0.000	777	953		1826	3.2	1.2
PBX9503	PBX9503	-175	[c]	2.159	2.289	2.265	2.265	3.8	CHNOX		1.599	1.144	0.560	1.132	0.000	0.000	853	1013		1914	3.2	1.1
pent	pentaerythritol tetranitrate	-407	[8]	1.582	2.531	1.265	3.796	0.0	CHNO	2.0	0.316	1.265	1.265	0.633	0.000	0.000	1483	1514	6.79	2523	3.3	0.9
PENTOLITE	PENTOLITE	-243	[c]	2.332	2.366	1.293	3.219	0.0	CHNO	3.0	1.314	1.183	1.018	0.647	0.000	0.000	1267	1398	5.79	2332	3.1	0.9
PETN/TNT (20/80)	PETN/TNT (20/80)	-144	[c]	2.782	2.267	1.310	2.872	0.0	CHNO	3.0	1.912	1.134	0.869	0.655	0.000	0.000	1138	1329	5.22	2210	3.0	1.0
PETN/TNT (60/40)	PETN/TNT (60/40)	-276	[c]	2.182	2.399	1.287	3.334	0.0	CHNO	3.0	1.114	1.199	1.067	0.644	0.000	0.000	1310	1422	5.99	2371	3.1	0.9
PETN/TNT/RDX (20/30/50)	PETN/TNT/RDX (20/30/50)	-72	[c]	1.916	2.517	2.000	2.902	0.0	CHNO	3.0	1.094	1.259	0.822	1.000	0.000	0.000	1319	1429	6.18	2379	3.3	0.9
pf	1-fluoro-2,4,6-trinitrobenzene	-268	[8]	2.596	0.865	1.298	2.596	8.2	CHNOX		1.515	0.433	1.082	0.649	0.000	0.000	848	999		1908	2.9	1.1
PICRATOL	PICRATOL	-236	[c]	2.747	2.324	1.479	2.747	0.0	CHNO	3.0	1.955	1.162	0.792	0.740	0.000	0.000	985	1181	4.93	2056	3.0	1.0
picric	trinitrophenol	-224	[8]	2.619	1.309	1.309	3.055	0.0	CHNO	3.0	1.419	0.655	1.200	0.655	0.000	0.000	1142	1283	5.17	2213	3.0	1.0
ppam	n-(2,2-nitropropyl)-n,2,2-trinitro-1-propanamine	-170	[48]	1.839	3.066	1.839	3.066	0.0	CHNO	3.0	1.073	1.533	0.766	0.920	0.000	0.000	1330	1437	6.35	2389	3.3	0.9
PRNQ/HMX/CARNAUBA (30/68/2)	PRNQ/HMX/CARNAUBA (30/68/2)	-73	[c]	1.882	4.175	2.658	2.247	0.0	CHNO	3.0	1.802	2.087	0.080	1.329	0.000	0.000	1029	1209	5.76	2101	3.5	1.0
PRNQ/NQ/HMX (34/35/31)	PRNQ/NQ/HMX (34/35/31)	-179	[c]	1.686	4.509	3.113	1.975	0.0	CHNO	5.0	1.686	1.975	0.000	1.557	0.279	0.000	794	962	5.41	1846	3.6	1.2
PYX/PE (95/5)	PYX/PE (95/5)	35	[c]	2.902	1.625	1.682	2.497	0.0	CHNO	3.0	2.060	0.813	0.842	0.841	0.000	0.000	1091	1297	4.94	2164	3.0	1.0
rdx	cyclomethylenetrinitramine	66	[8]	1.351	2.701	2.701	2.701	0.0	CHNO	3.0	0.675	1.351	0.675	1.351	0.000	0.000	1415	1482	6.78	2464	3.5	0.9
RDX/ESTANE (80/20)	RDX/ESTANE (80/20)	-137	[c]	2.107	3.660	2.199	2.513	0.0	CHNO	3.0	1.766	1.830	0.341	1.099	0.000	0.000	1065	1242	5.66	2138	3.3	1.0
RDX/EVA (80/20)	RDX/EVA (80/20)	66	[c]	2.291	4.380	2.161	2.363	0.0	CHNO	3.0	2.204	2.190	0.086	1.081	0.000	0.000	1192	1413	5.90	2262	3.4	0.9
RDX/EVA (95/5)	RDX/EVA (95/5)	66	[c]	1.586	3.121	2.566	2.617	0.0	CHNO	3.0	1.058	1.560	0.528	1.283	0.000	0.000	1359	1465	6.57	2415	3.4	0.9
RDX/EXON (90/10)	RDX/EXON (90/10)	-30	[c]	1.452	2.646	2.434	2.434	6.9	CHNOX		0.897	1.323	0.555	1.217	0.000	0.000	1168	1257		2239	3.4	1.0
RDX/GAP (84/16)	RDX/GAP (84/16)	214	[4]	1.657	3.214	2.708	2.433	0.0	CHNO	3.0	1.244	1.607	0.413	1.354	0.000	0.000	1407	1531	6.63	2457	3.5	0.9
RDX/HTPB (80/20)	RDX/HTPB (80/20)	52	[c]	2.512	4.410	2.180	2.178	0.0	CHNO	4.0	2.512	2.178	0.000	1.090	0.027	0.000	1060	1311	5.49	2133	3.3	1.0
RDX/HTPB (82/18)	RDX/HTPB (82/18)	25	[c]	2.352	4.243	2.228	2.266	0.0	CHNO	3.0	2.280	2.121	0.072	1.114	0.000	0.000	1092	1320	5.63	2165	3.3	1.0
RDX/HTPB (85/15)	RDX/HTPB (85/15)	56	[c]	2.222	3.983	2.310	2.309	0.0	CHNO	3.0	2.063	1.992	0.159	1.155	0.000	0.000	1150	1356	5.81	2221	3.4	1.0
RDX/PIB (91/9)	RDX/PIB (91/9)	33	[c]	1.818	3.578	2.458	2.508	0.0	CHNO	3.0	1.459	1.789	0.359	1.229	0.000	0.000	1260	1405	6.26	2325	3.4	0.9
RDX/SYLGARD (85/15)	RDX/SYLGARD (85/15)	-224	[3]	1.529	3.407	2.310	2.487	6.1	CHNOX		1.137	1.704	0.392	1.155	0.000	0.000	1016	1130		2088	3.5	1.0
RDX/TATB/HTPB (65/20/15)	RDX/TATB/HTPB (65/20/15)	14	[c]	2.417	3.908	2.235	2.234	0.0	CHNO	3.0	2.277	1.954	0.140	1.117	0.000	0.000	1047	1275	5.45	2120	3.3	1.0
RDX/TATB/HTPB (70/15/15)	RDX/TATB/HTPB (70/15/15)	24	[c]	2.368	3.927	2.253	2.252	0.0	CHNO	3.0	2.223	1.963	0.145	1.127	0.000	0.000	1073	1295	5.54	2146	3.3	1.0
RDX/TATB/HTPB (75/10/15)	RDX/TATB/HTPB (75/10/15)	35	[c]	2.319	3.945	2.272	2.271	0.0	CHNO	3.0	2.170	1.973	0.149	1.136	0.000	0.000	1098	1315	5.63	2171	3.3	1.0
RDX/TFNA (65/35)	RDX/TFNA (65/35)	-189	[c]	1.512	2.643	2.263	2.516	7.2	CHNOX		0.914	1.322	0.597	1.131	0.000	0.000	1045	1137		2118	3.4	1.0
RDX/TNT (30/70)	RDX/TNT (30/70)	-35	[c]	2.563	2.351	1.735	2.660	0.0	CHNO	3.0	1.821	1.176	0.742	0.867	0.000	0.000	1160	1342	5.40	2232	3.1	1.0
RDX/TNT (50/50)	RDX/TNT (50/50)	-6	[c]	2.216	2.451	2.011	2.671	0.0	CHNO	3.0	1.493	1.226	0.723	1.006	0.000	0.000	1233	1382	5.79	2300	3.2	0.9
RDX/TNT (60/40)	RDX/TNT (60/40)	8	[c]	2.043	2.501	2.149	2.677	0.0	CHNO	3.0	1.330	1.251	0.713	1.075	0.000	0.000	1269	1402	5.98	2334	3.3	0.9
RDX/TNT (64/36)	RDX/TNT (64/36)	14	[c]	1.974	2.521	2.204	2.680	0.0	CHNO	3.0	1.264	1.261	0.710	1.102	0.000	0.000	1284	1410	6.06	2347	3.3	0.9
RDX/TNT (65/35)	RDX/TNT (65/35)	16	[c]	1.957	2.526	2.218	2.680	0.0	CHNO	3.0	1.248	1.263	0.709	1.109	0.000	0.000	1287	1412	6.08	2351	3.3	0.9
RDX/TNT (70/30)	RDX/TNT (70/30)	23	[c]	1.870	2.551	2.287	2.683	0.0	CHNO	3.0	1.166	1.276	0.704	1.144	0.000	0.000	1306	1422	6.18	2367	3.3	0.9
RDX/TNT (75/25)	RDX/TNT (75/25)	30	[c]	1.783	2.576	2.356	2.686	0.0	CHNO	3.0	1.084	1.288	0.699	1.178	0.000	0.000	1324	1432	6.28	2384	3.3	0.9
RDX/TNT (77/23)	RDX/TNT (77/23)	33	[c]	1.749	2.586	2.384	2.688	0.0	CHNO	3.0	1.052	1.293	0.697	1.192	0.000	0.000	1331	1436	6.32	2390	3.4	0.9
RDX/TNT (78/22)	RDX/TNT (78/22)	34	[c]	1.732	2.591	2.398	2.688	0.0	CHNO	3.0	1.035	1.296	0.696	1.199	0.000	0.000	1335	1438	6.34	2393	3.4	0.9
RDX/TNT (80/20)	RDX/TNT (80/20)	37	[c]	1.697	2.601	2.425	2.689	0.0	CHNO	3.0	1.003	1.301	0.694	1.213	0.000	0.000	1342	1442	6.38	2400	3.4	0.9
RDX/TNT (90/10)	RDX/TNT (90/10)	52	[c]	1.524	2.651	2.563	2.695	0.0	CHNO	3.0	0.839	1.326	0.685	1.282	0.000	0.000	1378	1462	6.58	2432	3.4	0.9
RDX/VITON (95/5)	RDX/VITON (95/5)	-26	[c]	1.417	2.660	2.566	2.566	3.3	CHNOX		0.799	1.330	0.618	1.283	0.000	0.000	1244	1324		2311	3.5	0.9
RDX/WAX (94/6)	RDX/WAX (94/6)	41	[c]	1.697	3.395	2.539	2.539	0.0	CHNO	3.0	1.276	1.697	0.421	1.270	0.000	0.000	1290	1418	6.38	2353	3.4	0.9
RDX/WAX (95/5)	RDX/WAX (95/5)	45	[c]	1.640	3.279	2.566	2.566	0.0	CHNO	3.0	1.176	1.640	0.463	1.283	0.000	0.000	1311	1428	6.44	2372	3.4	0.9
RX23	RX23	-405	[c]	0.000	6.820	3.822	2.474	0.0	HNO	5.0	0.000	2.474	0.000	1.911	0.936	0.000	1025	1025	7.38	2097	4.4	1.0
RX26	RX26	-76	[c]	1.959	2.722	2.423	2.487	0.0	CHNO	3.0	1.396	1.361	0.563	1.211	0.000	0.000	1101	1241	5.69	2174	3.3	1.0
RX27	RX27	158	[c]	3.004	0.989	1.906	1.906	5.7	CHNOX		2.299	0.495	0.706	0.953	0.000	0.000	878	1108		1941	2.9	1.1
RX36	RX36	183	[c]	1.866	1.480	2.426	2.426	3.3	CHNOX		1.023	0.740	0.843	1.213	0.000	0.000	1301	1403		2363	3.2	0.9
RX41	RX41	-129	[c]	1.341	1.703	2.414	2.817	3.3	CHNOX		0.358	0.852	0.983	1.207	0.000	0.000	1251	1287		2317	3.4	0.9
RX45	RX45	36	[c]	1.569	2.232	3.680	1.472	3.8	CHNOX		1.391	1.116	0.178	1.840	0.000	0.000	709	849		1745	3.5	1.2
RX47	RX47	-30	[c]	2.312	1.481	2.167	2.167	5.7	CHNOX		1.599	0.740	0.713	1.084	0.000	0.000	909	1069		1975	3.1	1.1
RX48	RX48	34	[c]	2.446	1.186	1.915	2.299	5.8	CHNOX		1.593	0.593	0.853	0.958	0.000	0.000	1020	1179		2092	3.0	1.0
RX52AE	RX52AE	-285	[c]	2.149	2.345	1.911	2.579	3.8	CHNOX		1.445	1.173	0.703	0.955	0.000	0.000	910	1055		1976	3.2	1.1
schembl	[2-nitro-3-(nitrooxy)-2-[(nitrooxy)methyl][propyl]-nitrate	-191	[48]	1.398	2.097	1.398	3.845	0.0	CHNO	2.0	0.000	1.049	1.398	0.699	0.000	0.000	1730	1730	7.38	2725	3.3	0.8
tacot	1,3,7,9-tetranitrobenzotriazolo-[2,1-a]benzotriazole	285	[8]	3.091	1.030	2.061	2.061	0.0	CHNO	3.0	2.318	0.515	0.773	1.030	0.000	0.000	1077	1309	4.68	2150	2.9	1.0
tat	1,3,5-triazido-2,4,6-triazine (cyanuric triazide)	1071	[47]	1.470	0.000	5.879	0.000	0.0	CN	4.0	1.470	0.000	0.000	2.940	0.000	0.000	924	1071	5.09	1991	3.6	1.1
tatb	1,3,5-triamino-2,4,6-trinitrobenzene	-143	[8]	2.324	2.324	2.324	2.324	0.0	CHNO	3.0	1.743	1.162	0.581	1.162	0.000	0.000	901	1075	4.97	1967	3.2	1.1
TATB/KELF (90/10)	TATB/KELF (90/10)	-268	[c]	2.285	2.140	2.092	2.092	7.6	CHNOX		1.774	1.070	0.511	1.046	0.000	0.000	653	831		1674	3.2	1.3
TATB/TNT (30/70)	TATB/TNT (30/70)	-98	[c]	2.855	2.238	1.622	2.546	0.0	CHNO	3.0	2.141	1.119	0.714	0.811	0.000	0.000	1006	1220	4.90	2078	3.0	1.0
tetryl	n-methyl-n-nitro-2,4,6-trinitroaniline	28	[48]	2.438	1.741	1.741	2.786	0.0	CHNO	3.0	1.480	0.871	0.958	0.871	0.000	0.000	1284	1432	5.64	2348	3.1	0.9
TKX-50/VITON (95/5)	TKX-50/VITON (95/5)	340	[c]	0.938	3.312	4.023	1.609	3.3	CHNOX		0.938	1.609	0.000	2.011	0.047	0.000	1177	1271		2247	3.8	1.0
tna	2,4,6-trinitroaniline	-78	[48]	2.630	1.753	1.753	2.630	0.0	CHNO	3.0	1.753	0.877	0.877	0.877	0.000	0.000	1078	1253	5.10	2151	3.0	1.0
tnan	2,4,6-trinitroanisole	-149	[48]	2.879	2.056	1.234	2.879	0.0	CHNO	3.0	1.954	1.028	0.925	0.617	0.000	0.000	1120	1315	5.09	2192	3.0	1.0
tnb	trinitrobenceno	42	[48]	2.815	1.408	1.408	2.815	0.0	CHNO	3.0	1.760	0.704	1.056	0.704	0.000	0.000	1266	1442	5.29	2331	2.9	0.9
tneof	tris(2,2,2-trinitroethyl)orthoformate	-232	[48]	1.265	1.265	1.627	3.796	0.0	CHNO	1.0	0.000	0.633	1.265	0.813	0.000	0.316	1324	1324	6.33	2384	3.2	0.9
tnetb	trinitroethyltrinitrobutyrate	-307	[48]	1.554	1.554	1.554	3.626	0.0	CHNO	2.0	0.129	0.777	1.424	0.777	0.000	0.000	1469	1481	6.59	2511	3.2	0.9

Fernando G. Bastante [1] *, María Araújo Fernández* [1] *, Eduardo Giráldez* [1] .
CINTECX, GESSMin group, University of Vigo

PREDICTIVE MODEL FOR EXPLOSIVE DETONATION PARAMETERS FROM AN EQUATION OF STATE BASED ON DETONATION VELOCITY. Physical Chemistry Chemical Physics 2022

DEoS DATABASE

EXPLOSIVES ***238***

CHNO Composition (mol/100g) *Other elements (% weight X)* *hierarchy* *[Cl+F+P+Si] as inerts*

Average values

Q_DEoS (cal/g)	1160
w (m/s per kg/m³)	3.37
Do (m/s)	2215
C (m/s per cal/g)	1.0

$$w = \left(\frac{\partial D}{\partial \rho_o}\right)_Q \qquad C = \left(\frac{\partial D}{\partial Q}\right)_{\rho_o}$$

Acronym	Name	ΔH°_{298} (cal/g)	reference	C	H	N	O	X: {Cl+F+P+Si}	Comp.	type (Xiong)	C (s)	H2O (g)	CO2 (g)	N2 (g)	H2 (g)	O2 (g)	Q_DEoS (cal/g)	Q_{KJ} (cal/g)	Phi (KJ)	Do (DEoS)	w (DEoS)	C (DEoS)
tnm	tetranitromethane	45	[47]	0.510	0.000	2.040	4.081	0.0	CNO	1.0	0.000	0.000	0.510	1.020	0.000	1.530	525	525	4.01	1501	3.1	1.4
TNM/BENZ (76.4/23.6)	TNM/BENZ (76.4/23.6)	70	[c]	2.202	1.813	1.559	3.118	0.0	CHNO	2.0	1.097	0.906	1.106	0.779	0.000	0.000	1524	1634	6.29	2557	3.1	0.8
TNM/NM (0.071/1)	TNM/NM (0.071/1)	-352	[c]	1.429	4.002	1.713	3.426	0.0	CHNO	3.0	0.716	2.001	0.712	0.856	0.000	0.000	1403	1474	6.94	2454	3.5	0.9
TNM/NM (0.25/1)	TNM/NM (0.25/1)	-226	[c]	1.136	2.726	1.817	3.635	0.0	CHNO	2.0	0.000	1.363	1.136	0.909	0.000	0.000	1630	1630	7.45	2645	3.4	0.8
TNM/NM (0.5/1)	TNM/NM (0.5/1)	-142	[c]	0.943	1.886	1.886	3.772	0.0	CHNO	1.0	0.000	0.943	0.943	0.943	0.000	0.472	1290	1290	6.52	2353	3.3	0.9
TNM/NM (60/40)	TNM/NM (60/40)	-684	[c]	1.554	4.993	1.224	3.697	0.0	CHNO	3.0	0.954	2.497	0.600	0.612	0.000	0.000	1228	1323	6.59	2295	3.5	0.9
TNM/NM (70/30)	TNM/NM (70/30)	-502	[c]	1.293	3.745	1.428	3.793	0.0	CHNO	2.0	0.333	1.873	0.960	0.714	0.000	0.000	1450	1483	7.11	2495	3.4	0.9
TNM/NM (80/20)	TNM/NM (80/20)	-320	[c]	1.032	2.497	1.632	3.889	0.0	CHNO	1.0	0.000	1.248	1.032	0.816	0.000	0.288	1373	1373	6.82	2427	3.3	0.9
TNM/NM (90/10)	TNM/NM (90/10)	-137	[c]	0.771	1.248	1.836	3.985	0.0	CHNO	1.0	0.000	0.624	0.771	0.918	0.000	0.909	949	949	5.53	2018	3.1	1.1
tnt	2,4,6-trinitrotoluene	-78	[47]	3.082	2.201	1.321	2.642	0.0	CHNO	3.0	2.311	1.101	0.770	0.660	0.000	0.000	1051	1282	4.84	2124	2.9	1.0
TNT/FOX-12(50/50)	TNT/FOX-12(50/50)	-242	[c]	2.019	2.774	2.334	2.516	0.0	CHNO	3.0	1.455	1.387	0.565	1.167	0.000	0.000	945	1090	5.30	2014	3.3	1.1
tntab	trinitrotriazidobenzene	803	[8]	1.785	0.000	3.570	1.785	0.0	CNO	3.0	0.892	0.000	0.892	1.785	0.000	0.000	1553	1643	6.27	2582	3.5	0.8
tntmta	trinitrosotrimethylenetriamine	387	[48]	1.723	3.446	3.446	1.723	0.0	CHNO	4.0	1.723	1.723	0.000	1.723	0.000	0.000	1211	1383	6.15	2279	3.5	0.9
TO/NM (14.5/85.5)	TO/NM (14.5/85.5)	-374	[c]	2.502	5.461	1.401	2.801	0.0	CHNO	3.0	2.467	2.731	0.035	0.700	0.000	0.000	991	1238	5.49	2062	3.3	1.0
ttnh	1,3,4,6-tetranitroglycouril	31	[48]	1.242	0.621	2.484	3.105	0.0	CHNO	1.0	0.000	0.310	1.242	1.242	0.000	0.155	1378	1378	6.38	2432	3.3	0.9
X-0341	X-0341	-196	[c]	2.259	2.250	2.226	2.226	3.8	CHNOX		1.708	1.125	0.550	1.113	0.000	0.000	801	972		1854	3.2	1.2
X-0342	X-0342	-186	[c]	2.212	2.268	2.244	2.244	3.8	CHNOX		1.657	1.134	0.555	1.122	0.000	0.000	825	991		1882	3.2	1.1
X-0343	X-0343	-177	[c]	2.166	2.286	2.262	2.262	3.8	CHNOX		1.607	1.143	0.559	1.131	0.000	0.000	850	1010		1909	3.2	1.1
X-0344	X-0344	-157	[c]	2.074	2.322	2.298	2.298	3.8	CHNOX		1.505	1.161	0.568	1.149	0.000	0.000	898	1048		1963	3.3	1.1

Fernando G. Bastante [1], *María Araújo Fernández* [1], *Eduardo Giráldez* [1].
CINTECX, GESSMin group, University of Vigo

PREDICTIVE MODEL FOR EXPLOSIVE DETONATION PARAMETERS FROM AN EQUATION OF STATE BASED ON DETONATION VELOCITY. Physical Chemistry Chemical Physics 2022

DEoS DATABASE

Number of Explosives 238

	Number of data D	Number of data P
KJ (only CHNO)	449	224
DEoS	519	263

residuals D

Statistics velocity	KJ	DEoS
RMRS	3.4%	1.7%
MAPR	2.5%	1.3%
P97,5	8.2%	3.9%

residuals P

Statistics pressure	KJ	DEoS
RMRS	7.0%	6.0%
MAPR	5.6%	4.9%
P97,5	17.0%	12.6%

Gamma (γ) correlation (CHNO explosives)

	KJ	DEoS
r	0.44	0.53

Jones and Grüneisen parameters (DEoS Model)

	α	Γ
average values	0.27	0.60
standar deviation	0.02	0.06

		experimental data			*calculated D*				*calculated P*										
Acr	density (g/cc)	Dexp (m/s)	Pexp (kbar)	reference	DKJ (m/s)	D_DEoS (m/s)	RRD KJ	RRD_DEoS	PKJ (kbar)	P_DEoS (kbar)	RRP KJ	RRP_DEoS		$\gamma_{experimental}$	γ_{KJ}	$\gamma_{\_DEoS}$		α	Γ
abh	1.64	7200	nan	[8]	7269	7138	1.0%	-0.9%	221	223								0.25	0.54
abh	1.78	7600	nan	[48]	7692	7545	1.2%	-0.7%	261	267								0.25	0.57
AFX902	1.74	8340	290	[8]		8191		-1.8%		279		-3.9%						0.33	0.80
bchmx	1.78	8780	nan	[40]	8807	8660	0.3%	-1.4%	342	346								0.26	0.60
bchmx	1.79	8650	nan	[4]	8842	8694	2.2%	0.5%	346	350								0.26	0.60
BCHMX/GAP (84/16)	1.62	8292	nan	[4]	8173	8078	-1.4%	-2.6%	278	279								0.25	0.57
BCHMX/PIB (91/9)	1.66	8266	nan	[44]	8066	8023	-2.4%	-2.9%	275	278								0.26	0.59
BCHMX/SYLGARD (85/15)	1.58	7858	nan	[3]		7612		-3.1%		236								0.27	0.61
BCHMX/VITON (95/5)	1.78	8520	nan	[24]		8464		-0.7%		328								0.27	0.61
BCHMX/VITON (95/5)	1.82	8740	nan	[24]		8600		-1.6%		344								0.27	0.62
BCHMX/VITON (97/3)[**]	1.79	8650	nan	[3]		8578		-0.8%		339								0.27	0.61
btf	1.76	8260	nan	[8]	8023	8250	-2.9%	-0.1%	282	315								0.26	0.57
btf	1.82	NaN	338	[2]	8213	8443			301	339	-10.9%	0.3%						0.26	0.58
btf	1.84	NaN	345	[2]	8276	8507			308	347	-10.8%	0.7%						0.26	0.58
btf	1.85	8490	340	[8]	8308	8539	-2.1%	0.6%	311	351	-8.5%	3.4%		2.92	3.10	2.84		0.26	0.59
btf	1.86	8490	360	[8]	8340	8572	-1.8%	1.0%	315	356	-12.6%	-1.2%		2.72	3.11	2.84		0.26	0.59
btf	1.90	8620	nan	[46]	8467	8701	-1.8%	0.9%	328	373								0.26	0.60
btnen	1.27	6130	nan	[30]	6676	6354	8.9%	3.7%	156	140								0.24	0.51
btnen	1.41	6880	nan	[30]	7135	6800	3.7%	-1.2%	193	175								0.24	0.53
btnen	1.63	7650	nan	[30]	7855	7499	2.7%	-2.0%	257	240								0.26	0.58
btnen	1.84	8460	nan	[50]	8556	8179	1.1%	-3.3%	329	316								0.27	0.62
btnen	1.87	8500	nan	[30]	8641	8262	1.7%	-2.8%	339	327								0.27	0.62
btnen	1.88	NaN	364	[29]	8677	8297			343	331	-5.8%	-9.0%						0.27	0.62
btnen	1.91	8660	nan	[30]	8772	8389	1.3%	-3.1%	353	343								0.27	0.63
btnen	1.92	8780	nan	[50]	8805	8421	0.3%	-4.1%	357	347								0.28	0.63
btnen	1.93	8657	357.6	[55]	8821	8437	1.9%	-2.5%	359	349	0.4%	-2.4%		3.03	3.17	2.93		0.28	0.63
btnen	1.95	8800	nan	[30]	8903	8516	1.2%	-3.2%	368	359								0.28	0.64
btnen	1.96	8850	nan	[48]	8936	8548	1.0%	-3.4%	372	364								0.28	0.64
BTNEN/BTF (60/40)	1.86	8700	nan	[50]	9043	8676	3.9%	-0.3%	370	367								0.26	0.57
BTNEN/HMX (30/70)	1.91	9020	nan	[50]	9316	9125	3.3%	1.2%	399	407								0.27	0.62
BTNEN/HMX (32/68)	1.88	8884	nan	[55]	9229	9030	3.9%	1.6%	388	394								0.27	0.62
BTNEN/RDX (56/44)	1.85	8701	nan	[55]	9226	8923	6.0%	2.6%	383	381								0.26	0.60
btneu	1.86	9000	nan	[48]	8971	8714	-0.3%	-3.2%	364	364								0.27	0.61
bttc	1.85	8060	nan	[48]	8258	7957	2.5%	-1.3%	307	299								0.27	0.63
cl-20	1.96	9440	nan	[44]	9690	9369	2.6%	-0.7%	438	446								0.26	0.60
cl-20	1.98	9473	nan	[4]	9761	9437	3.0%	-0.4%	447	456								0.27	0.60
CL20/GAP (84/16)	1.73	8676	nan	[4]	8479	8362	-2.3%	-3.6%	311	316								0.26	0.58
CL-20/HTPB (91/9)	1.84	8850	nan	[9]	8857	8692	0.1%	-1.8%	353	362								0.26	0.59
CL-20/HTPB (92/8)	1.86	9052	nan	[9]	8975	8793	-0.8%	-2.9%	364	374								0.26	0.59
CL-20/PIB (91/9)	1.77	8594	nan	[44]	8664	8499	0.8%	-1.1%	330	334								0.26	0.58
CL20/SYLGARD (85/15)	1.66	8277	nan	[3]		7861		-5.0%		264								0.27	0.61
COMP B	1.56	7480	nan	[10]	7490	7436	0.1%	-0.6%	227	227								0.26	0.57
COMP B	1.61	7670	nan	[10]	7651	7600	-0.3%	-0.9%	242	243								0.26	0.58
COMP B	1.67	7868	272	[34]	7843	7796	-0.3%	-0.9%	261	264	-4.2%	-3.0%		2.80	2.94	2.85		0.26	0.59
COMP B	1.67	7690	256.5	[34]	7847	7800	2.0%	1.4%	261	264	1.7%	3.0%		2.85	2.94	2.85		0.26	0.59
COMP B	1.67	7890	267	[34]	7856	7810	-0.4%	-1.0%	262	265	-1.9%	-0.7%		2.90	2.95	2.85		0.26	0.59
COMP B	1.69	7840	267.5	[34]	7914	7868	0.9%	0.4%	268	272	0.0%	1.5%		2.89	2.96	2.86		0.26	0.60
COMP B	1.70	7850	283	[34]	7940	7895	1.1%	0.6%	270	274	-4.6%	-3.0%		2.70	2.97	2.86		0.26	0.60
COMP B	1.70	7750	272	[34]	7950	7904	2.6%	2.0%	271	276	-0.4%	1.3%		2.76	2.97	2.86		0.26	0.60
COMP B	1.71	8022	293	[34]	7979	7934	-0.5%	-1.1%	274	279	-6.5%	-4.8%		2.76	2.98	2.87		0.26	0.60
COMP B	1.72	7920	295	[8]	8004	7960	1.1%	0.5%	276	282	-6.3%	-4.5%		2.66	2.99	2.87		0.27	0.60
COMP B	1.72	7990	nan	[10]	8004	7960	0.2%	-0.4%	276	282								0.27	0.60
COMP B	1.73	7980	297.7	[34]	8033	7990	0.7%	0.1%	279	285	-6.2%	-4.2%		2.70	2.99	2.87		0.27	0.60
COMP B	1.73	7950	263	[34]	8036	7993	1.1%	0.5%	280	285	6.3%	8.5%		3.16	3.00	2.87		0.27	0.60
COMP B	1.73	7886	275	[34]	8036	7993	1.9%	1.4%	280	285	1.7%	3.8%		2.91	3.00	2.87		0.27	0.60
COMP B	1.73	8000	300	[34]	8046	8003	0.6%	0.0%	281	287	-6.5%	-4.5%		2.70	3.00	2.87		0.27	0.60
COMP C3	1.60	7630	nan	[8]	7643	7633	0.2%	0.0%	241	243								0.26	0.59
COMP C4	1.66	8370	nan	[8]	7979	8007	-4.7%	-4.3%	269	275								0.27	0.61
daaf	1.69	7930	306	[17]	7611	7913	-4.0%	-0.2%	247	269	-19.4%	-12.2%		2.46	2.96	2.93		0.28	0.63
DAAF/HMX/VITON (45/50/5)	1.72	8120	nan	[35]		8054		-0.8%		283								0.28	0.64
DAAF/HMX/VITON (60/35/5)	1.70	7970	nan	[35]		7921		-0.6%		270								0.28	0.64
DAAF/HMX/VITON (80/15/5)	1.67	7760	nan	[35]		7731		-0.4%		253								0.28	0.65
DAAF/RDX/VITON (60/35/5)	1.67	7910	nan	[35]		7820		-1.1%		260								0.28	0.64
DAAF/RDX/VITON (80/15/5)	1.66	7760	nan	[35]		7698		-0.8%		249								0.28	0.64
DAAF/VITON (95/5)	1.65	7660	nan	[35]		7596		-0.8%		241								0.28	0.65
datb	1.78	7600	251	[8]	7503	7605	-1.3%	0.1%	248	261	-1.2%	4.0%		3.10	3.04	2.94		0.28	0.64
datb	1.79	7520	259	[10]	7526	7630	0.1%	1.5%	250	264	-3.4%	1.8%		2.90	3.05	2.95		0.28	0.64
datb	1.79	7585	257	[34]	7532	7637	-0.7%	0.7%	251	264	-2.4%	2.9%		3.01	3.05	2.95		0.28	0.64
datb	1.80	7600	251	[8]	7562	7668	-0.5%	0.9%	254	268	1.0%	6.7%		3.14	3.06	2.95		0.28	0.65

Fernando G. Bastante [1], *María Araújo Fernández* [1], *Eduardo Giráldez* [1].
CINTECX, GESSMin group, University of Vigo

PREDICTIVE MODEL FOR EXPLOSIVE DETONATION PARAMETERS FROM AN EQUATION OF STATE BASED ON DETONATION VELOCITY. Physical Chemistry Chemical Physics 2022

DEoS DATABASE

Number of Explosives 238

	Number of data	
	D	***P***
KJ (only CHNO)	449	224
DEoS	519	263

residuals D

Statistics *velocity*	***KJ***	**DEoS**
RMRS	*3.4%*	*1.7%*
MAPR	*2.5%*	*1.3%*
P97,5	*8.2%*	*3.9%*

residuals P

Statistics *pressure*	***KJ***	**DEoS**
RMRS	*7.0%*	*6.0%*
MAPR	*5.6%*	*4.9%*
P97,5	*17.0%*	*12.6%*

Gamma (γ) correlation (CHNO explosives)

	KJ	**DEoS**
r	*0.44*	*0.53*

Jones and Grüneisen parameters (DEoS Model)

	α	Γ
average values	*0.27*	*0.60*
standar deviation	*0.02*	*0.06*

		experimental data			***calculated D***				***calculated P***										
Acr	**density (g/cc)**	**Dexp (m/s)**	**Pexp (kbar)**	**reference**	**DKJ (m/s)**	**D_DEoS (m/s)**	**RRD KJ**	**RRD_DEoS**	**PKJ (kbar)**	**P_DEoS (kbar)**	**RRP KJ**	**RRP_DEoS**		$\gamma_{experimental}$	γ_{KJ}	$\gamma_{\_DEoS}$		α	Γ
datb	1.84	7690	nan	[48]	7679	7793	-0.1%	1.3%	265	282								0.28	0.66
degn	1.38	6760	nan	[8]	7054	6843	4.4%	1.2%	185	174								0.24	0.53
degn	1.38	6600	nan	[48]	7068	6856	7.1%	3.9%	186	175								0.24	0.53
dina	1.00	5950	nan	[33]	5947	5763	-0.1%	-3.1%	102	94								0.22	0.45
dina	1.36	7000	nan	[16]	7157	6971	2.2%	-0.4%	189	178								0.24	0.53
dina	1.48	7400	nan	[16]	7560	7374	2.2%	-0.4%	224	214								0.25	0.55
dina	1.55	7580	nan	[16]	7795	7609	2.8%	0.4%	245	236								0.25	0.57
dina	1.60	7720	nan	[23]	7963	7777	3.1%	0.7%	261	254								0.26	0.58
dina	1.64	7800	nan	[16]	8098	7911	3.8%	1.4%	275	268								0.26	0.58
dina	1.67	8000	nan	[48]	8198	8011	2.5%	0.1%	285	279								0.26	0.59
dipam	1.76	7400	nan	[8]	7482	7452	1.1%	0.7%	245	253								0.27	0.60
dipam	1.79	7500	nan	[48]	7570	7542	0.9%	0.6%	253	262								0.27	0.61
dipetn	1.63	7530	nan	[48]	7930	7661	5.3%	1.7%	262	251								0.26	0.57
dipicrylamine	1.60	7140	nan	[48]	7082	6988	-0.8%	-2.1%	207	207								0.25	0.55
dmtnb	1.60	6820	nan	[48]	6972	6884	2.2%	0.9%	200	199								0.26	0.57
dmttp	1.60	6800	nan	[48]	6816	6786	0.2%	-0.2%	191	192								0.26	0.58
dnaf	1.77	9100	nan	[47]	8938	9005	-1.8%	-1.0%	351	377								0.25	0.57
dnaf	1.88	9450	nan	[47]	9325	9389	-1.3%	-0.6%	396	431								0.26	0.59
dnaf	1.94	9700	nan	[21]	9536	9598	-1.7%	-1.0%	421	463								0.26	0.60
DNAN/RDX/NTO (40/20/40)	1.64	7190	220	[53]	7151	7256	-0.5%	0.9%	214	220	-2.9%	0.1%		2.84	2.91	2.91		0.27	0.62
dnb	1.49	6100	nan	[48]	6158	6195	1.0%	1.6%	149	151								0.25	0.56
dndmo	1.52	7100	nan	[48]	7124	7126	0.3%	0.4%	202	200								0.26	0.59
dnff	1.86	8930	nan	[35]	8704	8880	-2.5%	-0.6%	343	381								0.26	0.59
dnmt	1.56	7850	nan	[35]	7602	7598	-3.2%	-3.2%	234	237								0.25	0.57
DNMT/HMX (49.5/50.5)	1.73	8390	nan	[35]	8351	8322	-0.5%	-0.8%	302	309								0.27	0.60
dnp	1.75	8100	nan	[35]	8121	8055	0.3%	-0.6%	288	295								0.26	0.59
dnq	1.88	9200	nan	[56]	8892	9010	-3.3%	-2.1%	360	382								0.29	0.67
dntfx	1.96	9660	nan	[56]	9500	9483	-1.7%	-1.8%	421	457								0.26	0.60
dp12	1.26	5970	125	[8]		5903		-1.1%		114		-9.1%						0.26	0.60
edad	1.30	6660	nan	[33]	6620	6754	-0.6%	1.4%	156	153								0.27	0.61
edad	1.60	7670	nan	[48]	7579	7862	-1.2%	2.5%	237	246								0.29	0.68
EDC-11	1.78	8213	315	[14]	8309	8255	1.2%	0.5%	304	312	-3.4%	-0.9%		2.82	3.04	2.89		0.27	0.61
EDC-24	1.78	8710	nan	[14]	8476	8491	-2.7%	-2.5%	316	327								0.27	0.63
edna	1.66	8240	nan	[48]	8122	8218	-1.4%	-0.3%	278	286								0.27	0.63
etdn	1.48	7300	nan	[48]	7971	7576	9.2%	3.8%	249	229								0.24	0.53
etn	1.65	7940	nan	[32]	8244	7825	3.8%	-1.5%	286	267								0.25	0.56
etn	1.68	7887	nan	[51]	8354	7928	5.9%	0.5%	297	278								0.25	0.57
etn	1.70	8027	nan	[32]	8415	7986	4.8%	-0.5%	303	285								0.26	0.57
etn	1.70	7994	nan	[51]	8428	7999	5.4%	0.1%	305	286								0.26	0.57
explosive d	1.48	6700	nan	[8]	6595	6604	-1.6%	-1.4%	170	168								0.26	0.59
explosive d	1.55	6850	nan	[8]	6801	6822	-0.7%	-0.4%	187	186								0.27	0.60
explosive d	1.63	7150	nan	[48]	7035	7071	-1.6%	-1.1%	206	209								0.27	0.62
fefo	1.59	7500	250	[8]		7148		-4.7%		209		-16.5%						0.27	0.61
fefo	1.61	7450	245	[8]		7212		-3.2%		215		-12.4%						0.27	0.62
FM1	1.51	6570	190	[8]		6976		6.2%		191		0.7%						0.26	0.59
fox-12	1.67	7970	261.1	[20]	7539	8025	-5.4%	0.7%	240	264	-7.9%	1.2%		3.05	2.94	3.06		0.30	0.71
fox-7	1.78	8375	284	[54]	8268	8395	-1.3%	0.2%	301	316	6.0%	11.3%		3.40	3.04	2.97		0.28	0.66
fox-7	1.78	8405	292	[54]	8268	8395	-1.6%	-0.1%	301	316	3.1%	8.3%		3.31	3.04	2.97		0.28	0.66
fox-7	1.89	8870	nan	[56]	8608	8760	-3.0%	-1.2%	338	361								0.29	0.68
FOX-7/EVA (95.1/4.9)	1.69	8110	251	[26]	7855	7978	-3.1%	-1.6%	263	273	4.8%	8.6%		3.42	2.96	2.94		0.28	0.64
FOX-7/EVA (95/5)	1.65	7730	241	[26]	7725	7838	-0.1%	1.4%	250	258	3.9%	7.0%		3.08	2.92	2.92		0.27	0.63
FOX-7/TNT (30/70)	1.62	7060	nan	[52]	7175	7160	1.6%	1.4%	214	216								0.26	0.59
FOX-7/TNT (60/40)	1.70	7600	nan	[52]	7679	7712	1.0%	1.5%	253	259								0.27	0.62
FOX-7/VITON (95/5)	1.85	8400	nan	[35]		8434		0.4%		326								0.30	0.70
FOX-7/WAX (98.5/1.5)	1.76	8335	nan	[1]	8136	8273	-2.4%	-0.7%	289	303								0.28	0.65
H2O2/H2O (90,5/9,5)[*]	1.39	6140	nan	[37]	5297	5731	-13.7%	-6.7%	105	107								0.35	0.85
ha	1.20	7320	nan	[19]	6311	7706	-13.8%	5.3%	134	169								0.34	0.82
hac	1.13	7570	166	[39]	7191	7498	-5.0%	-1.0%	165	170	-0.6%	2.3%		2.89	2.53	2.73		0.24	0.54
HAC/W (60/40)	1.09	6270	nan	[39]	5861	6380	-6.5%	1.8%	107	112								0.28	0.65
HAC/W (62/38)	1.09	6350	nan	[39]	5951	6446	-6.3%	1.5%	110	115								0.28	0.64
HAC/W (69/31)	1.10	6630	nan	[39]	6226	6655	-6.1%	0.4%	121	125								0.27	0.61
HAC/W (78/26)	1.11	7070	nan	[39]	6574	6938	-7.0%	-1.9%	136	139								0.26	0.58
HAC/W (88/12)	1.12	7390	nan	[39]	6875	7201	-7.0%	-2.6%	150	153								0.25	0.56
HAC/W (93/7)	1.12	7470	nan	[39]	7013	7328	-6.1%	-1.9%	156	160								0.25	0.55
HAC/W (98/2)	1.13	7540	nan	[39]	7146	7454	-5.2%	-1.1%	163	167								0.25	0.54
hco	1.79	8520	nan	[33]	8748	8499	2.7%	-0.2%	339	337								0.26	0.59
hmx	1.00	5800	110	[8]	6043	5937	4.2%	2.4%	105	100	-4.1%	-9.1%		2.06	2.46	2.52		0.22	0.46
hmx	1.18	6670	155	[8]	6658	6563	-0.2%	-1.6%	147	140	-5.3%	-9.6%		2.39	2.56	2.63		0.23	0.50
hmx	1.20	6580	160	[8]	6727	6632	2.2%	0.8%	152	145	-5.1%	-9.3%		2.25	2.58	2.64		0.23	0.50

Fernando G. Bastante [1], *María Araújo Fernández* [1], *Eduardo Giráldez* [1].
CINTECX, GESSMin group, University of Vigo

PREDICTIVE MODEL FOR EXPLOSIVE DETONATION PARAMETERS FROM AN EQUATION OF STATE BASED ON DETONATION VELOCITY. Physical Chemistry Chemical Physics 2022

DEoS DATABASE

Number of Explosives 238

	Number of data	
	D	***P***
KJ (only CHNO)	449	224
DEoS	519	263

residuals D

Statistics velocity	***KJ***	***DEoS***
RMRS	*3.4%*	*1.7%*
MAPR	*2.5%*	*1.3%*
$P_{97,5}$	*8.2%*	*3.9%*

residuals P

Statistics pressure	***KJ***	***DEoS***
RMRS	*7.0%*	*6.0%*
MAPR	*5.6%*	*4.9%*
$P_{97,5}$	*17.0%*	*12.6%*

Gamma (γ) correlation (CHNO explosives)

	KJ	***DEoS***
r	*0.44*	*0.53*

Jones and Grüneisen parameters (DEoS Model)

	α	Γ
average values	*0.27*	*0.60*
standar deviation	*0.02*	*0.06*

		experimental data			***calculated D***				***calculated P***										
Acr	**density (g/cc)**	**Dexp (m/s)**	**Pexp (kbar)**	**reference**	**D_{KJ} (m/s)**	**D_{DEoS} (m/s)**	**RRD_{KJ}**	**RRD_{DEoS}**	**P_{KJ} (kbar)**	**P_{DEoS} (kbar)**	**RRP_{KJ}**	**RRP_{DEoS}**		**$\gamma_{experimental}$**	**γ_{KJ}**	**γ_{DEoS}**		**α**	**Γ**
hmx	1.40	7300	210	[8]	7410	7328	1.5%	0.4%	207	201	-1.6%	-4.2%		2.55	2.72	2.74		0.25	0.54
hmx	1.60	7910	280	[8]	8093	8024	2.3%	1.4%	270	269	-3.6%	-3.8%		2.58	2.88	2.82		0.26	0.58
hmx	1.72	8480	nan	[29]	8503	8441	0.3%	-0.5%	312	316								0.27	0.60
hmx	1.77	8500	323	[38]	8674	8615	2.0%	1.4%	330	338	2.3%	4.5%		2.96	3.03	2.89		0.27	0.61
hmx	1.80	NaN	361	[2]	8776	8719			342	351	-5.4%	-2.9%						0.27	0.62
hmx	1.81	8780	nan	[29]	8817	8761	0.4%	-0.2%	346	356								0.27	0.62
hmx	1.88	9050	nan	[50]	9032	8980	-0.2%	-0.8%	371	385								0.28	0.63
hmx	1.89	9100	405	[8]	9083	9032	-0.2%	-0.7%	377	392	-7.0%	-3.2%		2.86	3.14	2.93		0.28	0.64
hmx	1.89	9110	390	[8]	9083	9032	-0.3%	-0.9%	377	392	-3.4%	0.5%		3.02	3.14	2.93		0.28	0.64
hmx	1.90	9110	393	[31]	9118	9067	0.1%	-0.5%	381	397	-3.1%	0.9%		3.01	3.15	2.94		0.28	0.64
hmx	1.90	9150	nan	[48]	9118	9067	-0.4%	-0.9%	381	397								0.28	0.64
HMX/EXON (91/9)	1.83	8665	343	[14]		8545		-1.4%		337		-1.6%						0.28	0.66
HMX/GAP (84/16)	1.64	8384	nan	[4]	8120	8083	-3.1%	-3.6%	276	280								0.26	0.58
HMX/HN (75/25)	1.86	9100	nan	[14]	9096	9126	0.0%	0.3%	374	391								0.28	0.65
HMX/PIB (91/9)	1.67	8318	nan	[44]	8004	8037	-3.8%	-3.4%	271	278								0.27	0.61
HMX/SYLGARD (85/15)	1.59	7936	nan	[3]		7633		-3.8%		237								0.27	0.63
HMX/TATB/VITON (10/80/10)	1.84	7400	245	[5]		7554		2.1%		255		4.2%						0.31	0.74
HMX/TATB/VITON (20/70/10)	1.84	7410	253	[5]		7671		3.5%		265		4.6%						0.31	0.73
HMX/TATB/VITON (30/60/10)	1.82	7640	260	[5]		7722		1.1%		267		2.6%						0.30	0.72
HMX/TATB/VITON (40/50/10)	1.83	7730	278	[5]		7868		1.8%		279		0.5%						0.30	0.71
HMX/TATB/VITON (50/40/10)	1.83	7910	290	[5]		7979		0.9%		288		-0.6%						0.30	0.70
HMX/TATB/VITON (60/30/10)	1.83	8120	300	[5]		8089		-0.4%		297		-0.9%						0.30	0.69
HMX/TATB/VITON (70/20/10)	1.83	8190	304	[5]		8198		0.1%		306		0.7%						0.29	0.68
HMX/TATB/VITON (80/10/10)	1.84	8240	312	[5]		8339		1.2%		319		2.3%						0.29	0.68
HMX/TNT (60/40)	1.60	7360	216	[38]	7605	7544	3.3%	2.5%	238	239	10.4%	10.4%		3.01	2.88	2.82		0.26	0.58
HMX/TNT (60/40)	1.63	7550	226	[38]	7701	7642	2.0%	1.2%	247	249	9.5%	10.0%		3.11	2.91	2.83		0.26	0.58
HMX/TNT (60/40)	1.67	7590	241	[38]	7829	7772	3.2%	2.4%	260	262	7.7%	8.9%		2.99	2.94	2.85		0.26	0.59
HMX/TNT (60/40)	1.70	7680	253	[38]	7926	7870	3.2%	2.5%	269	273	6.4%	7.9%		2.96	2.97	2.86		0.26	0.60
HMX/TNT (60/40)	1.75	8000	nan	[52]	8086	8033	1.1%	0.4%	285	291								0.27	0.61
HMX/TNT (60/40)	1.80	8160	320	[8]	8247	8196	1.1%	0.4%	302	310	-5.7%	-3.0%		2.75	3.06	2.89		0.27	0.62
HMX/TNT (70/30)	1.60	7520	227	[38]	7728	7665	2.8%	1.9%	246	246	8.4%	8.4%		2.99	2.88	2.82		0.26	0.58
HMX/TNT (70/30)	1.64	7680	243	[38]	7858	7797	2.3%	1.5%	259	260	6.4%	7.0%		2.98	2.92	2.83		0.26	0.59
HMX/TNT (70/30)	1.68	7810	257	[38]	7989	7930	2.3%	1.5%	271	274	5.6%	6.7%		2.99	2.95	2.85		0.26	0.59
HMX/TNT (70/30)	1.70	7900	267	[38]	8054	7996	2.0%	1.2%	278	282	4.1%	5.5%		2.97	2.97	2.86		0.26	0.60
HMX/TNT (70/30)	1.77	8192	295	[45]	8283	8228	1.1%	0.4%	301	308	2.1%	4.6%		3.03	3.03	2.89		0.27	0.61
HMX/TNT (75/25)	1.82	8550	306.5	[34]	8516	8463	-0.4%	-1.0%	324	334	5.7%	9.0%		3.34	3.08	2.90		0.27	0.62
HMX/TNT (75/25)	1.81	8480	nan	[8]	8480	8426	0.0%	-0.6%	320	329								0.27	0.62
HMX/TNT (78/22)	1.82	NaN	342	[8]	8553	8499			327	337	-4.5%	-1.6%						0.27	0.62
HMX/TNT (80/20)	1.61	7730	242	[38]	7884	7818	2.0%	1.1%	257	257	6.3%	6.3%		2.98	2.89	2.82		0.26	0.58
HMX/TNT (80/20)	1.64	7820	251	[38]	7983	7919	2.1%	1.3%	267	268	6.3%	6.8%		3.00	2.92	2.84		0.26	0.59
HMX/TNT (80/20)	1.68	7950	265	[38]	8116	8054	2.1%	1.3%	280	283	5.7%	6.7%		3.01	2.95	2.85		0.26	0.59
HMX/TNT (80/20)	1.71	8050	278	[38]	8215	8155	2.0%	1.3%	290	294	4.4%	5.9%		2.99	2.98	2.86		0.26	0.60
HMX/TNT (80/20)	1.82	8523	331	[45]	8579	8526	0.7%	0.0%	329	339	-0.7%	2.3%		2.99	3.08	2.91		0.27	0.62
HMX/TNT (89/11)	1.84	8778	352	[45]	8766	8713	-0.1%	-0.7%	345	357	-1.9%	1.4%		3.03	3.09	2.91		0.27	0.63
HMX/TNT (90/10)	1.60	7850	247	[38]	7972	7904	1.6%	0.7%	262	262	6.0%	5.9%		2.99	2.88	2.82		0.26	0.58
HMX/TNT (90/10)	1.65	8000	266	[38]	8140	8076	1.8%	0.9%	279	280	4.7%	5.3%		2.97	2.92	2.84		0.26	0.59
HMX/TNT (90/10)	1.71	8200	288	[38]	8342	8281	1.7%	1.0%	299	303	3.9%	5.3%		2.99	2.98	2.87		0.27	0.60
HMX/TNT (90/10)	1.75	8320	303	[38]	8477	8418	1.9%	1.2%	313	319	3.4%	5.4%		3.00	3.01	2.88		0.27	0.61
hn	1.63	8691	nan	[14]	7920	8354	-8.9%	-3.9%	261	279								0.30	0.71
hnab	1.60	7310	205	[8]	7196	7091	-1.6%	-3.0%	213	215	4.1%	4.7%		3.17	2.88	2.75		0.25	0.54
hnb	1.97	9340	430	[8]	9338	9250	0.0%	-1.0%	408	437	-5.2%	1.7%		3.00	3.21	2.85		0.26	0.59
hnb	1.97	9300	420	[55]	9348	9260	0.5%	-0.4%	409	439	-2.7%	4.5%		3.06	3.22	2.86		0.26	0.60
hnb	1.97	9335	400	[34]	9348	9260	0.1%	-0.8%	409	439	2.2%	9.7%		3.30	3.22	2.86		0.26	0.60
hnb	2.00	9500	nan	[46]	9440	9349	-0.6%	-1.6%	420	452								0.26	0.60
hnbp	1.60	7100	nan	[48]	7075	6945	-0.4%	-2.2%	206	206								0.25	0.54
hnetn	1.86	7580	nan	[46]	7373	7496	-2.7%	-1.1%	246	256								0.31	0.73
hns	1.00	5100	73	[8]	5131	5082	0.6%	-0.3%	76	75	4.1%	2.2%		2.56	2.46	2.46		0.22	0.44
hns	1.20	5740	115	[8]	5711	5653	-0.5%	-1.5%	109	107	-4.8%	-6.7%		2.44	2.58	2.58		0.23	0.48
hns	1.40	6340	160	[8]	6291	6224	-0.8%	-1.8%	149	148	-6.9%	-7.7%		2.52	2.72	2.67		0.24	0.51
hns	1.60	6800	nan	[8]	6871	6795	1.0%	-0.1%	195	196								0.25	0.55
hns	1.66	7030	215	[8]	7045	6967	0.2%	-0.9%	209	213	-2.6%	-1.0%		2.82	2.93	2.78		0.25	0.56
hns	1.70	7000	210	[38]	7161	7081	2.3%	1.2%	220	224	4.6%	6.8%		2.97	2.97	2.80		0.25	0.57
hns	1.70	7000	nan	[8]	7161	7081	2.3%	1.2%	220	224								0.25	0.57
hns	1.74	7130	nan	[48]	7277	7195	2.1%	0.9%	230	236								0.26	0.58
HZ/HN (21/79)	1.44	8600	nan	[14]	7888	8425	-8.3%	-2.0%	239	255								0.29	0.68
HZ/HN (70/30)	1.14	8025	nan	[14]	6625	7904	-17.4%	-1.5%	141	170								0.33	0.79
IMX-104	1.72	7705	nan	[36]	7414	7578	-3.8%	-1.6%	237	250								0.28	0.65
IMX-104	1.76	7714	nan	[43]	7512	7685	-2.6%	-0.4%	247	261								0.28	0.66
ipn	1.04	5400	nan	[48]	5474	5429	1.4%	0.5%	89	83								0.24	0.52

Fernando G. Bastante [1], *María Araújo Fernández* [1], *Eduardo Giráldez* [1].
CINTECX, GESSMin group, University of Vigo

PREDICTIVE MODEL FOR EXPLOSIVE DETONATION PARAMETERS FROM AN EQUATION OF STATE BASED ON DETONATION VELOCITY. Physical Chemistry Chemical Physics 2022

DEoS DATABASE

Number of Explosives 238

	Number of data	
	D	***P***
KJ (only CHNO)	449	224
DEoS	519	263

residuals D

Statistics velocity	***KJ***	***DEoS***
RMRS	*3.4%*	*1.7%*
MAPR	*2.5%*	*1.3%*
$P_{97,5}$	*8.2%*	*3.9%*

residuals P

Statistics pressure	***KJ***	***DEoS***
RMRS	*7.0%*	*6.0%*
MAPR	*5.6%*	*4.9%*
$P_{97,5}$	*17.0%*	*12.6%*

Gamma (γ) correlation (CHNO explosives)

	KJ	***DEoS***
r	*0.44*	*0.53*

Jones and Grüneisen parameters (DEoS Model)

	α	Γ
average values	*0.27*	*0.60*
standar deviation	*0.02*	*0.06*

		experimental data			***calculated D***				***calculated P***										
Acr	**density (g/cc)**	**Dexp (m/s)**	**Pexp (kbar)**	**reference**	**D_{KJ} (m/s)**	**D_{DEoS} (m/s)**	**RR_D KJ**	**RR_{D_DEoS}**	**P_{KJ} (kbar)**	**P_{DEoS} (kbar)**	**RR_P KJ**	**RR_{P_DEoS}**		**$\gamma_{experimental}$**	**γ_{KJ}**	**$\gamma_{\_DEoS}$**		**α**	**Γ**
LLM-105/VITON (95/5)	1.78	7980	nan	[35]		7880		-1.3%		285								0.27	0.60
LLM-175/VITON (95/5)	1.65	7730	nan	[35]		7472		-3.3%		241								0.26	0.58
LX-01	1.24	6840	nan	[8]	6952	6739	1.6%	-1.5%	166	155								0.23	0.50
LX-01	1.31	NaN	156	[10]	7195	6979			186	174	19.0%	11.3%						0.24	0.51
LX-04	1.86	8460	350	[8]		8281		-2.1%		314		-10.2%						0.30	0.71
LX-04	1.87	8480	320	[13]		8308		-2.0%		317		-0.8%						0.30	0.71
LX-04	1.87	8480	345	[34]		8305		-2.1%		317		-8.1%						0.30	0.71
LX-04	1.87	8540	nan	[10]		8315		-2.6%		318								0.30	0.71
LX-07	1.85	8590	377.3	[34]		8479		-1.3%		332		-11.9%						0.29	0.68
LX-07	1.87	8640	nan	[8]		8547		-1.1%		341								0.29	0.68
LX-09	1.86	8820	366.3	[34]		8855		0.4%		371		1.4%						0.28	0.63
LX-09	1.84	8810	377	[8]		8783		-0.3%		362		-4.0%						0.27	0.63
LX-10	1.84	8810	372	[34]		8662		-1.7%		349		-6.1%						0.28	0.65
LX-10	1.86	8820	375	[8]		8728		-1.0%		358		-4.6%						0.28	0.65
LX-10	1.87	8850	375	[10]		8762		-1.0%		362		-3.4%						0.28	0.65
LX-11	1.86	8320	nan	[8]		8027		-3.5%		291								0.32	0.75
LX-14	1.81	8760	nan	[14]	8643	8629	-1.3%	-1.5%	332	344								0.27	0.63
LX-14	1.83	8800	370	[8]	8710	8698	-1.0%	-1.2%	340	353	-8.2%	-4.7%		2.83	3.09	2.93		0.28	0.63
LX-14	1.84	8830	370	[8]	8743	8733	-1.0%	-1.1%	344	357	-7.1%	-3.5%		2.88	3.09	2.93		0.28	0.63
LX-14	1.87	8840	nan	[9]	8844	8836	0.0%	0.0%	355	371								0.28	0.64
LX-15	1.58	6840	nan	[8]		6591		-3.6%		181								0.25	0.56
LX-17	1.91	7630	260	[8]		7807		2.3%		283		8.9%						0.31	0.74
manitrol	1.75	8260	nan	[48]	8522	8068	3.2%	-2.3%	317	298								0.26	0.58
md	1.73	9000	nan	[48]	8849	8804	-1.7%	-2.2%	339	344								0.27	0.62
MEN-II	1.02	5490	nan	[8]	5626	5590	2.5%	1.8%	93	86								0.24	0.54
metn	1.46	7180	nan	[48]	7378	7145	2.8%	-0.5%	211	199								0.25	0.54
nag	1.65	8600	nan	[48]	7904	8505	-8.1%	-1.1%	263	293								0.30	0.71
ng	1.59	7650	253	[10]	8133	7726	6.3%	1.0%	272	252	7.3%	-0.3%		2.68	2.87	2.76		0.25	0.55
ng	1.59	7580	nan	[14]	8133	7726	7.3%	1.9%	272	252								0.25	0.55
ng	1.60	7700	253	[8]	8168	7759	6.1%	0.8%	275	256	8.7%	1.1%		2.75	2.88	2.77		0.25	0.55
ng	1.60	7740	nan	[48]	8168	7759	5.5%	0.2%	275	256								0.25	0.55
nm	1.13	6250	128	[31]	6372	6238	2.0%	-0.2%	130	121	1.3%	-5.8%		2.44	2.53	2.64		0.23	0.50
nm	1.13	6250	133	[31]	6372	6238	2.0%	-0.2%	130	121	-2.5%	-9.4%		2.31	2.53	2.64		0.23	0.50
nm	1.13	6370	125	[34]	6379	6245	0.1%	-2.0%	130	121	4.1%	-3.2%		2.67	2.53	2.64		0.23	0.50
nm	1.13	6280	120	[8]	6379	6245	1.6%	-0.6%	130	121	8.5%	0.8%		2.71	2.53	2.64		0.23	0.50
nm	1.13	6350	125	[8]	6379	6245	0.5%	-1.6%	130	121	4.1%	-3.2%		2.65	2.53	2.64		0.23	0.50
nm	1.13	6299	134	[34]	6389	6256	1.4%	-0.7%	131	122	-2.3%	-9.2%		2.35	2.53	2.64		0.23	0.50
nm	1.14	6370	nan	[48]	6413	6280	0.7%	-1.4%	132	123								0.23	0.50
nmet	1.21	6750	nan	[48]	7031	6728	4.2%	-0.3%	167	152								0.23	0.49
no	1.30	5620	103	[14]	5785	5613	2.9%	-0.1%	119	106	15.9%	2.6%		2.99	2.64	2.88		0.27	0.61
nona	1.70	7400	nan	[8]	7359	7217	-0.6%	-2.5%	232	234								0.25	0.56
nona	1.78	7560	nan	[48]	7597	7448	0.5%	-1.5%	254	259								0.26	0.57
nq	1.00	5460	nan	[33]	5448	5612	-0.2%	2.8%	86	84								0.25	0.55
nq	1.40	NaN	158	[18]	6680	7119			168	178	6.3%	12.9%						0.29	0.66
nq	1.51	7540	nan	[15]	7031	7549	-6.8%	0.1%	196	214								0.30	0.69
nq	1.55	7650	nan	[8]	7142	7684	-6.6%	0.4%	206	226								0.30	0.70
nq	1.62	7930	nan	[8]	7357	7948	-7.2%	0.2%	225	251								0.31	0.72
nq	1.63	7980	nan	[15]	7385	7982	-7.5%	0.0%	227	254								0.31	0.72
nq	1.63	NaN	256	[29]	7385	7982			227	254	-11.2%	-0.7%						0.31	0.72
nq	1.64	7940	nan	[29]	7403	8004	-6.8%	0.8%	229	257								0.31	0.73
nq	1.65	7980	nan	[29]	7453	8065	-6.6%	1.1%	234	263								0.31	0.73
nq	1.70	8200	nan	[48]	7604	8249	-7.3%	0.6%	248	281								0.31	0.74
nq	1.72	NaN	245	[8]	7665	8325			254	289	3.5%	18.1%						0.32	0.75
nq	1.78	8590	nan	[8]	7850	8551	-8.6%	-0.5%	272	314								0.32	0.76
NQ/ESTANE (95/5)	1.70	8280	268	[14]	7460	8128	-9.9%	-1.8%	238	272	-11.0%	1.4%		3.35	2.97	3.13		0.32	0.76
NQ/TNT(35/65)	1.66	NaN	212	[18]	7243	7373			221	230	4.4%	8.4%						0.28	0.63
NQ/TNT(50/50)	1.67	NaN	221	[18]	7340	7564			228	240	3.1%	8.7%						0.28	0.65
NQ/TNT(50/50)	1.66	7400	nan	[18]	7334	7557	-0.9%	2.1%	227	240								0.28	0.65
NQ/TNT(50/50)	1.64	7280	nan	[18]	7274	7490	-0.1%	2.9%	222	233								0.28	0.65
NQ/TNT(50/50)	1.64	7620	nan	[18]	7259	7474	-4.7%	-1.9%	220	231								0.28	0.65
NQ/TNT(50/50)	1.64	7430	nan	[18]	7253	7467	-2.4%	0.5%	220	231								0.28	0.65
NQ/TNT(80/20)	1.69	7833	nan	[18]	7528	7987	-3.9%	2.0%	242	266								0.30	0.71
NQ/TNT(90/10)	1.70	8022	nan	[18]	7585	8136	-5.5%	1.4%	246	276								0.31	0.73
NQ/TNT(95/5)	1.69	8056	nan	[18]	7564	8156	-6.1%	1.2%	244	275								0.31	0.73
nto	1.00	5269	nan	[33]	5275	5321	0.1%	1.0%	80	77								0.24	0.51
nto	1.80	8020	nan	[35]	7660	8028	-4.5%	0.1%	260	287								0.30	0.70
nto	1.83	8090	nan	[35]	7749	8129	-4.2%	0.5%	269	298								0.30	0.71
nto	1.86	8200	nan	[35]	7839	8231	-4.4%	0.4%	278	310								0.30	0.71
nto	1.87	8180	nan	[35]	7868	8264	-3.8%	1.0%	281	314								0.30	0.72

Fernando G. Bastante [1], *María Araújo Fernández* [1], *Eduardo Giráldez* [1].
CINTECX, GESSMin group, University of Vigo

PREDICTIVE MODEL FOR EXPLOSIVE DETONATION PARAMETERS FROM AN EQUATION OF STATE BASED ON DETONATION VELOCITY. Physical Chemistry Chemical Physics 2022

DEoS DATABASE

Number of Explosives 238

	Number of data	
	D	***P***
KJ (only CHNO)	449	224
DEoS	519	263

residuals D

Statistics *velocity*	***KJ***	**DEoS**
RMRS	*3.4%*	*1.7%*
MAPR	*2.5%*	*1.3%*
P97,5	*8.2%*	*3.9%*

residuals P

Statistics *pressure*	***KJ***	**DEoS**
RMRS	*7.0%*	*6.0%*
MAPR	*5.6%*	*4.9%*
P97,5	*17.0%*	*12.6%*

Gamma (γ) correlation (CHNO explosives)

	KJ	**DEoS**
r	*0.44*	*0.53*

Jones and Grüneisen parameters (DEoS Model)

	α	Γ
average values	*0.27*	*0.60*
standar deviation	*0.02*	*0.06*

		experimental data			***calculated D***				***calculated P***									
Acr	**density (g/cc)**	**Dexp (m/s)**	**Pexp (kbar)**	**reference**	**DKJ (m/s)**	**D_DEoS (m/s)**	**RRD KJ**	**RRD_DEoS**	**PKJ (kbar)**	**P_DEoS (kbar)**	**RRP KJ**	**RRP_DEoS**		$\gamma_{experimental}$	γ_{KJ}	$\gamma_{\_DEoS}$	α	Γ
nto	1.87	8220	nan	[35]	7868	8264	-4.3%	0.5%	281	314							0.30	0.72
NTO/RDX/TNT (50/12/38)	1.79	7660	265	[22]	7722	7852	0.8%	2.5%	264	279	-0.5%	5.3%		2.97	3.05	2.96	0.28	0.65
NTO/TNT (30/70)	1.64	6900	nan	[52]	7060	7097	2.3%	2.9%	209	213							0.27	0.60
NTO/TNT (50/50)	1.71	7370	226	[22]	7317	7430	-0.7%	0.8%	230	240	1.9%	6.3%		3.11	2.98	2.93	0.28	0.63
NTO/TNT (60/40)	1.69	7300	nan	[52]	7279	7425	-0.3%	1.7%	226	237							0.28	0.64
NTO/TNT (60/40)	1.78	7840	256	[22]	7546	7713	-3.8%	-1.6%	251	267	-2.0%	4.1%		3.27	3.04	2.97	0.28	0.66
OCTOL	1.81	8476	343	[14]	8494	8440	0.2%	-0.4%	321	330	-6.4%	-3.7%		2.79	3.07	2.90	0.27	0.62
OCTOL	1.81	8450	338	[8]	8497	8443	0.6%	-0.1%	321	331	-4.9%	-2.1%		2.82	3.07	2.90	0.27	0.62
ont	1.80	7330	nan	[48]	7457	7360	1.7%	0.4%	247	254							0.26	0.58
PAX-41	1.70	7830	nan	[35]	7843	7825	0.2%	-0.1%	264	269							0.27	0.60
PBX-9007	1.64	8090	nan	[8]	7776	7807	-3.9%	-3.5%	253	259							0.26	0.60
PBX-9007	1.60	NaN	265	[10]	7647	7673			241	245	-9.0%	-7.6%					0.26	0.59
PBX-9010	1.78	8363	319	[55]		8301		-0.7%		310		-3.0%					0.28	0.65
PBX-9010	1.78	8370	328	[8]		8297		-0.9%		309		-5.7%					0.28	0.65
PBX-9011	1.77	8500	324	[8]	8304	8337	-2.3%	-1.9%	303	314	-6.5%	-3.2%		2.95	3.03	2.92	0.27	0.63
PBX-9205	1.67	8170	nan	[8]	7982	7994	-2.3%	-2.1%	270	276							0.27	0.60
PBX-9404	1.84	8800	365	[14]		8769		-0.4%		360		-1.3%					0.28	0.63
PBX-9404	1.84	8800	375	[8]		8769		-0.4%		360		-4.0%					0.28	0.63
PBX-9407	1.60	7910	287	[8]		7855		-0.7%		256		-10.8%					0.26	0.60
PBX-9408	1.84	8787	nan	[14]		8770		-0.2%		361							0.28	0.63
PBX9501	1.83	8802	nan	[7]	8774	8743	-0.3%	-0.7%	345	357							0.27	0.63
PBX9501	1.84	8830	nan	[8]	8801	8771	-0.3%	-0.7%	348	361							0.28	0.63
PBX9502	1.91	7710	nan	[8]		7906		2.5%		292							0.31	0.72
PBX9502	1.90	7710	289	[10]		7858		1.9%		287		-0.7%					0.31	0.72
PBX9503	1.90	7710	nan	[8]		8043		4.3%		303							0.30	0.71
pent	1.23	6370	139	[8]	6839	6546	7.4%	2.8%	160	146	15.1%	5.3%		2.59	2.60	2.60	0.23	0.48
pent	1.23	6364	143.2	[25]	6832	6539	7.4%	2.7%	159	146	11.4%	1.9%		2.47	2.59	2.60	0.23	0.48
pent	1.26	6590	160	[8]	6942	6644	5.3%	0.8%	168	154	4.9%	-3.8%		2.42	2.62	2.61	0.23	0.49
pent	1.38	6910	173	[34]	7352	7036	6.4%	1.8%	201	186	16.4%	7.5%		2.81	2.70	2.67	0.24	0.51
pent	1.45	7178	207.4	[25]	7585	7259	5.7%	1.1%	222	206	6.9%	-0.7%		2.60	2.76	2.70	0.24	0.53
pent	1.45	7180	208	[8]	7592	7265	5.7%	1.2%	222	207	6.9%	-0.7%		2.59	2.76	2.70	0.24	0.53
pent	1.50	7480	240	[8]	7763	7429	3.8%	-0.7%	238	222	-0.9%	-7.4%		2.50	2.80	2.73	0.24	0.53
pent	1.53	7490	225	[34]	7865	7527	5.0%	0.5%	248	232	10.0%	3.0%		2.81	2.82	2.74	0.25	0.54
pent	1.60	7737	263.7	[34]	8095	7746	4.6%	0.1%	270	254	2.3%	-3.5%		2.63	2.88	2.77	0.25	0.55
pent	1.60	7900	nan	[10]	8105	7756	2.6%	-1.8%	271	255							0.25	0.55
pent	1.60	7750	266	[8]	8105	7756	4.6%	0.1%	271	255	1.8%	-4.0%		2.61	2.88	2.77	0.25	0.55
pent	1.66	7926	nan	[51]	8320	7962	5.0%	0.5%	292	278							0.25	0.56
pent	1.67	7980	300	[10]	8344	7985	4.6%	0.1%	295	280	-1.7%	-6.5%		2.54	2.94	2.80	0.25	0.57
pent	1.70	8070	307	[8]	8447	8083	4.7%	0.2%	306	292	-0.4%	-5.0%		2.61	2.97	2.81	0.26	0.57
pent	1.70	8082	302.1	[25]	8457	8093	4.6%	0.1%	307	293	1.5%	-3.1%		2.68	2.97	2.81	0.26	0.57
pent	1.76	8260	nan	[10]	8652	8279	4.7%	0.2%	328	315							0.26	0.58
pent	1.76	8270	310	[8]	8652	8279	4.6%	0.1%	328	315	5.7%	1.6%		2.88	3.02	2.83	0.26	0.58
pent	1.76	8270	337	[8]	8652	8279	4.6%	0.1%	328	315	-2.8%	-6.5%		2.57	3.02	2.83	0.26	0.58
pent	1.76	8263	314.3	[25]	8662	8289	4.8%	0.3%	329	316	4.6%	0.6%		2.83	3.02	2.83	0.26	0.58
pent	1.77	8300	335	[14]	8686	8312	4.7%	0.1%	331	319	-1.1%	-4.8%		2.64	3.03	2.83	0.26	0.58
PENTOLITE	1.64	7530	nan	[8]	7612	7416	1.1%	-1.5%	243	237							0.25	0.57
PENTOLITE	1.64	7520	256.3	[34]	7625	7428	1.4%	-1.2%	244	239	-4.9%	-6.9%		2.63	2.92	2.80	0.25	0.57
PENTOLITE	1.64	7520	252	[34]	7625	7428	1.4%	-1.2%	244	239	-3.2%	-5.3%		2.69	2.92	2.80	0.25	0.57
PENTOLITE	1.65	7465	nan	[14]	7644	7447	2.4%	-0.2%	246	241							0.26	0.57
PENTOLITE	1.66	7448	241	[34]	7675	7478	3.1%	0.4%	249	244	3.2%	1.1%		2.82	2.93	2.81	0.26	0.57
PENTOLITE	1.68	7650	251	[8]	7739	7540	1.2%	-1.4%	255	250	1.4%	-0.3%		2.92	2.95	2.82	0.26	0.58
PENTOLITE	1.68	7520	nan	[10]	7739	7540	2.9%	0.3%	255	250							0.26	0.58
PENTOLITE	1.70	7530	nan	[8]	7802	7602	3.6%	1.0%	261	257							0.26	0.58
PENTOLITE	1.71	7750	nan	[8]	7833	7633	1.1%	-1.5%	264	260							0.26	0.58
PETN/TNT (20/80)	1.59	6980	180	[45]	7075	6975	1.4%	-0.1%	205	204	14.1%	13.3%		3.30	2.87	2.79	0.25	0.57
PETN/TNT (60/40)	1.65	7530	242	[45]	7772	7542	3.2%	0.2%	254	247	4.9%	2.1%		2.87	2.92	2.80	0.25	0.57
PETN/TNT (60/40)	1.67	7525	231	[45]	7836	7605	4.1%	1.1%	260	254	12.6%	9.8%		3.09	2.94	2.81	0.26	0.57
PETN/TNT (60/40)	1.68	7610	248	[45]	7868	7636	3.4%	0.3%	263	257	6.1%	3.6%		2.92	2.95	2.81	0.26	0.57
PETN/TNT/RDX (20/30/50)	1.71	7890	266.5	[45]	8094	7974	2.6%	1.1%	282	282	5.7%	6.0%		2.99	2.98	2.85	0.26	0.59
pf	1.83	7290	270	[8]		7201		-1.2%		240		-11.2%					0.28	0.65
PICRATOL	1.63	6970	nan	[8]	6997	6989	0.4%	0.3%	204	206							0.26	0.60
picric	1.60	7100	nan	[8]	7073	6943	-0.4%	-2.2%	206	204							0.25	0.56
picric	1.71	7350	nan	[48]	7401	7268	0.7%	-1.1%	236	236							0.26	0.58
picric	1.71	7260	nan	[8]	7401	7268	1.9%	0.1%	236	236							0.26	0.58
picric	1.76	7570	nan	[8]	7550	7416	-0.3%	-2.0%	249	251							0.26	0.59
ppam	1.73	8100	nan	[48]	8268	8125	2.1%	0.3%	296	296							0.26	0.60
PRNQ/HMX/CARNAUBA (30/68/2)	1.64	7900	nan	[35]	7589	7803	-3.9%	-1.2%	241	253							0.28	0.64
PRNQ/NQ/HMX (34/35/31)	1.59	7710	nan	[35]	7204	7647	-6.6%	-0.8%	213	230							0.30	0.70
PYX/PE (95/5)	1.56	7097	nan	[14]	6782	6766	-4.4%	-4.7%	186	188							0.25	0.56

Fernando G. Bastante [1], *María Araújo Fernández* [1], *Eduardo Giráldez* [1].
CINTECX, GESSMin group, University of Vigo

PREDICTIVE MODEL FOR EXPLOSIVE DETONATION PARAMETERS FROM AN EQUATION OF STATE BASED ON DETONATION VELOCITY. Physical Chemistry Chemical Physics 2022

DEoS DATABASE

Number of Explosives 238

	Number of data	
	D	***P***
KJ (only CHNO)	449	224
DEoS	519	263

residuals D

Statistics *velocity*	***KJ***	**DEoS**
RMRS	*3.4%*	*1.7%*
MAPR	*2.5%*	*1.3%*
$P_{97,5}$	*8.2%*	*3.9%*

residuals P

Statistics *pressure*	***KJ***	**DEoS**
RMRS	*7.0%*	*6.0%*
MAPR	*5.6%*	*4.9%*
$P_{97,5}$	*17.0%*	*12.6%*

Gamma (γ) correlation (CHNO explosives)

	KJ	**DEoS**
r	*0.44*	*0.53*

Jones and Grüneisen parameters (DEoS Model)

	α	Γ
average values	*0.27*	*0.60*
standar deviation	*0.02*	*0.06*

		experimental data			***calculated D***				***calculated P***									
Acr	**density (g/cc)**	**Dexp (m/s)**	**Pexp (kbar)**	**reference**	**D_{KJ} (m/s)**	**D_{DEoS} (m/s)**	**RRD_{KJ}**	**RRD_{DEoS}**	**P_{KJ} (kbar)**	**P_{DEoS} (kbar)**	**RRP_{KJ}**	**RRP_{DEoS}**		**$\gamma_{experimental}$**	**γ_{KJ}**	**γ_{DEoS}**	**α**	**Γ**
rdx	1.00	5981	nan	[14]	6049	5942	1.1%	-0.7%	106	100							0.22	0.46
rdx	1.00	6100	89	[8]	6049	5942	-0.8%	-2.6%	106	100	18.7%	12.6%		3.18	2.46	2.52	0.22	0.46
rdx	1.00	6030	108	[38]	6049	5942	0.3%	-1.5%	106	100	-2.2%	-7.2%		2.37	2.46	2.52	0.22	0.46
rdx	1.07	6260	116	[34]	6289	6185	0.5%	-1.2%	121	115	4.3%	-1.0%		2.61	2.50	2.56	0.23	0.47
rdx	1.10	6180	122	[8]	6391	6290	3.4%	1.8%	128	121	4.8%	-0.4%		2.44	2.51	2.58	0.23	0.48
rdx	1.10	6115	112.7	[34]	6391	6290	4.5%	2.9%	128	121	13.4%	7.8%		2.65	2.51	2.58	0.23	0.48
rdx	1.17	6648	134.4	[34]	6641	6543	-0.1%	-1.6%	145	139	8.2%	3.1%		2.86	2.56	2.62	0.23	0.49
rdx	1.20	6770	152	[8]	6733	6637	-0.5%	-2.0%	152	145	0.1%	-4.4%		2.62	2.58	2.64	0.23	0.50
rdx	1.22	6609	148.9	[34]	6788	6693	2.7%	1.3%	156	149	4.9%	0.3%		2.57	2.59	2.65	0.23	0.50
rdx	1.29	7000	164	[34]	7041	6950	0.6%	-0.7%	176	169	7.2%	3.2%		2.85	2.64	2.68	0.24	0.52
rdx	1.29	7036	166.2	[38]	7041	6950	0.1%	-1.2%	176	169	5.8%	1.8%		2.84	2.64	2.68	0.24	0.52
rdx	1.29	7000	166	[8]	7041	6950	0.6%	-0.7%	176	169	5.9%	1.9%		2.81	2.64	2.68	0.24	0.52
rdx	1.40	7460	213	[8]	7417	7333	-0.6%	-1.7%	207	201	-2.8%	-5.4%		2.66	2.72	2.74	0.25	0.54
rdx	1.46	7600	211	[8]	7622	7542	0.3%	-0.8%	225	221	6.7%	4.6%		3.00	2.77	2.76	0.25	0.55
rdx	1.46	7600	208	[34]	7622	7542	0.3%	-0.8%	225	221	8.3%	6.1%		3.05	2.77	2.76	0.25	0.55
rdx	1.46	7626	209.8	[38]	7622	7542	-0.1%	-1.1%	225	221	7.3%	5.2%		3.05	2.77	2.76	0.25	0.55
rdx	1.59	8077	259	[38]	8066	7994	-0.1%	-1.0%	267	266	3.1%	2.7%		3.00	2.87	2.82	0.26	0.58
rdx	1.60	8250	nan	[10]	8101	8029	-1.8%	-2.7%	270	270							0.26	0.58
rdx	1.60	8130	263	[8]	8101	8029	-0.4%	-1.2%	270	270	2.8%	2.6%		3.02	2.88	2.82	0.26	0.58
rdx	1.66	8240	nan	[8]	8306	8237	0.8%	0.0%	291	293							0.26	0.59
rdx	1.71	NaN	314	[2]	8477	8411			309	313	-1.6%	-0.4%					0.27	0.60
rdx	1.72	8460	313	[8]	8511	8446	0.6%	-0.2%	313	317	-0.1%	1.3%		2.93	2.99	2.87	0.27	0.60
rdx	1.72	8528	310	[38]	8511	8446	-0.2%	-1.0%	313	317	0.8%	2.3%		3.04	2.99	2.87	0.27	0.60
rdx	1.72	8460	308.5	[34]	8511	8446	0.6%	-0.2%	313	317	1.3%	2.7%		2.99	2.99	2.87	0.27	0.60
rdx	1.76	8622	325	[34]	8655	8592	0.4%	-0.3%	328	335	0.9%	3.0%		3.03	3.02	2.89	0.27	0.61
rdx	1.77	8700	338	[8]	8682	8620	-0.2%	-0.9%	331	338	-2.1%	0.0%		2.96	3.03	2.89	0.27	0.61
rdx	1.80	8750	341	[8]	8785	8724	0.4%	-0.3%	342	351	0.4%	3.0%		3.04	3.06	2.90	0.27	0.62
rdx	1.80	8754	347	[31]	8785	8724	0.3%	-0.3%	342	351	-1.4%	1.2%		2.98	3.06	2.90	0.27	0.62
rdx	1.80	8800	nan	[48]	8785	8724	-0.2%	-0.9%	342	351							0.27	0.62
rdx	1.80	NaN	350	[31]	8785	8724			342	351	-2.2%	0.3%					0.27	0.62
rdx	1.80	NaN	385	[31]	8785	8724			342	351	-11.1%	-8.8%					0.27	0.62
RDX/ESTANE (80/20)	1.20	6290	nan	[28]	6150	6148	-2.2%	-2.3%	127	123							0.24	0.52
RDX/EVA (80/20)	1.28	6500	nan	[28]	6538	6557	0.6%	0.9%	151	148							0.24	0.53
RDX/EVA (95/5)	1.56	7630	nan	[22]	7847	7803	2.8%	2.3%	250	249							0.26	0.58
RDX/EVA (95/5)	1.63	8248	269	[26]	8065	8027	-2.2%	-2.7%	271	273	0.8%	1.5%		3.12	2.91	2.84	0.26	0.59
RDX/EXON (90/10)	1.79	8404	320	[14]		8374		-0.4%		317		-0.9%					0.28	0.65
RDX/GAP (84/16)	1.59	8074	nan	[4]	7976	7949	-1.2%	-1.6%	261	263							0.26	0.58
RDX/HTPB (80/20)	1.43	7200	nan	[28]	6767	6878	-6.0%	-4.5%	175	177							0.26	0.57
RDX/HTPB (82/18)	1.52	7526	nan	[4]	7132	7239	-5.2%	-3.8%	203	207							0.26	0.59
RDX/HTPB (85/15)	1.43	7200	nan	[28]	6958	7017	-3.4%	-2.5%	185	186							0.25	0.57
RDX/PIB (91/9)	1.61	8055	nan	[44]	7814	7836	-3.0%	-2.7%	253	256							0.26	0.59
RDX/SYLGARD (85/15)	1.54	7682	nan	[3]		7429		-3.3%		218							0.27	0.62
RDX/TATB/HTPB (65/20/15)	1.49	7100	nan	[28]	6927	7035	-2.4%	-0.9%	189	192							0.26	0.59
RDX/TATB/HTPB (70/15/15)	1.47	7120	nan	[28]	6921	7015	-2.8%	-1.5%	187	189							0.26	0.58
RDX/TATB/HTPB (75/10/15)	1.45	7150	nan	[28]	6913	6994	-3.3%	-2.2%	184	186							0.26	0.57
RDX/TFNA (65/35)	1.75	8220	324	[14]		8088		-1.6%		289		-10.8%					0.28	0.66
RDX/TNT (30/70)	1.64	7230	nan	[52]	7354	7305	1.7%	1.0%	226	229							0.26	0.58
RDX/TNT (50/50)	1.63	7660	231	[8]	7579	7522	-1.1%	-1.8%	240	241	3.7%	4.3%		3.14	2.91	2.83	0.26	0.58
RDX/TNT (50/50)	1.65	7540	251	[45]	7642	7586	1.4%	0.6%	246	248	-2.2%	-1.3%		2.74	2.92	2.83	0.26	0.58
RDX/TNT (60/40)	1.49	7195	192	[38]	7256	7189	0.8%	-0.1%	207	204	7.8%	6.4%		3.02	2.79	2.77	0.25	0.55
RDX/TNT (60/40)	1.52	7250	200	[38]	7352	7287	1.4%	0.5%	215	213	7.7%	6.7%		2.99	2.82	2.78	0.25	0.56
RDX/TNT (60/40)	1.54	7300	206	[38]	7417	7352	1.6%	0.7%	221	220	7.3%	6.6%		2.98	2.83	2.79	0.25	0.56
RDX/TNT (60/40)	1.59	7415	219	[38]	7577	7515	2.2%	1.3%	236	236	7.6%	7.6%		2.99	2.87	2.81	0.26	0.57
RDX/TNT (60/40)	1.68	7640	nan	[52]	7866	7808	3.0%	2.2%	263	266							0.26	0.59
RDX/TNT (60/40)	1.72	7890	287	[8]	7995	7938	1.3%	0.6%	276	281	-3.9%	-2.3%		2.73	2.99	2.86	0.26	0.60
RDX/TNT (60/40)	1.72	7840	287	[22]	7995	7938	2.0%	1.3%	276	281	-3.9%	-2.3%		2.68	2.99	2.86	0.26	0.60
RDX/TNT (60/40)	1.73	NaN	268	[31]	8027	7971			279	284	4.1%	6.0%					0.27	0.60
RDX/TNT (60/40)	1.73	7977	275	[31]	8027	7971	0.6%	-0.1%	279	284	1.5%	3.4%		3.00	3.00	2.87	0.27	0.60
RDX/TNT (60/40)	1.73	NaN	292	[31]	8027	7971			279	284	-4.5%	-2.7%					0.27	0.60
RDX/TNT (60/40)	1.74	8090	nan	[8]	8059	8003	-0.4%	-1.1%	282	288							0.27	0.60
RDX/TNT (60/40)	1.79	8130	309	[45]	8220	8166	1.1%	0.4%	299	307	-3.3%	-0.7%		2.83	3.05	2.89	0.27	0.61
RDX/TNT (64/36)	1.71	8030	294	[14]	8024	7966	-0.1%	-0.8%	277	282	-5.7%	-4.2%		2.76	2.98	2.86	0.26	0.60
RDX/TNT (65/35)	1.72	8040	292	[8]	8060	8002	0.2%	-0.5%	280	285	-4.0%	-2.4%		2.81	2.99	2.86	0.26	0.60
RDX/TNT (70/30)	1.49	7290	197	[38]	7374	7304	1.2%	0.2%	214	211	8.5%	7.0%		3.02	2.79	2.77	0.25	0.55
RDX/TNT (70/30)	1.52	7370	207	[38]	7472	7403	1.4%	0.5%	222	220	7.5%	6.3%		2.99	2.82	2.78	0.25	0.56
RDX/TNT (70/30)	1.55	7460	216	[38]	7570	7503	1.5%	0.6%	231	230	7.1%	6.4%		2.99	2.84	2.80	0.25	0.57
RDX/TNT (70/30)	1.59	7580	227	[38]	7701	7635	1.6%	0.7%	243	243	7.2%	7.1%		3.02	2.87	2.81	0.26	0.57
RDX/TNT (70/30)	1.59	7580	216	[45]	7701	7635	1.6%	0.7%	243	243	12.7%	12.5%		3.23	2.87	2.81	0.26	0.57
RDX/TNT (70/30)	1.73	8060	nan	[8]	8158	8099	1.2%	0.5%	288	293							0.27	0.60

Fernando G. Bastante [1] *, María Araújo Fernández* [1] *, Eduardo Giráldez* [1] *.*
CINTECX, GESSMin group, University of Vigo

PREDICTIVE MODEL FOR EXPLOSIVE DETONATION PARAMETERS FROM AN EQUATION OF STATE BASED ON DETONATION VELOCITY. Physical Chemistry Chemical Physics 2022

DEoS DATABASE

Number of Explosives 238

	Number of data	
	D	***P***
KJ (only CHNO)	449	224
DEoS	519	263

residuals D

Statistics *velocity*	***KJ***	**DEoS**
RMRS	*3.4%*	*1.7%*
MAPR	*2.5%*	*1.3%*
P97,5	*8.2%*	*3.9%*

residuals P

Statistics *pressure*	***KJ***	**DEoS**
RMRS	*7.0%*	*6.0%*
MAPR	*5.6%*	*4.9%*
P97,5	*17.0%*	*12.6%*

Gamma (γ) correlation (CHNO explosives)

	KJ	**DEoS**
r	*0.44*	*0.53*

Jones and Grüneisen parameters (DEoS Model)

	α	Γ
average values	*0.27*	*0.60*
standar deviation	*0.02*	*0.06*

		experimental data			***calculated D***				***calculated P***										
Acr	**density (g/cc)**	**Dexp (m/s)**	**Pexp (kbar)**	**reference**	**DKJ (m/s)**	**D_DEoS (m/s)**	**RRD KJ**	**RRD_DEoS**	**PKJ (kbar)**	**P_DEoS (kbar)**	**RRP KJ**	**RRP_DEoS**		$\gamma_{experimental}$	γ_{KJ}	$\gamma_{\_DEoS}$		α	Γ
RDX/TNT (75/25)	1.62	7950	265	[8]	7861	7795	-1.1%	-1.9%	257	257	-3.1%	-2.9%		2.86	2.90	2.83		0.26	0.58
RDX/TNT (75/25)	1.74	8200	316	[10]	8256	8196	0.7%	0.0%	296	302	-6.3%	-4.5%		2.70	3.00	2.87		0.27	0.60
RDX/TNT (75/25)	1.76	8300	323.3	[34]	8312	8253	0.1%	-0.6%	302	308	-6.6%	-4.6%		2.74	3.02	2.88		0.27	0.61
RDX/TNT (75/25)	1.76	8300	316	[8]	8322	8263	0.3%	-0.4%	303	310	-4.1%	-2.0%		2.84	3.02	2.88		0.27	0.61
RDX/TNT (77/23)	1.74	8250	313	[8]	8282	8222	0.4%	-0.3%	298	304	-4.8%	-3.0%		2.78	3.00	2.87		0.27	0.60
RDX/TNT (77/23)	1.75	8274	316	[34]	8321	8262	0.6%	-0.1%	302	308	-4.4%	-2.4%		2.80	3.01	2.88		0.27	0.61
RDX/TNT (77/23)	1.76	8290	313	[34]	8331	8272	0.5%	-0.2%	303	310	-3.1%	-1.1%		2.85	3.02	2.88		0.27	0.61
RDX/TNT (78/22)	1.76	8310	317	[8]	8361	8302	0.6%	-0.1%	306	312	-3.5%	-1.4%		2.83	3.02	2.88		0.27	0.61
RDX/TNT (80/20)	1.50	7500	210	[38]	7525	7452	0.3%	-0.6%	224	221	6.5%	5.0%		3.02	2.80	2.78		0.25	0.56
RDX/TNT (80/20)	1.53	7570	222	[38]	7624	7553	0.7%	-0.2%	233	230	4.8%	3.7%		2.95	2.82	2.79		0.25	0.56
RDX/TNT (80/20)	1.56	7675	231	[38]	7724	7654	0.6%	-0.3%	242	240	4.7%	4.0%		2.98	2.85	2.80		0.26	0.57
RDX/TNT (80/20)	1.60	7745	242	[38]	7857	7789	1.4%	0.6%	254	254	5.1%	5.0%		2.97	2.88	2.82		0.26	0.58
RDX/TNT (90/10)	1.51	7570	217	[38]	7676	7601	1.4%	0.4%	234	231	7.7%	6.2%		2.99	2.81	2.78		0.25	0.56
RDX/TNT (90/10)	1.55	7740	231	[38]	7811	7738	0.9%	0.0%	246	244	6.6%	5.7%		3.02	2.84	2.80		0.25	0.57
RDX/TNT (90/10)	1.59	7840	247	[38]	7945	7875	1.3%	0.4%	259	258	4.9%	4.6%		2.96	2.87	2.82		0.26	0.58
RDX/TNT (90/10)	1.61	7910	256	[38]	8013	7943	1.3%	0.4%	266	266	3.8%	3.7%		2.93	2.89	2.83		0.26	0.58
RDX/VITON (95/5)	1.76	8424	nan	[44]		8387		-0.4%		316								0.28	0.63
RDX/WAX (94/6)	1.66	8380	nan	[24]	8055	8068	-3.9%	-3.7%	274	279								0.27	0.60
RDX/WAX (95/5)	1.64	8100	nan	[24]	8031	8027	-0.9%	-0.9%	270	274								0.26	0.60
RX23	1.42	8640	258	[8]	7811	8343	-9.6%	-3.4%	232	247	-10.1%	-4.4%		3.11	2.73	3.01		0.29	0.68
RX26	1.84	8240	340	[8]	8172	8285	-0.8%	0.5%	300	318	-11.7%	-6.4%		2.67	3.09	2.97		0.28	0.66
RX27	1.64	6930	200	[8]		6673		-3.7%		189		-5.7%						0.27	0.60
RX36	1.83	8510	335	[8]		8295		-2.5%		323		-3.5%						0.27	0.61
RX41	1.86	8810	350	[8]		8595		-2.4%		348		-0.4%						0.28	0.64
RX45	1.75	7710	250	[8]		7871		2.1%		263		5.3%						0.32	0.75
RX47	1.82	7660	260	[8]		7638		-0.3%		267		2.6%						0.29	0.66
RX48	1.85	7760	263	[8]		7696		-0.8%		278		5.9%						0.28	0.64
RX52AE	1.78	7570	nan	[10]		7665		1.3%		263								0.29	0.66
schembl	1.64	8190	nan	[48]	8592	8119	4.9%	-0.9%	309	289								0.25	0.54
tacot	1.85	7250	nan	[8]	7440	7531	2.6%	3.9%	250	270								0.27	0.61
tat	1.02	5500	nan	[41]	5301	5619	-3.6%	2.2%	83	87								0.24	0.52
tat	1.50	7300	nan	[27]	6723	7327	-7.9%	0.4%	178	205								0.28	0.64
tat	1.54	7500	nan	[11]	6842	7469	-8.8%	-0.4%	188	217								0.28	0.65
tatb	1.83	7580	260	[8]	7608	7826	0.4%	3.2%	259	280	-0.3%	7.6%		3.04	3.09	3.01		0.29	0.68
tatb	1.85	7660	259	[8]	7667	7890	0.1%	3.0%	265	287	2.3%	10.8%		3.19	3.10	3.01		0.29	0.68
tatb	1.88	7760	nan	[8]	7755	7986	-0.1%	2.9%	274	298								0.30	0.69
tatb	1.90	7860	315	[14]	7799	8034	-0.8%	2.2%	278	303	-11.7%	-3.7%		2.72	3.14	3.03		0.30	0.69
tatb	1.94	7990	nan	[48]	7930	8178	-0.7%	2.3%	291	321								0.30	0.70
TATB/KELF (90/10)	1.91	7630	nan	[14]		7728		1.3%		276								0.32	0.76
TATB/TNT (30/70)	1.65	6930	nan	[52]	7028	7046	1.4%	1.7%	208	212								0.26	0.60
tetryl	1.20	6340	nan	[8]	6139	6035	-3.2%	-4.8%	126	122								0.23	0.48
tetryl	1.36	6680	142	[8]	6638	6526	-0.6%	-2.3%	162	158	14.4%	11.2%		3.27	2.69	2.67		0.24	0.51
tetryl	1.44	6875	nan	[10]	6887	6772	0.2%	-1.5%	182	178								0.24	0.53
tetryl	1.61	7580	226	[8]	7417	7294	-2.1%	-3.8%	228	227	0.7%	0.3%		3.09	2.89	2.78		0.25	0.56
tetryl	1.68	7500	239	[8]	7635	7509	1.8%	0.1%	248	249	3.7%	4.2%		2.95	2.95	2.81		0.26	0.57
tetryl	1.70	7560	nan	[48]	7698	7571	1.8%	0.1%	254	256								0.26	0.57
tetryl	1.71	7850	nan	[8]	7729	7602	-1.5%	-3.2%	257	259								0.26	0.58
tetryl	1.73	7720	nan	[8]	7791	7663	0.9%	-0.7%	263	266								0.26	0.58
TKX-50/VITON (95/5)	1.77	8690	nan	[35]		8926		2.7%		352								0.29	0.68
tna	1.72	7300	nan	[48]	7382	7368	1.1%	0.9%	235	241								0.27	0.60
tnan	1.61	6800	nan	[48]	7046	6945	3.6%	2.1%	205	205								0.25	0.57
tnb	1.69	7350	nan	[48]	7429	7286	1.1%	-0.9%	236	237								0.25	0.56
tneof	1.80	8160	nan	[48]	8489	8090	4.0%	-0.9%	320	305								0.26	0.60
tnetb	1.23	6280	nan	[49]	6739	6481	7.3%	3.2%	155	144								0.23	0.48
tnetb	1.33	6640	nan	[49]	7076	6804	6.6%	2.5%	182	169								0.23	0.50
tnetb	1.39	6860	nan	[49]	7278	6998	6.1%	2.0%	198	185								0.24	0.51
tnetb	1.45	7090	nan	[42]	7480	7191	5.5%	1.4%	216	203								0.24	0.52
tnetb	1.48	7180	nan	[49]	7582	7288	5.6%	1.5%	225	212								0.24	0.53
tnetb	1.50	7240	nan	[42]	7649	7353	5.6%	1.6%	231	218								0.24	0.53
tnetb	1.54	7390	nan	[42]	7784	7482	5.3%	1.2%	244	231								0.25	0.54
tnetb	1.55	7400	nan	[42]	7818	7514	5.6%	1.5%	247	234								0.25	0.54
tnetb	1.56	7450	nan	[42]	7851	7546	5.4%	1.3%	250	237								0.25	0.54
tnetb	1.58	7550	nan	[42]	7919	7611	4.9%	0.8%	256	244								0.25	0.55
tnetb	1.60	7700	nan	[42]	7986	7675	3.7%	-0.3%	263	251								0.25	0.55
tnetb	1.61	7740	nan	[42]	8020	7708	3.6%	-0.4%	266	254								0.25	0.55
tnetb	1.65	7870	nan	[42]	8155	7837	3.6%	-0.4%	280	268								0.25	0.56
tnetb	1.67	7960	nan	[42]	8222	7901	3.3%	-0.7%	286	275								0.25	0.56
tnetb	1.68	7990	nan	[49]	8256	7934	3.3%	-0.7%	290	279								0.25	0.57
tnetb	1.70	8050	nan	[42]	8323	7998	3.4%	-0.6%	297	286								0.25	0.57

Fernando G. Bastante [1], *María Araújo Fernández* [1], *Eduardo Giráldez* [1].
CINTECX, GESSMin group, University of Vigo

PREDICTIVE MODEL FOR EXPLOSIVE DETONATION PARAMETERS FROM AN EQUATION OF STATE BASED ON DETONATION VELOCITY. Physical Chemistry Chemical Physics 2022

DEoS DATABASE

Number of Explosives 238

	Number of data D	Number of data P
KJ (only CHNO)	449	224
DEoS	519	263

residuals D — Statistics *velocity*

	KJ	DEoS
RMRS	3.4%	1.7%
MAPR	2.5%	1.3%
P97,5	8.2%	3.9%

residuals P — Statistics *pressure*

	KJ	DEoS
RMRS	7.0%	6.0%
MAPR	5.6%	4.9%
P97,5	17.0%	12.6%

Gamma (γ) correlation (CHNO explosives)

	KJ	DEoS
r	0.44	0.53

Jones and Grüneisen parameters (DEoS Model)

	α	Γ
average values	0.27	0.60
standar deviation	0.02	0.06

	experimental data				*calculated D*				*calculated P*									
Acr	density (g/cc)	Dexp (m/s)	Pexp (kbar)	reference	DKJ (m/s)	D_DEoS (m/s)	RRD KJ	RRD_DEoS	PKJ (kbar)	P_DEoS (kbar)	RRP KJ	RRP_DEoS		γ experimental	γ KJ	γ _DEoS	α	Γ
tnetb	1.71	8100	nan	[49]	8357	8031	3.2%	-0.9%	300	290							0.26	0.57
tnetb	1.74	8210	nan	[42]	8458	8127	3.0%	-1.0%	311	301							0.26	0.58
tnetb	1.76	8290	nan	[42]	8525	8192	2.8%	-1.2%	318	309							0.26	0.58
tnetb	1.77	8310	nan	[42]	8559	8224	3.0%	-1.0%	322	313							0.26	0.58
tnetb	1.78	8300	nan	[48]	8593	8257	3.5%	-0.5%	325	317							0.26	0.58
tnetb	1.78	8260	nan	[42]	8593	8257	4.0%	0.0%	325	317							0.26	0.58
tnetb	1.78	8460	nan	[10]	8593	8257	1.6%	-2.4%	325	317							0.26	0.58
tnetb	1.79	8270	nan	[34]	8626	8289	4.3%	0.2%	329	321							0.26	0.59
tnm	1.64	6360	159	[8]	6332	6540	-0.4%	2.8%	168	172	5.6%	7.9%		3.17	2.92	3.09	0.31	0.73
tnm	1.64	6480	165	[14]	6332	6540	-2.3%	0.9%	168	172	1.8%	4.0%		3.17	2.92	3.09	0.31	0.73
tnm	1.65	6450	155	[8]	6359	6571	-1.4%	1.9%	170	174	9.7%	12.3%		3.43	2.92	3.09	0.31	0.73
TNM/BENZ (76.4/23.6)	1.36	6850	nan	[14]	7019	6794	2.5%	-0.8%	182	173							0.23	0.49
TNM/NM (0.071/1)	1.20	6570	138	[14]	6799	6602	3.5%	0.5%	155	143	12.2%	4.0%		2.74	2.57	2.64	0.23	0.50
TNM/NM (0.25/1)	1.31	6880	156	[14]	7453	7148	8.3%	3.9%	199	184	27.8%	17.9%		2.97	2.65	2.64	0.23	0.50
TNM/NM (0.5/1)	1.40	6780	168	[14]	7265	6911	7.2%	1.9%	198	179	18.1%	6.7%		2.82	2.72	2.72	0.24	0.53
TNM/NM (60/40)	1.15	6360	132	[31]	6470	6284	1.7%	-1.2%	136	124	2.9%	-5.8%		2.52	2.54	2.65	0.24	0.51
TNM/NM (70/30)	1.24	6790	160	[6]	7033	6767	3.6%	-0.3%	170	156	6.4%	-2.6%		2.57	2.60	2.64	0.23	0.50
TNM/NM (80/20)	1.35	6790	180	[6]	7265	6919	7.0%	1.9%	194	175	7.5%	-2.8%		2.46	2.68	2.69	0.24	0.52
TNM/NM (90/10)	1.48	6760	187	[6]	6944	6605	2.7%	-2.3%	189	169	0.9%	-9.8%		2.62	2.78	2.83	0.26	0.58
tnt	1.00	5111	64	[38]	5112	5053	0.0%	-1.1%	75	73	17.9%	13.8%		3.08	2.46	2.51	0.22	0.45
tnt	1.00	5000	67	[8]	5112	5053	2.2%	1.1%	75	73	12.6%	8.7%		2.73	2.46	2.51	0.22	0.45
tnt	1.33	6076	nan	[38]	6063	6017	-0.2%	-1.0%	133	130							0.24	0.52
tnt	1.36	6200	124	[8]	6152	6107	-0.8%	-1.5%	140	137	12.5%	10.5%		3.22	2.69	2.70	0.24	0.52
tnt	1.38	6212	nan	[31]	6201	6157	-0.2%	-0.9%	143	141							0.24	0.53
tnt	1.42	6363	nan	[31]	6320	6277	-0.7%	-1.3%	152	150							0.24	0.54
tnt	1.45	NaN	161	[38]	6398	6356			158	156	-2.1%	-3.1%					0.25	0.54
tnt	1.45	6500	144	[8]	6412	6371	-1.3%	-2.0%	159	157	10.2%	9.2%		3.25	2.76	2.74	0.25	0.54
tnt	1.54	6736	nan	[34]	6681	6643	-0.8%	-1.4%	180	180							0.25	0.56
tnt	1.57	6814	nan	[34]	6747	6711	-1.0%	-1.5%	185	186							0.25	0.57
tnt	1.58	6880	184	[34]	6788	6752	-1.3%	-1.9%	188	190	2.4%	3.0%		3.06	2.87	2.80	0.25	0.57
tnt	1.59	6872	nan	[10]	6814	6778	-0.8%	-1.4%	191	192							0.26	0.57
tnt	1.59	6940	202	[38]	6817	6781	-1.8%	-2.3%	191	192	-5.6%	-4.8%		2.79	2.87	2.80	0.26	0.57
tnt	1.59	6950	nan	[34]	6817	6781	-1.9%	-2.4%	191	192							0.26	0.57
tnt	1.59	6940	176.5	[10]	6817	6781	-1.8%	-2.3%	191	192	8.1%	8.9%		3.34	2.87	2.80	0.26	0.57
tnt	1.60	6700	189	[53]	6831	6796	2.0%	1.4%	192	194	1.6%	2.4%		2.79	2.88	2.81	0.26	0.57
tnt	1.61	6842	nan	[34]	6860	6825	0.3%	-0.2%	194	196							0.26	0.57
tnt	1.62	6883	nan	[10]	6889	6854	0.1%	-0.4%	197	199							0.26	0.57
tnt	1.63	NaN	210	[34]	6932	6898			200	203	-4.5%	-3.3%					0.26	0.58
tnt	1.63	7070	205	[8]	6932	6898	-1.9%	-2.4%	200	203	-2.2%	-1.0%		2.97	2.91	2.82	0.26	0.58
tnt	1.63	6940	190	[34]	6938	6904	0.0%	-0.5%	201	204	5.8%	7.2%		3.14	2.91	2.82	0.26	0.58
tnt	1.63	7070	205	[34]	6938	6904	-1.9%	-2.3%	201	204	-2.0%	-0.7%		2.98	2.91	2.82	0.26	0.58
tnt	1.64	6940	nan	[48]	6961	6928	0.3%	-0.2%	203	206							0.26	0.58
tnt	1.64	6930	210	[8]	6961	6928	0.5%	0.0%	203	206	-3.4%	-2.0%		2.75	2.92	2.82	0.26	0.58
tnt	1.64	6950	190	[31]	6961	6928	0.2%	-0.3%	203	206	6.8%	8.3%		3.17	2.92	2.82	0.26	0.58
tnt	1.64	6958	192	[31]	6961	6928	0.0%	-0.4%	203	206	5.7%	7.2%		3.14	2.92	2.82	0.26	0.58
tnt	1.64	NaN	195	[53]	6961	6928			203	206	4.1%	5.5%					0.26	0.58
tnt	1.64	NaN	217	[14]	6961	6928			203	206	-6.5%	-5.2%					0.26	0.58
TNT/FOX-12(50/50)	1.65	7120	221	[18]	7317	7471	2.8%	4.9%	225	234	1.9%	5.8%		2.79	2.93	2.94	0.28	0.64
tntab	1.74	8580	nan	[8]	8247	8647	-3.9%	0.8%	296	338							0.26	0.59
tntmta	1.49	7300	nan	[14]	7355	7542	0.8%	3.3%	213	221							0.26	0.59
tntmta	1.57	7800	nan	[48]	7615	7825	-2.4%	0.3%	236	248							0.27	0.60
TO/NM (14.5/85.5)	1.09	5840	100	[14]	5716	5674	-2.1%	-2.8%	101	96	1.3%	-4.3%		2.71	2.51	2.66	0.24	0.51
ttnh	2.01	9150	nan	[48]	9214	8991	0.7%	-1.7%	401	412							0.28	0.64
X-0341	1.90	7816	nan	[7]		7931		1.5%		294							0.31	0.72
X-0342	1.90	7866	nan	[7]		7979		1.4%		298							0.30	0.71
X-0343	1.90	7915	nan	[7]		8029		1.4%		302							0.30	0.71
X-0344	1.89	8046	nan	[7]		8121		0.9%		309							0.30	0.70

[*] D KJ = 6482 m/s and D TW = 6266 m/s with H2O(l) instead of H2O(g)

[**] 3% of Viton B in the composition as 3% Viton A in the calculation

references

[1]	A. Belaada and W. A. Trzciński, 1,1-Diamino-2,2-dinitroethene (DADNE, FOX-7) – Properties and Formulations (a Review), Cent. Eur. J. Energ. Mater. 2016, 2(13), 527–544.
[2]	A. Dolgoborodov, M. Brajnikov, M. Makhov, N. Safronov, V. Kirilenko, Detonation parameters of pressed charges of benzotrifuroxane. Combust. Explos. Shock Waves 2013, 49, 723–730.
[3]	A. Elbeih, M. M. Mohamed, T. Wafy, Sensitivity and detonation characteristics of selected nitramines bonded by sylgard binder, Propellants Explos. Pyrotech. 2016, 41(6), 1044–1049.
[4]	A. K. Hussein, A. Elbeih, S. Zeman, The effect of glycidyl azide polymer on the stability and explosive properties of different interesting nitramines. RSC Adv. 2018, 8,17272-17278.
[5]	A. Singh, M. Kumar, P. Soni, M. Singh, A. Srivastava, Mechanical and explosive properties of plastic bonded explosives based on mixture of HMX and TATB. Def. Sci. J. 2013, 63(6), 622-629.
[6]	A. V. Utkin, V. M. Mochalova, A. M. Astakhov, V. E. Rykova, S. A. Koldunov, Structure of detonation waves in mixtures of tetranitromethane with nitrobenzene and methanol. Combust. Explos. Shock Waves 2020, 56, 556–565.
[7]	A. W. Campbell, H. L. Flaugh, A. Popolato, A. J. B. Ramsay, Customized explosives based on plastic-bonded mixtures to TATB and HMX, Seventh Symposium (International) on Detonation, Annapolis, 19 Jun 1981, Los Alamos National Lab. (LANL), MD, USA 1981.
[8]	B. C. McGee, M. L. Hobbs, M. R. Baer, Exponential 6 Parameterization for the JCZ3-EOS, Report SAND98-1191, Sandia National Laboratories, Albuquerque, NM, USA 1998.
[9]	B. Le Roux, M. Golfier, M. Rat, S. Lecume, Development of a cast plastic bonded explosive with high CL20 content, Insensitive munitions & energetic materials technology symposium, Bristol, 24-28 april 2006, NDIA, MSIAC and IMEMG, UK 2006.
[10]	B. M. Dobratz, P. C. Crawford, LLNL Explosives: Handbook Properties of Chemical Explosives and Explosive Simulants, Lawrence Livermore National Laboratory, California, CA, USA 1985.
[11]	B. T. Fedoroff, O. E. Sheffield, Encyclopedia of explosives and related items, PATR 2700, Vol. 2, p. B270, Picatinny Arsenal, Dover, NJ, USA 1962.
[12]	B. T. Fedoroff, O. E. Sheffield, Encyclopedia of explosives and related items, PATR 2700, Vol. 5, p. E124, Picatinny Arsenal, Dover, NJ, USA 1962.
[13]	C. M. Tarver, Ignition and growth reactive flow modeling of detonating LX-04 using recent and older experimental data, AIP Conference Proceedings 1979, 100042 (2018)
[14]	C.L. Mader, Numerical Modeling of Explosives and Propellants, Third Edition, CRC Press, 2008.
[15]	D. Price, A. R. Clairmont Jr.,(1968), The Response of Nitroguanidine to a Strong Shock, NOLTR 67-169, US Naval Ordnance Laboratory, White Oak, MD, USA 1968.
[16]	D. Price, The detonation velocity-loading density relation for selected explosives and mixtures of explosives, J. Energ. Mater. 1983, 1(1), 55-82.
[17]	E.G. Francois, D.E. Chavez, J.T. Mang, V.E. Sanders, J.M. Lloyd, Shock sensitivity of Diaminoazoxyfurazan (DAAF) using an instrumented Small Scale Gap Test, LA-UR-08-07858, 40th International Conference of ICT, Los Alamos National Laboratories, Los Alamos, NM, USA, 2009
[18]	E-C Koch, Insensitive high explosives: IV. Nitroguanidine — Initiation & detonation, Def. Technol. 2019, 15(4), 467-487.
[19]	G. S. Yakovleva, R. K. Kurbangalina, L. N. Stesik, Rate of detonation of hydrazonium azide. Combust. Explos. Shock Waves 1974, 10, 233-235.
[20]	H. Östmark, A. Helte, T.E. Carlsson, N-guanylurea-dinitramide (FOX-12): A new extremely insensitive energetic material for explosives applications, Thirteenth International Detonation Symp., Norfolk, 23-28 Jul 2006, Office of Naval Research, VA, USA 2006.
[21]	I. Zhukov, G. Kozak, Calculation of thermochemical and explosive characteristics of furoxanes. Central Eur. J. Energ. Mater. 2008, 5(34), 45-54.
[22]	J. P. Lu, Evaluation of the Thermo Chemical Code Cheetah 2.0 for Modeling Explosives Performance. Report DSTO-TR-1199, Aeronautical and Maritime Research Laboratory, Melbourne, AU 2001.
[23]	J. R. Stine, On predicting properties of explosives – detonation velocity. J. Energ. Mater. 1990, 8(1-2), 41-73.
[24]	J. Rećko, R. Lewczuk, L. Szymańczyk, S. Zeman, Study on explosive properties of BCHMX. Proceedings of the 22nd Seminar on New Trends in Research of Energetic Materials : NTREM, Pardubice, 10-12 April 2019, University of Pardubice, CZ 2019.
[25]	L. G. Green, E. L. Lee, Detonation pressure measurements on PETN, Proceedings of the 13th International Detonation Symposium, Norfolk, VA, United States 2006, pp. 1144-1150.
[26]	M. A. Daniel, P. J. Davies, I. J. Lochert, FOX-7 for Insensitive Boosters, Report DSTO-TR-2449, Defence Science and Technology Organisation, Weapons Systems DIV, Edinburgh, AU 2010.
[27]	M. A. Ilyushin, I. V. Tselinsky, I. V Shugalei, Environmentally friendly energetic materials for initiation devices. Cent. Eur. J. Energ. Mater. 2012, 9(4), 293-327.
[28]	M. D. Joseph, S. K. Jangid,, R. S. Satpute, B. G. Polke, T. Nath, S. N. Asthana, A. S. Rao, Studies on Advanced RDX/TATB-Based Low Vulnerable Sheet Explosives with HTPB Binder, Propellants Explos. Pyrotech.- 2009, 34, 326–330.
[29]	M. F. Gogulya, M. N. Makhov, A. Yu. Dolgoborodov, M. A. Brazhnikov, V. I. Arkhipov, V. G. Shchetinin, Mechanical sensitivity and detonation parameters of aluminized explosives. Combust. Explos. Shock Waves 2004, 40, 445-457.
[30]	M. F. Gogulya, M. N. Makhov, M. A. Brazhnikov, A. Yu. Dolgoborodov, Detonation velocity of BTNEN/Al. Combust. Explos. Shock Waves 2006, 42, 480-485.
[31]	M. J. Kamlet, J. M. Short, The chemistry of detonations. VI. A Rule for Gamma as a criterion for choice among conflicting detonation pressure measurements, Combust. Flame 1980, 38, 221-230.
[32]	M. Künzel, R. Matyáš, O. Vodochodský, J. Pachman, Explosive properties of melt cast erythritol tetranitrate (ETN). Cent. Eur. J. Energ. Mater. 2017, 14(2), 418-429.
[33]	N. V. Kozyrev, Reparametrization of the BKW equation of state for CHNO explosives which release no condensed carbon upon detonation. Cent. Eur. J. Energ. Mater. 2015, 12(4), 651-669.
[34]	P. Cooper, Explosives Engineering, Wiley-VCH, NY, USA 1996.
[35]	P. Samuels, K. Spangler, D. Iwaniuk, R. Cornell, E. L. Baker, L. I. Stiel, Detonation performance analyses for recent energetic molecules, AIP Conference Proceedings 1979, 2018, 150033.
[36]	R. E. Cornell, E. T. Wrobel, An experimental investigation of corner-turning performance in a large double cylinder of highly-insensitive explosive. Propellants Explos. Pyrotech. 2021, 46, 378-388.
[37]	R. Engelke, S. A. Sheffield, L. L. Davis, Experimental and Predicted Detonation Parameters for Liquid-Phase H202/H20 Mixtures, J. Phys. Chem. 2000, 104, 6894-6898.
[38]	R. JeremiĆ, J. Bogdanov, Development of a new model for the calculation of the detonation parameters of high explosives, J. Serb. Chem. Soc. 2012, 77-3, 371–380.
[39]	R. K. Kurbangalina, E. A. Patskov, L. N. Stesik, G. Yakovleva, Detonation of liquid hydrazoic acid and its aqueous solutions. J. Appl. Mech. Tech. Phys. 1970, 11, 672-677.
[40]	R. Lewczuk, P. Koślik, J. Rećko, Performance of BCHMX in small charges. Propellants Explos. Pyrotech. 2020, 45, 581-586.
[41]	R. Meyer, J. Köhler, A. Homburg, Explosives, Wiley-VCH Verlag GmbH, Weinheim, 2007.
[42]	S. A. Kolesnikov, A. V. Utkin, Nonclassical steady-state detonation regimes in pressed TNETB. Combust. Explos. Shock Waves 2007, 43, 710–716.
[43]	S. W. Vincent, S. I. Jackson, C. Chiquete, M. Short, The geometric scaling of IMX-104 explosive: Detonation velocity versus charge size for cylindrical rate sticks and slab tests, in: Proc. 15th International Detonation Symposium (Eds.: J. Carney and J. Maienschein), Office of Naval Research, 2015, p. 534.
[44]	S. Zeman, A. Elbeih, Z. Akštein. Preliminary study on several plastic bonded explosives based on cyclic nitramines. Chin. J. Energ. Mater. 2011, 19 (1), 8-12.
[45]	V. Džingalašević, G. Antić, D. Mlađenović, Ratio of detonation pressure and critical pressure of high explosives with different compounds. Sci. Tech. Rev. 2004, 3-4, 72-76.
[46]	V. I. Pepekin, B. L. Korsunskii, Y. N. Matyushin, Explosive properties of furoxanes. Combust. Explos. Shock Waves 2008, 44, 110-114.
[47]	V. I. Pepekin, Limiting detonation velocities and limiting propelling powers of organic explosives. Dokl. Phys. Chem. 2007, 414, 159-161.
[48]	V. I. Pepekin, S. A. Gubin, Methods of calculating the detonation parameters of explosives, Khimicheskaya fizika 2003, 22(9), 72–97. [in Russian]
[49]	V. M. Mochalova, A. V. Utkin, A. V. Anan'in, Effect of the degree of dispersion on the detonation wave structure in pressed TNETB. Combust. Explos. Shock Waves 2007, 43, 575–579.
[50]	V. Pepekin, Development of High Efficiency Energetic Explosives, 22nd International Pyrotechnics Seminar, Fort Collins, 15-19 July 1996, The International Pyrotechnics Society, Colorado, USA 1996.
[51]	V. W. Manner, D. N. Preston, B. C. Tappan, V. E. Sanders, G. W. Brown, E. Hartline, B. Jensen, Explosive performance properties of erythritol tetranitrate (ETN). Propellants Explos. Pyrotech. 2015, 40(4), 460-462.
[52]	V. S. Mishra, S. R. Vadali, A. L. Bhagat, R. K. Garg, V. M. Kugaonkar, S. Raman, R. K. Sinha, S. Asthana, Studies on NTO-, FOX-7- and DNAN-based melt cast formulations. Cent. Eur. J. Energ. Mater. 2017, 14, 403–417.
[53]	W. A. Trzcinski, S. Cudzilo, S. Dipak, M. Nita, A comparison of the sensitivity and performance characteristics of melt-pour explosives with TNT and DNAN binder. Cent. Eur. J. Energ., Mat. 2014, 11: 445-455
[54]	W. A. Trzciński, S. Cudziło, Z. Chyłek, L. Szymańczyk, Detonation properties of 1,1-diamino-2,2-dinitroethene (DADNE). J. Hazard. Mater. 2008, 157 (2-3): 605-612.
[55]	W. Xiong, A simple method for calculating detonation parameters of explosives, J. Energ. Mater. 1985, 3(4), 263-277.
[56]	Y. A. Bogdanova, S. A. Gubin, B. L. Korsunskii, V. I. Pepekin, Detonation characteristics of powerful insensitive explosives. Combust. Explos. Shock Waves 2009, 45, 738-743.
[57]	Y. A. Bogdanova, S. A. Gubin, A. A. Anikeev, S. B. Victorov, Thermodynamic modelling of detonation H-N-O high explosives, J. Phys.: Conf. Ser. 2015, 751, 012018.
[c]	calculated value