An Improved Simple Method for the Calculation of the Detonation Performance of CHNOFCl, Aluminized and Ammonium Nitrate Explosives

Mohammad Hossein KESHAVARZ, Mohammad KAMALVAND, Mohammad JAFARI, Ahmad ZAMANI

S.I.

Appendix A

Glossary of compound names and heats of formation for pure as well as composite explosives on the basis of 100 g for mixtures of different compounds

No.	Abbreviation	Full name or composition	Chemical formula	$\Delta_f H^\circ$(c) (kJ mol^{-1})
1	ABH	Azobis (2,2',4,4',6,6'-hexanitrobiphenyl)	$C_{24}H_6N_{14}O_{24}$	485.34 [12]
2	Alex 20	44/32/20/4 RDX/TNT/Al/Wax	$C_{1.783}H_{2.469}N_{1.613}O_{2.039}Al_{0.7335}$	-7.61
3	Alex 32	37/28/31/4 RDX/TNT/Al/Wax	$C_{1.647}H_{2.093}N_{1.365}O_{1.744}Al_{1.142}$	-9.33
4	AMATEX-20	42/20/38 AN/RDX/TNT	$C_{1.44}H_{1.38}N_{1.04}O_{1.54}(AN)_{0.53}$	-95.77
5	AMATEX-40	21/41/38 AN/RDX/TNT	$C_{1.73}H_{1.95}N_{1.61}O_{2.11}(AN)_{0.26}$	-197.49
6	AMATOL80/20	80/20 AN/TNT	$C_{0.62}H_{0.44}N_{0.26}O_{0.53}(AN)_1$	-371.25
7	AN	Ammonium Nitrate	NH_4NO_3 or $H_4N_2O_3$	-365.14 [6]
8	AN/Al (90/10)	--	$Al_{0.37}(AN)_{1.125}$ or $H_{4.5}N_{2.25}O_{3.37}Al_{0.37}$	-412.42
9	AN/Al (80/20)	--	$Al_{0.74}(AN)_1$ or $H_4N_2O_3Al_{0.74}$	-368.32
10	AN/Al (70/30)	--	$Al_{1.11}(AN)_{0.875}$ or $H_{3.5}N_{1.75}O_{2.62}Al_{1.11}$	-324.55

No.	Abbreviation	Full name or composition	Chemical formula	$\Delta_f H^{\circ}$(c) (kJ mol^{-1})
11	BTF	Benzotris(1,2,5-oxadiazole-1-oxide)	$C_6N_6O_6$	602.50 [12]
12	COMP A-3	91/9 RDX/WAX	$C_{1.87}H_{3.74}N_{2.46}O_{2.46}$	11.88 [12]
13	COMP B	63/36/1 RDX/TNT/wax	$C_{2.03}H_{2.64}N_{2.18}O_{2.67}$	5.36 [6]
14	COMP C-3	77/4/10/5/1/3 RDX/TNT/DNT/MNT/NC/Tetryl	$C_{1.90}H_{2.83}N_{2.34}O_{2.60}$	-26.99 [12]
15	COMP C-4	91/5.3/2.1/1.6 RDX/TNT/MNT/NC	$C_{1.82}H_{3.54}N_{2.46}O_{2.51}$	13.93 [12]
16	Cyclotol-50/50	50/50 RDX/TNT	$C_{2.22}H_{2.45}N_{2.01}O_{2.67}$	0.04
17	Cyclotol-60/40 (or COMP B-3)	60/40 RDX/TNT	$C_{2.04}H_{2.50}N_{2.15}O_{2.68}$	4.81 [6]
18	Cyclotol-65/35	65/35 RDX/TNT	$C_{1.96}H_{2.53}N_{2.22}O_{2.68}$	8.33
19	Cyclotol-70/30	70/30 RDX/TNT	$C_{1.87}H_{2.56}N_{2.29}O_{2.68}$	11.13
20	Cyclotol-75/25	75/25 RDX/TNT	$C_{1.78}H_{2.58}N_{2.36}O_{2.69}$	13.4 [6]
21	Cyclotol-77/23	77/23 RDX/TNT	$C_{1.75}H_{2.59}N_{2.38}O_{2.69}$	14.98
22	Cyclotol-78/22	78/22 RDX/TNT	$C_{1.73}H_{2.59}N_{2.40}O_{2.69}$	15.52
23	DATB	1,3-Diamino-2,4,6-trinitrobenzene	$C_6H_5N_5O_6$	-98.74 [12]
24	Destex	74.766/18.691/4.672/1.869 TNT/Al/Wax/Graphite	$C_{2.791}H_{2.3121}N_{0.987}O_{1.975}Al_{0.6930}$	-34.39
25	DIPAM (Dipicramide)	2.2' ,4,4' ,6,6' –Hexanitro-[1,1-biphenyl]-3,3'-diamine	$C_{12}H_6N_8O_{12}$	-14.90 [38]

No.	Abbreviation	Full name or composition	Chemical formula	$\Delta_f H^\theta$(c) (kJ mol^{-1})
26	DIPAM (Dipicramide)	2.2' ,4,4' ,6,6' –Hexanitro-[1,1-biphenyl]-3,3'-diamine	$C_{12}H_6N_8O_{12}$	-28.45 [12]
27	EXP D	Ammonium picrate or Explosive D	$C_6H_6N_4O_7$	-393.30 [12]
28	EDC-11	64/4/30/1/1 HMX/RDX/TNT/Wax/Trylene	$C_{1.986}H_{2.78}N_{2.23}O_{2.63}$	4.52
29	EDC-24	95/5 HMX/Wax	$C_{1.64}H_{3.29}N_{2.57}O_{2.57}$	18.28
30	HBX-3	31/29/35/5/0.5 RDX/TNT/AL/WAX/$CaCl_2$	$C_{1.66}H_{2.18}N_{1.21}O_{1.60}Al_{1.29}Ca_{0.005}Cl_{0.009}$	-8.71 [19]
31	HMX	Cyclotetramethylenetetranitramine	$C_4H_8N_8O_8$	74.98 [12]
32	HMX/Al (80/20)	--	$C_{1.08}H_{2.16}N_{2.16}O_{2.16}Al_{0.715}$	20.21
33	HMX/Al (70/30)	--	$C_{0.944}H_{1.888}N_{1.888}O_{1.888}Al_{1.11}$	17.66
34	HMX/Al (60/40)	--	$C_{0.812}H_{1.624}N_{1.624}O_{1.624}Al_{1.483}$	15.19
35	HMX/Exon (90.54/9.46)	--	$C_{1.43}H_{2.61}N_{2.47}O_{2.47}F_{0.15}Cl_{0.10}$	-1026.80
36	HNAB	2,2',4,4',6,6'-Hexanitroazobenzene	$C_{12}H_4N_8O_{12}$	284.09 [12]
37	Liquid TNT	--	$C_7H_5N_3O_6$	-53.26
38	LX-04	85/15 HMX/Viton	$C_{5.485}H_{9.2229}N_8O_8F_{1.747}$	-89.96 [6]
39	LX-07	90/10 HMX/Viton	$C_{1.48}H_{2.62}N_{2.43}O_{2.43}F_{0.35}$	-51.46 [6]
40	LX-09	93/4.6/2.4 HMX/DNPA/FEFO	$C_{1.43}H_{2.74}N_{2.59}O_{2.72}F_{0.02}$	8.38 [6]
41	LX-10	95/5 HMX/Viton	$C_{1.42}H_{2.66}N_{2.57}O_{2.57}F_{0.17}$	-13.14 [6]

No.	Abbreviation	Full name or composition	Chemical formula	$\Delta_f H^\circ$(c) (kJ mol^{-1})
42	LX-11	80/20 HMX/Viton	$C_{1.61}H_{2.53}N_{2.16}O_{2.16}F_{0.70}$	-128.57 [6]
43	LX-14	95.5/4.5 HMX/Estane 5702-F1	$C_{1.52}H_{2.92}N_{2.59}O_{2.66}$	6.28 [12]
44	LX-15	95/5 HNS-I/Kel-F 800	$C_{3.05}H_{1.29}N_{1.27}O_{2.53}Cl_{0.04}F_{0.3}$	-18.16 [6]
45	LX-17	92.5/7.5 TATB/Kel-F 800	$C_{2.29}H_{2.18}N_{2.15}O_{2.15}Cl_{0.054}F_{0.2}$	-100.58 [6]
46	MEN-II	72.2/23.4/4.4 Nitromethane/Methanol/Ethylene diamine	$C_{2.06}H_{7.06}N_{1.33}O_{3.10}$	-310.87 [6]
47	MINOL-2	40/40/20 AN/TNT/Al	$C_{1.23}H_{0.88}N_{0.53}O_{1.06}Al_{0.74}(AN)_{0.5}$	-194.26 [6]
48	NM	Nitromethane	$C_1H_3N_1O_2$	-112.97 [12]
49	NONA	2,2',2",4,4',4",6,6',6"-Nonanitro-m-terphenyl	$C_{18}H_5N_9O_{18}$	114.64 [12]
50	NQ	Nitroguanidine	$CH_4N_4O_2$	-92.47 [6]
51	NM/UP (60/40)	60/40 Nitromethane/UP; UP=90/10 $CO(NH_2)_2HClO_4/H_2O$	$C_{1.207}H_{4.5135}N_{1.432}O_{3.309}Cl_{0.2341}$	11.51
52	Octol-76/23	76.3/23.7 HMX/TNT	$C_{1.76}H_{2.58}N_{2.37}O_{2.69}$	12.76
53	Octol-75/25	75/25 HMX/TNT	$C_{1.78}H_{2.58}N_{2.36}O_{2.69}$	11.63 [6]
54	Octol-60/40	60/40 HMX/TNT	$C_{2.04}H_{2.50}N_{2.15}O_{2.68}$	4.14
55	PBX-9007	90/9.1/0.5/0.4 RDX/Polystyrene/DOP/Resin	$C_{1.97}H_{3.22}N_{2.43}O_{2.44}$	29.83 [12]
56	PBX-9010	90/10 RDX/Kel-F	$C_{1.39}H_{2.43}N_{2.43}O_{2.43}Cl_{0.09}F_{0.26}$	-32.93 [6]

No.	Abbreviation	Full name or composition	Chemical formula	$\Delta_f H^\circ$(c) (kJ mol^{-1})
57	PBX-9011	90/10 HMX/Estane	$C_{1.73}H_{3.18}N_{2.45}O_{2.61}$	-16.95 [12]
58	PBX-9205	92/6/2 RDX/Polystyrene/DOP	$C_{1.83}H_{3.14}N_{2.49}O_{2.51}$	24.31 [12]
59	PBX-9407	94/6 RDX/Exon 461	$C_{1.41}H_{2.66}N_{2.54}O_{2.54}Cl_{0.07}F_{0.09}$	3.39 [6]
60	PBX-9501	95/2.5/2.5 HMX/Estane/BDNPA-F	$C_{1.47}H_{2.86}N_{2.60}O_{2.69}$	9.62 [12]
61	PBX-9502	95/5 TATB/Kel-F 800	$C_{2.3}H_{2.23}N_{2.21}O_{2.21}Cl_{0.04}F_{0.13}$	-87.15 [6]
62	PBX-9503	15/80/5 HMX/TATB/KEL-F 800	$C_{2.16}H_{2.28}N_{2.26}O_{2.26}Cl_{0.038}$	-74.01 [6]
63	PBXC-9	75/20/5 HMX/Al/Viton	$C_{1.15}H_{2.14}N_{2.03}O_{2.03}F_{0.17}Al_{0.74}$	113.01
64	PBXC-116	86/14 RDX/Binder	$C_{1.968}H_{3.7463}N_{2.356}O_{2.4744}$	4.52
65	PBXC-117	71/17/12 RDX/Al/Binder	$C_{1.65}H_{3.1378}N_{1.946}O_{2.048}Al_{0.6303}$	-65.56
66	PBXC-119	82/18 HMX/Binder	$C_{1.817}H_{4.1073}N_{2.2149}O_{2.6880}$	18.28
67	Pentolite-50/50	50/50 TNT/PETN	$C_{2.33}H_{2.37}N_{1.29}O_{3.22}$	-100.01
68	PETN	Pentaerythritol tetranitrate	$C_5H_8N_4O_{12}$	-538.48 [6]
69	PF	1-Fluoro-2,4,6-trinitrobenzene	$C_6H_2N_3O_6F$	-224.72
70	RDX	Cyclomethylenetrinitramine	$C_3H_6N_6O_6$	61.55 [6]
71	RDX/Al (90/10)	--	$C_{1.215}H_{2.43}N_{2.43}O_{2.43}Al_{0.371}$	24.89
72	RDX/Al (80/20)	--	$C_{1.081}H_{2.161}N_{2.161}O_{2.161}Al_{0.715}$	22.13
73	RDX/Al (70/30)	--	$C_{0.945}H_{1.89}N_{1.89}O_{1.89}Al_{1.11}$	19.37

No.	Abbreviation	Full name or composition	Chemical formula	$\Delta_f H^\circ$(c) (kJ mol^{-1})
74	RDX/Al (60/40)	--	$C_{0.81}H_{1.62}N_{1.62}O_{1.62}Al_{1.483}$	16.61
75	RDX/Al (50/50)	--	$C_{0.675}H_{1.35}N_{1.35}O_{1.35}Al_{1.853}$	13.85
76	RDX/TFNA (65/35)	--	$C_{1.54}H_{2.64}N_{2.2}O_{2.49}F_{0.44}$	-823.83
77	RDX/Exon (90.1/9.9)	--	$C_{1.44}H_{2.6}N_{2.44}O_{2.44}F_{0.17}Cl_{0.11}$	-195.48
78	TATB	1,3,5-Triamino-2,4,6-trinitrobenzene	$C_6H_6N_6O_6$	-154.18 [6]
79	TATB/HMX/Kel-F (45/45/10)	--	$C_{1.88}H_{2.37}N_{2.26}O_{2.26}F_{0.28}Cl_{0.06}$	-478
80	Tetryl	N-Methyl-N-nitro-2,4,6-trinitroaniline	$C_7H_5N_5O_8$	19.54 [6]
81	TFENA	2,2,2-Trifluoroethylnitramine	$C_2H_3N_2O_2F_3$	-694.54
82	TFET	2,4,6-Trinitrophenyl-2,2,2-trifluoroethylnitramine	$C_8H_4N_5O_8F_3$	-576.8
83	TNT	2,4,6-Trinitrotoluene	$C_7H_5N_3O_6$	-67.07 [18]
84	TNTAB	Trinitrotriazidobenzene	$C_6N_{12}O_6$	1129.68 [12]
85	TNT/Al (89.4/10.6)	--	$C_{2.756}H_{1.969}N_{1.181}O_{2.362}Al_{0.393}$	-24.73
86	TNT/Al (78.3/21.7)	--	$C_{2.414}H_{1.724}N_{1.034}O_{2.069}Al_{0.804}$	-21.63
87	Toluene/Nitromethane(14.5/85.5)	--	$C_{2.503}H_{5.461}N_{1.4006}O_{2.8013}$	-160.71
88	Torpex	42/40/18 RDX/TNT/Al	$C_{1.8}H_{2.015}N_{1.663}O_{2.191}Al_{0.6674}$	-0.17
89	Tritonal	80/20 TNT/Al	$C_{2.465}H_{1.76}N_{1.06}O_{2.11}Al_{0.741}$	-23.64

Appendix B

Some examples of the calculation of the detonation velocities for different ideal or non-ideal high explosives.

Path	Name	ρ_0 g/cm^3	$D_{Exp.}$ km/s	Ref.	moles of products/moles of high explosive												α moles/g HE	$\overline{Mw}_g$ g/moles	Q_d kJ/g	$D_{Pred.}$ km/s
					HF	HCl	N_2	CO	CO_2	H_2	H_2O	O_2	C(s)	Al_2O_3(s)	Al(s)	AN(s)				
2a	AN (Pure)	1.05	4.50	[11]	-	-	0.78	-	-	-	1.56	0.39	-	-	-	0.22	0.0341	22.87	1.12	4.43
2b	AN/Al (70/30)	1.05	5.40	[11]	-	-	0.81	-	-	1.62	0.01	0.41	-	0.54	0.03	0.06	0.0285	13.80	6.17	4.99
2c	LX-17	1.91	7.63	[12]	0.2	0.05	1.08	2.15	-	0.96	-	-	0.14	-	-	-	0.0444	22.12	1.95	7.69
2d	DEGN	1.38	6.76	[12]	-	-	1.00	4.00	-	1.00	3.00	-	-	-	-	-	0.0459	21.79	3.83	6.93
2e	ANFO 6/94	0.88	5.50	[11]	-	-	1.00	0.09	0.28	-	2.36	-	-	-	-	-	0.0437	23.03	3.69	5.10
2f	NG	1.59	7.58	[11]	-	-	1.50	-	3.00	-	2.50	0.25	-	-	-	-	0.0319	32.15	6.23	7.89