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The Insensitive High Explosive Triaminotrinitrobenzene (TATB): Development and Characterization – 1888 to 1994

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GLOSSARY

This list includes acronyms, chemical names and formulae, and code names and designations for triaminotrinitrobenzene (TATB) and TATB formulations included in this compilation. For formulations, the weight percent (wt%) is implied. The formulations are listed alphabetically in decreasing order of wt% of TATB.

at %	atom percent	
ADNT	ammonium 3,5-dinitro-1,2,4-triazolate	
ADPA	American Defense Preparedness Association	
AFM	atomic force microscopy	
AN	ammonium nitrate	
APS	American Physical Society	
ARC	accelerating-rate calorimetry	
ARDC	Army Research and Development Center/ Command, Dover, NJ	
AWRE	Atomic Weapon Research Establishment	
$BaCO_3$	barium carbonate	
BET	Brunauer-Emmett-Teller (ACS J. 60, 309[1938] particle size distribution)	
BKW	Becker-Kistiakowsky-Wilson (EOS)	
BTF	benzotris[1,2,5]oxadiazole,1,4,7-trioxide,	
cgs	centimeter-gram-second system of measurement	
CEF	tris-β-chloroethyl phosphate	
C-J	Chapman-Jouguet	
$ClSO_3H$	chlorosulfonic acid	
Comp B-3	RDX/TNT 60/40, Composition B-3	
CRT	chemical reactivity test	
Cu	Copper	
Cyclotol 75/25	RDX/TNT 75/25	
DAGMAR	Direct Analysis Generated Modified Arrhenius Rate	
DATB	1,3-diamino-2,4,6-trinitrobenzene	
DATB/Estane/$BaCO_3$ 37/9.5/53/0.5		X-0262
DATB/Estane/oxamide 55.5/14.3/30.2		X-0263
DATB/HMX/Viton 20/70/10		LX-03-0
DATB/Talc/Estane 42.8/46.2/11.0		
DATB/TiO_2/Estane 37.4/53/9.6		
DATB/Viton 95/5		X-0299
DATB recycl/DATB raw/Viton A 63.33/31.67/5		
DATB/Viton A/$BaCO_3$		X-0264
DDT	deflagration-to-detonation transition	
DMF	dimethylformamide	
DMSO	dimethyl sulfoxide	
DNPA	dinitropropylacrylate	
DNT3CB, T3	1,3-dinitro-2,4,6-trichlorobenzene	
DNT4CB, T4	1,3-dinitro-2,4,5,6-tetrachlorobenzene	
DOP	dioctylphthalate	
DPE	diphenyl ether	
DSC	differential scanning calorimetry	
DSD	detonation shock dynamics	

DSD	detonation shock dynamics	
DTA	differential thermal analysis	
EAK	ethylene diammonium dinitrate/ammonium nitrate/potassium nitrate eutectic explosives	
EDD	ethylenediamine dinitrate	
EOS	equation of state	
Fairy Dust	AN/ADNT 2/1 molar ratio	
FSO_3H	fluorosulfonic acid	
F_3CSO_3H	trifluoromethylsulfonic acid	
HE	high explosive	
HMX	1,3,5,7-tetranitro-1,3,5,7-tetrazacyclooctane	
HNB	hexanitrobenzene	
HNS	2,2',4,4',5,5'-hexanitrostilbene	
H_2SO_4	sulfuric acid	
ICT	Institute for Chemical Technology, Fraunhofer Institute, Karlsruhe, Germany	
IHE	insensitive high explosive	
IR	infrared spectroscopy	
JWL	Jones-Wilkins-Lee (EOS)	
$KClO_4$	potassium perchlorate	
LANL	Los Alamos National Laboratory	
LLNL	Lawrence Livermore National Laboratory	
LSGT	large-scale gap test	
LSTX	large-scale time-to-explosion test	
LX-03-0	DATB/HMX/Viton 20/70/10	
LX-10-0	HMX/Viton A 95/5	
LX-10-1	HMX/Viton A 94.5/5.5	
LX-17-0	TATB/Kel-F 800 92.5/7.5	RX-03-BB, made with dry-aminated TATB
LX-17-1	TATB/Kel-F 800 92.5/7.5	made with wet-aminated TATB
MEK	methyl ethyl ketone	
MHSMP	Mason & Hanger, Silas Mason Co., Inc., Pantex Plant	
MLM	Mound Laboratory	
MNTCB	see TCNB	
NC	nitrocellulose	
NQ	nitroguanidine	
NAWC	Naval Air Warfare Center	
NH_4Cl	ammonium chloride	
NMR	nuclear magnetic resonance	
NSWC	Naval Surface Warfare Center	
OB	oxygen balance	
ODTX	one-dimensional time-to-explosion test	
Pb	lead	
$PbCrO_4$	lead chromate	
PBX	plastic-bonded explosive	
PBX 9404	HMX/NC/CEF 94/3/3	
PBX 9502	TATB/Kel-F 800 95/5	X-0290, RX-03-AR, RX-03-AU
PBX 9503	TATB/HMX/Kel-F 800 80/15/5	
	TATB/HMX/Kel-F 800/dye 79.8/15/5/0.2	X-0433

PBXW-7	TATB/RDX/PTFE 60/35/5	
PE	polyethylene	
PETN	pentaerythritol tetranitrate	
PNF	synthetic rubber	
ppm	parts per million	
PS	polystyrene	
PTFE	poly(tetrafluoroethylene)	
PXGT	Pantex gap text	
PVF	poly(vinylidine fluoride)	
PYX	2,6-bis(picrylamino)-3,5-dinitropyridine	
RDX	1,3,5-trinitro-1,3,5-triazacyclohexane	
RT	room temperature, ambient	
RX-03-AB	See X-0219	
RX-03-AE	TATB/Estane 5702 F-1 94/6	
RX-03-AF	TATB/Viton A 91/9	
RX-03-AH	TATB/Kel-F 800 91/9	
RX-03-AI	TATB/Kel-F 800 90/10	
RX-03-AJ	TATB/Estane 5702 F-1 97/3	
RX-03-AR	See RX-03-AU, X-0290, PBX 9502	
RX-03-AT	TATB/Viton A 95.5/4.5	
RX-03-AU	See PBX 9502, X-0290	
RX-03-BB	TATB/Kel-F 800 92.5/7.5	RX-03-BC, LX-17-0
RX-03-BC	See LX-17-0	
RX-03-CK	TATB/Phenoxy 92.5/7.5	
RX-03-DA	TATB/HMX/Kraton 48/48/4	
RX-03-DD	TATB/HMX/Kraton/Vistanex 48/48/2/2	
RX-03-DH	TATB/TNT 95/5	
RX-03-DI	TATB/Phenoxy PKHJ 96.3/3.7	
RX-03-DU	TATB/Kraton 70-3608 96.22/3.78	
RX-03-DY	TATB/Phenoxy PKHJ 97.5/2.5	
RX-03-EJ	TATB/Kel-F 800/Al 74/6/20	
RX-03-EK	TATB/Kel-F 800/Al 83.25/6.75/10	
RX-03-EL	TATB/Kel-F 800/Al 64.75/5.25/30	
RX-03-EM	TATB/Kel-F 800/Al 55.5/4.5/40	
RX-03-ER	TATB/Kel-F 800/AP/Al 74.0/6.0/12.4/7.6	
RX-03-EY	TATB/Kraton G1650/Tufflo Oil 6026 96.15/2.56/1.29	
RX-26-AF	TATB/HMX/Estane 57-2-F1 46.64/49.28/4.10	
RX-26-AX	TATB/HMX/Kraton 1650 47.1/49.7/3.2	
RX-34-AD	TATB/BTF/NH_4ClO_4 35.42/2.50/61.08	
RX-34-AG	TATB/BTF/NH_4ClO_4 31.99/10.0/58.01	
RX-36-AA	TATB/HMX/BTF 32/36.7/31.3	
RX-36-AB	TATB/BTF 50.6/49.4	
RX-36-AC	TATB/HMX/BTF 15.2/69.9/14.9	
RX-36-AD	TATB/HMX/BTF 58.6/22.4/19.0	
RX-36-AF	TATB/HMX 46.6/53.4	
RX-36-AG	TATB/HMX/BTF 19.7/22.6/57.7	
RX-36-AI	TATB/HMX/BTF/Viton 14.44/66.40/14.16/5.0	
SDT	shock-to-detonation transition	
SEM	scanning electron microscopy	
SI	International System of Units	
SNL	Sandia National Laboratories	
SNLA	Sandia National Laboratories Albuquerque	

SNLL	Sandia National Laboratories Livermore	
SRI	Stanford Research Institute	
SSGT	small-scale gap test	
STP	standard temperature and pressure	
T3	1,3,5-trichloro-2,4-dinitrobenzene, see DNT3CB	
T4	1,2,3,5-tetrachloro-4,6-dinitrobenzene, see DNT4CB	
Ta	tantalum	
TATB	1,3,5-triamino-2,4,6-trinitrobenzene	
TATB/acrylate binder 70/30		
TATB/AN 1/9 molar ratio		
TATB/AN/ADNT 28.4/27.0/44.6, 1.3/2/1 molar ratio		
TATB/AN/ADNT 1.3/4/3 molar ratio		
TATB/AN/EDD 50/25/25		
TATB/BTF 50.6/49.4		RX-36-AB
TATB/BTF/NH_4ClO_4 36.42/2.50/61.08		RX-34-AD
TATB/BTF/NH_4ClO_4 31.99/10.0/58.01		RX-34-AG
TATB/Cu 50/50 vol%		
TATB/Dapon M 95/5		X-0253
TATB/Dapon M 90/10		
TATB/EAK 20/80		
TATB/Elwax/B^2 wax 94/3/3		
TATB/Elwax/B^2 wax 90/5/5		
TATB/Epoxy HG18 95/5		
TATB/Estane 5702 F-1 97/3		RX-03-AJ
TATB/Estane 5702 F-1 94/6		RX-03-AE
TATB/Estane 5714-F1 95/5		X-0238
TATB/Fairy Dust 90/10		
TATB/HMX 85/15		
TATB/HMX 75/25		
TATB/HMX 46.6/53.4		RX-36-AF
TATB/HMX/AN/ADNT 21.2/36.9/20.0/21.9		
TATB/HMX/binder		RX-26-xx
TATB/HMX/BTF 58.6/22.4/19.0		RX-36-AD
TATB/HMX/BTF 15.2/69.9/14.9		RX-36-AC
TATB/HMX/BTF/Viton 14.44/66.40/14.16/5.0		RX-36-AI
TATB/HMX/Estane 70/25/5		
TATB/HMX/Estane 60.9/35/4.1		X-0450
TATB/HMX/Estane 5/92/3		
TATB/HMX/Estane 2/95/3		
TATB/HMX/Estane 5702-F1 46.64/49.28/4.10		RX-26-AF
TATB/HMX/Estane/Ca stearate 0-10/≤95/0-5/0-0.5		X-0272
TATB/HMX/Estane/dye 69.8/24.9/4.9/0.4		X-0396
TATB/HMX/Estane/dye 60.6/34.9/4.1/0.4		X-0450
TATB/HMX/Estane/dye 50.8/45.9/3/0.3		X-0371
TATB/HMX/Kel-F 0-92/0-92/9-15		X-0219
TATB/HMX/Kel-F 800 92.5/5/2.5		X-0353

TATB/HMX/Kel-F 800 90.25/4.75/5	X-0341
TATB/HMX/Kel-F 800 87.5/10/2.5	X-0354
TATB/HMX/Kel-F 800 85.5/9.5/5	X-0342
TATB/HMX/Kel-F 800 85/12.5/2.5	X-0358
TATB/HMX/Kel-F 800 82.5/15/2.5	X-0355
TATB/HMX/Kel-F 800 80.75/14.25/5	X-0343
TATB/HMX/Kel-F 800 80/15/5	PBX 9503
TATB/HMX/Kel-F 800 77.5/20/2.5	X-0356
TATB/HMX/Kel-F 800 75/20/5	X-0321
TATB/HMX/Kel-F 800 71.25/23.75/5	X-0344
TATB/HMX/Kel-F 800 70/25/5	
TATB/HMX/Kel-F 800 70/20/10	
TATB/HMX/Kel-F 800 60/35/5	X-0320
TATB/HMX/Kel-F 800 50/45/5	X-0319
TATB/HMX/Kel-F 800 47.5/45/7.5	X-0319
TATB/HMX/Kel-F 800 45/45/10	X-0219
TATB/HMX/Kel-F 800/dye 89.85/4.75/5/0.4	X-0431
TATB/HMX/Kel-F 800/dye 80.35/14.25/5/0.4	X-0343
TATB/HMX/Kel-F 800/blue pigment 44.73/45/10/0.27	X-0219
TATB/HMX/Kel-F 800/dye 37.8/57/5/0.2	
TATB/HMX/Kel-F 800/dye 19.8/70/10/0.2	
TATB/HMX/Kel-F 800/dye 18.8/76/5/0.2	
TATB/HMX/Kel-F 800/dye 2.8/92/5/0.2	
TATB/HMX/Kel-F 800/dye 79.8/15/5/0.2	X-0433, PBX 9503
TATB/HMX/Kel-F 800/purple dye 79.8/15/5/0.2	X-0351
TATB/HMX/Kel-F 800/blue pigment 49.73/45/5/0.27	X-0319
TATB/HMX/Kel-F 800/blue pigment 49.6/45/5/0.4	X-0319
TATB/HMX/Kel-F 800/dye 44.6/45/10/0.4	X-0219
TATB/HMX/Kel-F 800/Hi Viz pigment 49.7/45/5/0.3	X-0319
TATB/HMX/Kel-F 800/red-orange pigment 49.02/44.12/4.90/1.96	X-0319
TATB/HMX/Kel-F 820-800 63/27/10	
TATB/HMX/Kel-F 820-800 40/50/10	
TATB/HMX/Kel-F 820-800 20/70/10	
TATB/HMX/Kraton 48/48/4	RX-03-DA
TATB/HMX/Kraton 1650 47.1/49.7/3.2	RX-26-AX
TATB/HMX/Kraton G-6500 70/25/5	
TATB/HMX/Kraton/Hyvac oil 70/25/2.24/2.76	
TATB/HMX/Kraton/Hyvac oil 51.4/46.3/1.03/1.27	
TATB/HMX/Kraton/Hyvac oil 43/55/0.9/1.10	
TATB/HMX/Kraton/Hyvac oil 29/70/0.45/0.55	
TATB/HMX/Kraton/Irganox 1010 24.3/72.97/1.3/1.4/0.03	X-0398

TATB/HMX/Kraton/Vistanex 48/48/2/2		RX-03-DD
TATB/HMX/W/PS/DOP 6.74/6.60/85.36/0.8/0.5		
TATB/$KClO_4$/Astrel-360	proprietary	
TATB/$KClO_4$/Dapon M/$PbCrO_4$	proprietary	
TATB/Kel-F/Cumar R-16 95/5/0.15		
TATB/Kel-F 800 99.5/0.5		X-0331
TATB/Kel-F 800 99/1		X-0332
TATB/Kel-F 800 98/2		X-0333
TATB/Kel-F 800 97.5/2.5		X-0297
TATB/Kel-F 800 95/5		X-0290, PBX 9502, RX-03-AR, RX-03-AU
TATB/Kel-F 800 92.5/7.5		RX-03-BB, LX-17, X-0291
TATB/Kel-F 800 91/9		RX-03-AH
TATB/Kel-F 800 90/10		RX-03-AB,RX-03-AI, X-0219
TATB/Kel-F 800/Al 83.25/6.75/10		RX-03-EK
TATB/Kel-F 800/Al 77/5/18		
TATB/Kel-F 800/Al 74/6/20		RX-03-EJ
TATB/Kel-F 800/Al 64.75/5.25/30		RX-03-EL
TATB/Kel-F 800/Al 55.5/4.5/40		RX-03-EM
TATB/Kel-F 800/AP/Al 74.0/6.0/12.4/7.6		RX-03-ER
TATB/Kel-F 800/Dapon M 94.85/5/0.15		
TATB/Kel-F 800/Dioctyl sebacate 95/4.8/0.2		X-0458
TATB/Kel-F 800/Fluorolube LG-160 90/8/2		
TATB/Kel-F 800/Fluorolube MO-10 90/8/2		
TATB/Kel-F 800/oil 90/5/5		
TATB/Kel-F 800/purple dye 79.5/15/5/0.5		X-0351
TATB/Kel-F 800/Kraton G-6500 94.8/5/0.2		
TATB/Kel-F 800/Lecithin 94.8/5/0.2		
TATB/Kel-F 800/phenolic microballoons		X-0394
TATB/Kel-F 800/PE fibers/Silane 186-A 94.85/4/5/0.15		X-0339
TATB/Kel-F 800/Versamid 125 94.8/5/0.2		
TATB/Kel-F 3700 90/10		X-0219
TATB/Kel-F 5500 95/5		X-0290
TATB/Kraton 98/2		X-0296
TATB/Kraton/Tufflo oil 95.13/3.24/1.63		
TATB/Kraton G-6500/Hivac oil 97.6/1.68/0.72		X-0345
TATB/Pb 50/50 vol%		
TATB/PBX 9502 machining scrap/Kel-F 800 66.5/30/3.5		PBX 9502
TATB/PBX 9502 machining scrap/Kel-F 800 47.5/50/2.5		PBX 9502
TATB/PETN 70/30		
TATB/PETN/Kel-F 800 75/20/5		

TATB/PETN/Kel-F 800 70/25/5		X-0407
TATB/PETN/Kel-F 800/blue dye 69.8/25.0/5.0/0.2		X-0407
TATB/PETN/Kel-F 800 65/30/5		
TATB/Phenoxy 96.9/3.1		X-0329
TATB/Phenoxy 92.5/7.5		RX-03-CK
TATB/Phenoxy PKHJ 96.3/3.7		RX-03-DI
TATB/PNF elastomer 90/10		
TATB/Polysar 306 95/5		X-0497
TATB/PS/DOP 94/4.5/1.5		
TATB/PS/poly(phenylene oxide) 97.2/2.52/0.28		X-0330
TATB/PVF 95.4/4.6		X-0500
TATB/PYX 50/50		
TATB/RDX 85/15		
TATB/RDX 80/20		
TATB/RDX 75/25		
TATB/RDX/acrylate 70/30 (90/10)		
TATB/RDX/acrylate 70/30 (70/30)		
TATB/RDX/PTFE 60/35/5		PBXW-7
TATB/Ta/Kel-F 800 65.2/31.0/3.8		
TATB/TNT 99.9/0.1		
TATB/TNT 95/5		RX-03-DH
TATB/TNT 60/40		
TATB/TNT 50/50		
TATB/TNT 40/60		
TATB/TNT 30/70		
TATB/TNT 20/80		
TATB/TNT 10/90		
TATB/TNT/Al 40/40/20		
TATB/TNT/Kel-F 800 94.9/0.1/5		
TATB/Vibrathane 5003 98/2		X-0219
TATB/Vibrathane 5003 95/5		X-0219
TATB/Vistalon 95/5		X-0498
TATB/Vistanex Tufflo 6026/D32 microballoons 86/12/2		
TATB/Viton 91/9		
TATB/Viton A 95/5		RX-03-AT
TATB/Viton A 91/9		RX-03-AF
TATB/W/PS/DOP 13.46/85.24/0.8/0.5		
TATB/Wax-10-200 90/8/2		
TBTNB	1,3,5-tribromo-2,4,6-trinitrobenzene	
TCA	trichloroaniline	
TCB	1,3,5-trichlorobenzene	
TCDNB	see DNT3CB,T3	
TCNB	2,4,6-trichloro-1-nitrobenzene	
TCTNB	2,4,6-trichloro-1,3,5-trinitrobenzene	
TGA	thermogravimetric analysis	
TLC	thin-layer chromatography	
TMD	theoretical maximum density	
TMTNB	1,3,5-trimethoxy-2,4,6-trinitrobenzene	
TNT	2,4,6-trinitrotoluene	
TOFMS	time-of-flight mass spectrometry	
TRISP	time-resolved infrared spectral photography	

UST	underwater sensitivity test	
vol %	volume percent	
VTS	vacuum thermal stability	
W	tungsten	
wt %	weight percent	
X-0219	TATB/HMX/Kel-F 800 45/45/10	RX-03-AB
	TATB/HMX/Kel-F 800/blue pigment 44.73/45/10/0.27	
	TATB/HMX/Kel-F 800/dye 44.6/45/10/0.4	
	TATB/Kel-F 800 90/10	
	TATB/Kel-F 3799 90/10	
	TATB/Vibrathane 5003 98/2	
	TATB/Vibrathane 5003 95/5	
X-0238	TATB/Estane 5714-F1	
X-0253	TATB/Dapon M 95/5	
X-0262	DATB/Estane/$BaCO_3$ 37/9.5/53.5	
X-0263	DATB/Estane/oxamide 55.5/14.3/30.2	
X-0264	DATB/Viton A/$BaCO_3$ 35.1/14.1/50.8	
X-0272	TATB/HMX/Estane/Ca stearate 0-10/≤95/0-5/0-0.5	
X-0290	TATB/Kel-F 800 95/5	PBX 9502
	TATB/Kel-F 5500 95/5	
X-0291	TATB/Kel-F 800 92.5/7.5	
X-0296	TATB/Kraton 98/2	
X-0297	TATB/Kel-F 800 97.5/2.5	
X-0299	DATB/Viton 95/5	
X-0319	TATB/HMX/Kel-F 800 50/45/5	
	TATB/HMX/Kel-F 800/dye 49.6/45/5/0.4	
	TATB/HMX/Kel-F 800/Hi Viz pigment 49.7/45/5/0.3	
	TATB/HMX/Kel-F 800/red-orange pigment 49.02/44.12/4.9/1.96	
	TATB/HMX/Kel-F 800 47.5/45/7.5	
X-0320	TATB/HMX/Kel-F 800 60/35/5	
X-0321	TATB/HMX/Kel-F 800 75/20/5	
X-0329	TATB/Phenoxy 96.9/3.1	
X-0330	TATB/PS/polyphenylene oxide 97.2/2.52/0.28	
X-0331	TATB/Kel-F 800 99.5/0.5	
X-0332	TATB/Kel-F 800 99/1	
X-0333	TATB/Kel-F 800 98/2	
X-0339	TATB/Kel-F 800/PE fibers 95.0/4.5/0.5	
	TATB/Kel-F 800/PE fibers/Silane 186-A 90.85/4/5/0.15	
X-0341	TATB/HMX/Kel-F 800 90.25/4.75/5	
	TATB/HMX/Kel-F 800/dye 89.85/4.75/5/0.4	
X-0342	TATB/HMX/Kel-F 800 85.5/9.5/5	
X-0343	TATB/HMX/Kel-F 800 80.75/14.25/5	
	TATB/HMX/Kel-F 800/dye 80.35/14.25/5/0.4	
X-0344	TATB/HMX/Kel-F 800 71.25/23.75/5	
	TATB/HMX/Kel-F 800 71/24/5	
X-0345	TATB/Kraton G-6500/Hivac oil 97.6/1.68/0.72	

X-0351	TATB/HMX/Kel-F 800 80/15/5/0.5	
	TATB/HMX/Kel-F 800/purple dye 79.8/15/5/0.2	
	TATB/HMX/Kel-F 800/blue pigment 92.23/5/2.5/0.27	
X-0353	TATB/HMX/Kel-F 800 92.5/5/2.5	
X-0354	TATB/HMX/Kel-F 800 87.5/10/2.5	
X-0355	TATB/HMX/Kel-F 800 82.5/15/2.5	
X-0356	TATB/HMX/Kel-F 800 77.5/20/2.5	
X-0358	TATB/HMX/Kel-F 800 85/12.5/2.5	
	TATB superf/HMX/Kel-F 800 85.0/12.5/2.5	
X-0371	TATB/HMX/Estane/dye 50.8/45.9/3/0.3	
X-0394	TATB/HMX/Estane 47.5/48.7/3.8	
	TATB/Kel-F 800/phenolic microballoons	
X-0396	TATB/HMX/Estane/dye 69.8/24.9/4.9/0.4	
X-0398	TATB/HMX/Kraton/Irganox 1010/dye 24.3/72.97/1.3/1.4/0.03	
X-0407	TATB/PETN/Kel-F 800/dye 69.8/25/5/0.2	PBX 9503
X-0433	TATB/HMX/Kel-F 800/dye 79.8/15/5/0.2	
X-0450	TATB/HMX/Estane 60.6/34.9/4.1/0.4	
X-0458	TATB/Kel-F 800/dioctyl sebacate 95/4.8/0.2	
X-0497	TATB/Polysar 306 95/5	
X-0498	TATB/Vistalon 404 95/5	
X-0500	TATB/PVF 95.4/4.6	
XPS	x-ray photoelectron spectroscopy	
XTX-8003	PETN/Sylgard 80/20	
YAG	yttrium-aluminum-garnet (laser)	
ZND	Zeldovich-Von Neumann-Doering (theory/model of detonation)	

Greek letters

α, β, γ	crystal angles
τ	temporal duration of applied pressure
γ	surface tension
μ	coefficient of static friction
ρ	density

THE INSENSITIVE HIGH EXPLOSIVE TRIAMINOTRINITROBENZENE (TATB): DEVELOPMENT AND CHARACTERIZATION - 1888 TO 1994

by

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ABSTRACT

Assembled in this report are data and references on TATB and its formulations from its first synthesis in 1888 to 1994. This compilation includes sections on synthesis and preparation, analytical methods, properties, performance, aging and compatibility, and on safety. The information is arranged in chronological order within each section. A bibliography rounds out the report.

INTRODUCTION

Many lives have been lost and much property has been damaged or destroyed in the past due to accidental explosions during mixing, processing, transportation, and storage of high explosives. During and after WWII, 1,3,5,7-tetranitro-1,3,5,7-tetrazacyclooctane (HMX, $C_4H_8N_8O_8$) , 2,4,6-trinitrotoluene (TNT, $C_7H_5N_3O_6$), and 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX, $C_3H_6N_6O_6$), were used in nuclear weapons and in propellants . When these explosives are used in nuclear weapons, the additional hazard of aerosolized-plutonium dispersal must be considered. Scattering of this long-lived isotope poses a grave danger to human life and to the environment. Therefore, the Department of Energy (DOE) and the Department of Defense (DoD) have incorporated insensitive high explosive (IHE) compositions in their nuclear arsenals.

Mixtures containing 1,3,5-triamino-2,4,6-trinitrobenzene (TATB, $C_6H_6N_6O_6$) are particularly attractive for use in modern ordnance and space applications because they satisfy requirements for high-temperature service and resistance to accidental initiation. Other insensitive explosives, for example 2,4,6-trinitro-1,3-benzenediamine (DATB, $C_6H_5N_5O_6$), and nitroguanidine (NQ, $CH_4N_4O_2$), are used; but these materials lack the high density, favorable performance, or high-temperature stability of TATB. TATB also was found to have a critical diameter smaller than TNT, which means that it sustains a high-order, steady-state detonation more easily, but it does not have a deflagration-to-detonation (DDT) response.

In the text below, developments after WWII will be described only for work done in the United States of America (USA)--at the Los Alamos National Laboratory (LANL), formerly the Los Alamos Scientific Laboratory (LASL), Los Alamos, New Mex.; Lawrence Livermore National Laboratory (LLNL), formerly the Lawrence Livermore Laboratory, Livermore, Calif.; Sandia National Laboratories (SNL), Albuquerque, New Mex. (SNLA) and Livermore, Calif. (SNLL); Army Research and Development Center (ARDC), formerly Picatinny Arsenal, Dover, N.J.; Naval Surface Warfare Center (NSWC), formerly Naval Ordnance Laboratory (NOL), Silver Spring, Md.,; the Naval Air Weapons Center (NAWC), formerly Naval Weapons Center (NWC), China Lake, Calif.; and Mound Laboratory (MLM), Miamisburg, Oh.; and at Mason & Hanger, Silas Mason Co., Inc., Pantex Plant (MHSMP), Amarillo, Tex. The research is arranged chronologically within sections and subsections. The tests used to characterize and evaluate TATB and its mixtures are identified but not described in detail. As problems and questions arose during the development processes of TATB and its mixtures, tests were used when available or new tests were designed and conducted.

Additional information and data can be obtained from the references in each section and from the bibliography at the end of this report. While extensive, this list of references is not complete. This report is intended as a "roadmap" to the development and characterization of TATB and its use in plastic-bonded explosive (PBX) formulations as insensitive high explosives (IHE). Research and development continue even today into new applications for this safe energetic material, identified as an IHE. To facilitate comparisons from different sources, units have been converted to the centimeter-gram-second (cgs) system or the International System (SI) of Units.

I. SYNTHESIS, PREPARATION, AND SCALE-UP

A. TATB

1. Specifications. "Material Specification for TATB (Triaminotrinitrobenzene), Los Alamos Scientific Laboratory 13Y-188025."

"Material Specification for Ultrafine TATB," Lawrence Livermore Laboratory RM 254959.

2. Laboratory-Scale Preparations. The first mention of TATB in the chemical literature occurred in 1888, when Jackson and Wing obtained this compound by mixing 1,3,5-tribromo-2,4,6-trinitrobenzene (TBTNB, $C_6Br_3N_3O_6$) with cold alcoholic ammonia.[I-1] The reaction was carried to completion by refluxing the mixture in a flask for about 30 min and adding more alcoholic ammonia as needed. The nearly insoluble TATB was filtered hot from the orange liquid, then washed with water and alcohol to give a pale yellow solid.

Jackson and Wing determined that TATB decomposes without melting at about 360°C; is nearly insoluble in water, alcohol, ether, benzene, chloroform, or glacial acetic acid; and dissolves in aniline, strong sulfuric acid, or nitrobenzene. These researchers were unable to react TATB with glacial acetic acid, acetylchloride, or acetic anhydride, even when they heated the mixtures to 150°C in sealed ampoules. They did not recognize TATB as an explosive, but they considered it an intermediary in the preparation of hexaminobenzene.

In 1887 Jackson and Wing had prepared 2,4,6-trichloro-1,3,5-trinitrobenzene (TCTNB, $C_6Cl_3N_3O_6$) in small yield, and had characterized it as nearly insoluble in water; less soluble in alcohol than 2,4,6-trichloro-1,3-dinitrobenzene (TCDNB, $C_6Cl_3HN_2O_4$), and easily soluble in ether, benzene, chloroform, acetone, glacial acetic acid, or carbon disulfide. However, alcohol was the best solvent.[I-2] The melting point was given as 187°C.

Palmer continued this work.[I-3] He repeated the synthesis described in Ref. I-1 and also attempted reduction of TATB with tin and hydrochloric acid to make hexaminobenzene. This attempt failed, as had Jackson's and Wing's.

Flürscheim and Holmes succeeded where earlier researchers had failed. They prepared TATB by adding pentanitroaniline ($C_6H_2N_6O_{10}$) to aqueous ammonia and then boiled the mixture. The result was TATB, nearly insoluble but crystallizable from aniline and meltable above 300°C. Then they prepared hexaminobenzene ($C_6H_{12}N_6$) by reducing TATB with phenylhydrazine.[I-4,I-5]

In 1937 Backer and van der Baan prepared TATB from the readily available TCTNB by reacting it with ammonia.[I-6] They obtained TATB as an orange powder in 80% yield.

After WWII and many problems with highly energetic materials, researchers in the United States began looking for safer, more heat-resistant explosives, mainly for space applications. In 1956 Taylor of NOL reported on the preparation of TATB from TBTNB according to Reference I-1, finding the product "...much superior to our present service explosives, and also possesses a higher crystal density, insensitivity to impact, and a higher detonation velocity than TNT...".[I-7] Looking for commercially available starting materials, Hill and Taylor of NOL in 1960 compared preparative procedures for TBTNB and TCTNB; and they selected TCTNB as the preferred starting material for the preparation of TATB.[I-8] Kaplan and Taylor of NOL refined the early procedure and patented the process in 1959.[I-9]

With guidance from the Navy, the Army also used this process. Blais, Warman, Siele, and Matsuguma of Picatinny Arsenal modified Backer and van der Baan's method to prepare TCTNB (Ref. I-6).[I-10]

Discussions between NOL and LANL in the late 1950s gave researchers at Los Alamos the idea that the high-temperature-stable explosive TATB might be usable in nuclear devices for

Plowshare applications. In 1960 researchers at the Kirov Institute in the USSR proposed the use of "TATB as a thermostable high explosive for deep blasthole drilling."[I-11]

Density measurements and performance calculations for DATB and TATB indicated that TATB would be the more powerful explosive. This led Schwartz at LANL, early in 1961, to prepare a sufficient quantity of TATB for evaluation. Initial preparation by the NOL method of ammonolysis of TCTNB in benzene produced an extremely fine powder (after a water wash) of <0.7 μ particle size containing about 1% chlorine. Batches prepared with more than 250 g of TCTNB resulted in larger particle sizes, averaging 5 μ, but these batches had a chlorine content of 5%. Improvements in the purification procedure produced TATB with chlorine content comparable to NOL's, 0.1% to 3.7%, with higher amounts of chlorine in the larger batches.

Schwartz's purification process for TATB, made by ammonolysis of TCTNB, involved the following steps:

1. Reprecipitate TATB in 100% H_2SO_4 (5 ml acid/g TATB) by slow addition, with rapid agitation, of an equal volume of cold water;
2. Filter and wash the product with distilled water until the washings are neutral;
3. Wash the filter cake with warm water in a Soxhlet continuous extractor for one week.

The dried product, 200 g from two batches, had the composition in wt % of

C: 27.9, H: 2.33, N: 32.6, $C\ell^-$: 0, SO_4^-: 0 (theoretical),

C: 27.44, H: 2.62, N: 32.44, $C\ell^-$: 0.01, SO_4^-: 0.9 (found), and a density of 1.93 g/cm^3.

Later in 1961 Schwartz prepared TATB from 1,3,5-trimethoxy-2,4,6-trinitrobenzene (TMTNB); but he abandoned that approach because the yield was only 58%, carbon was 2% high and nitrogen 1.1% low.

Research on TATB synthesis and characterization resumed in 1964, when it was realized that TATB possessed qualities that made it desirable for use in nuclear weapons. TATB proved very insensitive in various tests, and safety of nuclear weapons had become a more important issue than performance. DOE provided funding for comprehensive, detailed studies of preparation and characterization, studies that continue into the present time. Many results from this effort have been documented and are supplemented here with excerpts and data from LANL, LLNL, and MHSMP internal and external reports.

Researchers at LANL recognized that starting materials and processing methods affected particle size and purity of the product, and therefore its performance. The purity of TATB improved as the starting materials and intermediate products were improved. Ungnade at LANL stated in a 1964 internal report that TATB could be prepared from trichloroaniline (TCA) in good yield, and be purified satisfactorily by using purified starting and intermediate materials. The resultant purified TATB was recovered in 88–95% yields with a crystal density of 1.926 g/cm^3 and 0.13% chlorine.

George and Coburn at LANL continued to look for alternate routes to a lower-cost, pure TATB product. In 1975 Coburn made chlorine-free TATB by treating TCTNB with sodium phenoxide and ammonia. This material became a primary standard for later syntheses and specifications. In 1979, Bissell and Swansiger at LLNL prepared chlorine-free TATB by amination of TMTNB. Yield was about 87%. They dissolved TMTNB in absolute methanol at 50 to 60°C, bubbled anhydrous ammonia through this hot solution, and obtained yellow solid TATB after sonication and filtering.

At this time LANL's Benziger began process-development work on the synthesis of TATB and the development of a pilot-plant process for large-scale manufacture. This research is described in Section I.A.3.

Since samples of TATB were sent to LLNL for study in the mid-1960s, scientists there developed the wet-amination process to prepare TATB, and subsequently they compounded many TATB-containing mixtures. They are presently working at LLNL on an extrusion-cast TATB formulation.

Starting and intermediate materials in the synthesis and scale-up to production of TATB were reported in detail by O'Keefe and Gurule of SNLA during 1977 and 1978.[I-12] Ease of preparation, impurities, and toxicity are some of the concerns addressed.

Rocketdyne (Division of Rockwell International Corporation) and others were unsuccessful in their attempts to scale up the nitration step in the production of TATB.[I-13]

Synthesis of TATB from a starting material other than the chlorine-containing 1,3,5-trichlorobenzene (TCB, $C_6H_3Cl_3$) was attempted by Ogimachi (Teledyne McCormick Selph for LLL). He started with 5-nitroisophthalic acid, which was esterified in methanol to dimethyl-5-nitroisophthalate, then converted to 5-nitroisophthalamide. K. Burgdorf's rearrangement resulted in 1,3-diamino-5-nitrobenzene. Nitration attempts were unsuccessful.[I-14]

Nielsen, Atkins, and Norris at Naval Air Weapons Center (NAWC) in 1979 described yet another route to TATB.[I-15] They reacted hexanitrobenzene (HNB) with ammonia in benzene solution and obtained TATB in 95% yield.

In the early 1980s Ott at LANL synthesized TATB by ammonolysis of 3,5-dichloro-2,4,6-trinitroanisole in toluene at room temperature. Yield of this high-purity (~0.8% chloride) product was >95%, but particle size was small. Attempts to run this reaction at temperatures of approximately 150°C to obtain larger particle size TATB have been unsuccessful, because several undesirable side reactions occurred. However, recrystallization of TATB from diphenyl ether seemed to give a better product than that obtained from solvents such as dimethylsulfoxide (DMSO) or dimethylformamide (DMF).[I-16] This process is now being studied by Quinlan at MHSMP.

3. Large-/Pilot Plant-Scale Preparations. The Navy decided to use the TCB process for preparation of TATB, based on a comparison of the then-existing methods by Kaplan and Taylor (NSWC) in 1958.[I-17]

Benziger's efforts at LANL were based on this early NSWC work. Even after Benziger issued his report on pilot-plant production of TATB in 1966,[I-18] work continued on small-scale efforts to improve the process, even to search for other starting materials and to better characterize the products. Impurities in TATB were traced back mainly to TCTNB (See Analyses, Section II).

The pilot-plant production method for TATB, developed by Benziger, was carried out by nitration of TCB to TCTNB, which was then aminated to TATB. This technology was transferred to MHSMP, where the process was optimized; and it was found that recycling toluene resulted in smaller TATB particles in subsequent runs.[I-19 to I-23] TATB, recycled from machine scrap and from PBXs in small batches exhibited satisfactory physical properties.[I-24] Major concerns were costs of starting materials, particle size of TATB, and purity of starting materials and product. In 1966 suppliers quoted prices of about $100/lb for 100-lb lots of TATB based on the following manufacturing process:

1. Chlorination of aniline to TCA;
2. Conversion of TCA to TCB by diazotization;
3. Nitration of TCB to TCTNB; and
4. Conversion of TCTNB to TATB by amination.

Improving the nitration and amination steps led to improved yields (95% in 6 hours vs. 72% in 24 hours), to reduced levels of NH_4Cl impurity, and to larger particle sizes (median size 40 µ rather than 20 µ). The larger particle size permitted reduction to 5% from 10% of a binder used to compound and press TATB mixtures. Nitration was improved by increasing the reaction temperature to 150°C from 135°C and using $NaNO_3$ instead of KNO_3. However, glass-lined reaction vessels had to be used to avoid degrading the product, because the reactants corroded stainless steel containers. Amination was improved by using toluene at 150°C with an ammonia pressure of 20 psig; this higher temperature led to production of large-particle-size TATB (≥45 µ). Also the inorganic impurity NH_4Cl was reduced by using water with the toluene. The cost of TATB had come down to about $30/lb by the mid-1980s.

Specifications had to be written to allow purchase of material from commercial sources. Characterization methods and tests had to be developed, and limits and tolerances had to be set for acceptance of commercial, as well as in-house, lots. The first specification for TATB molding powder was written in 1976 and revised when better test methods were developed. The Los Alamos material specification for TATB is also used at LLNL and MHSMP (see I.A.1. above).

Limits on impurities, particle sizes, and analytical procedures were specified for:

1. Total chlorine;
2. DMSO-soluble content;
3. Ash content;
4. Volatiles;
5. Particle-size distribution;
6. Foreign particles/inclusions; and
7. Color.

4. Processing

a. Particle Size/Surface Area. Particle-size distributions for the various types of TATB are:

Class	NH_4Cl (wt%)	Sieve Openg. (microns)	Weight % passing
Regular (dry-aminated)	1	20 45	15-35 60 median
Regular (wet-aminated)	0.1	20 45	15-50 75 maximum
Regular (damp-aminated, micronized)		~20	
Superfine (dry-aminated)		20 <45	70 minimum 95 minimum
Fine (emulsion-aminated)		0.5-5	
Fine (wet-aminated)		20	
Ultrafine		<20	
Crash-precipitated		20	20-25

Mortensen at LANL carried out routine determinations of the specific surface area of TATB received from Pantex. Photelometer sedimentation results were in the range of 450 - 900 cm^2/g.

Particle-size distributions were determined by Baytos at LANL. He reported in 1984 a typical particle-size distribution curve, comparing photelometer and Microtrac results, shown in Fig. I-1.

In the mid-1970s, Benziger patented his process to produce high-purity TATB.[I-24] He reported continuous processing with quantitative yields (>90%) and larger particle size. He presented summaries of LANL development, manufacture, and applications up to 1980 at American Defense Preparedness Assoication (ADPA) meetings and at the 1981 Annual Conference of the Fraunhofer Institute of Chemical Technology (ICT), July 1-3, 1981.[I-25 to I-28]

Process development and improvement continued into the 1980s to achieve control of impurities and particle sizes of TATB. As characterization and formulation efforts for TATB progressed, the need to produce lots of varying particle sizes for different applications became apparent. Coarse, regular, fine, superfine, and ultrafine lots were prepared by dry, wet, emulsion, or damp amination processes and by air-jet micronizing. Benziger was issued a patent for fine TATB in 1984.[I-29]

b. Purification/Moisture. Purification, i. e., elimination of impurities, and particle-size improvements were achieved through recrystallization, washing, filtration, drying, sieving, and grinding. In 1981, Kolb and Garza at LLNL explored the possibility of purifiying TATB by sublimation, because TATB has a relatively high vapor pressure at ≥100°C (see Section III.B.1.i.).[I-30] They determined by high-performance liquid chromatography (HPLC), electron spectroscopy for chemical analysis (ESCA), and scanning electron microscopy (SEM) that most of the impurities were carried along and redeposited. Firsich of Mound Laboratory (MLM) also reported successful purification of TATB by sublimation at an ADPA meeting in 1983.[I-31]

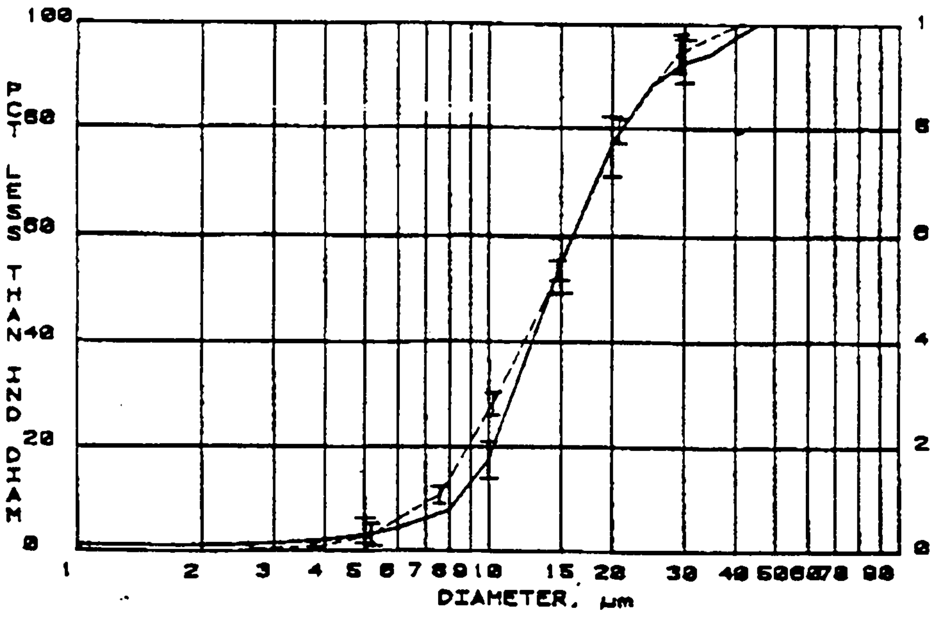

Fig. I-1. Cumulative plot of particle-size distribution of superfine TATB. The solid line represents the photelometer data; the dashed line, the Microtrac data. Error bars are shown at comparable diameters, one standard deviation from four trials.

In 1988, MLM's Thorpe and Fairheller reported that they obtained detonator-grade TATB with 25-30 m^3/g surface area by using fluid energy milling.[I-32] In 1990, Firsich, Thorpe, and Cox at MLM, in a study on processing methods, determined that ..." there is no single-step process that will produce the purity and surface area needed to qualify TATB as detonator-grade" explosive.[I-33] They recommended a three-step method:[I-36]

1. Crash precipitation in water of TATB dissolved in H_2SO_4; this gives fine-particle-size (25 m^2/g) TATB;
2. High-temperature recrystallization in DMSO from a temperature above 125°C, minimizing the occluded solvent; or using a different solvent to accomplish the same purpose; and
3. Use milling or another suitable method to obtain maximum surface area.

A study of the effect of oven-drying on the moisture content of water-aminated, dry aminated, and emulsion-aminated TATB was done by Copeland at MHSMP.[I-34] The results are summarized in Table I-1.

Coating TATB pellets with Parylene proved of some value in slightly reducing moisture take-up.[I-35]

TABLE I-1. Average % Moisture Content of TATB After Drying at 100°C

Process	Drying time (h)			
	0	24	48	72
Water-aminated	3	0.12	0.09	0.06
Dry-aminated	2.9	0.12	0.09	0.06
Emulsion-aminated	0.16	0.10	0.09	0.09

In 1992, Cady at LANL summarized his experiences with growing TATB crystals by amination of TCTNB in dry toluene (the dry-amination process). After washing with water, the resultant crystal shows a swiss-cheese pattern in SEM photographs. Cady concludes that the collapse of these voids inside the crystal will produce hot spots, which will provide a mechanism for initiation (see also Section IV.D.1.b). This effect might help explain TATB's unusually small failure diameter.[I-36]

B. TATB Formulations

Many mixtures of TATB were compounded with other explosives, metals, binders, sensitizers, wetting/surface-active agents, and other materials during the course of these studies. Only the formulations characterized in detail and tested extensively for specific applications are listed in the subsequent sections. Livermore experimental formulations are designated RX-xx-XX, and LX-xx-x after they have been qualified for use. Los Alamos experimental formulations are designated X-xxxx, and PBX xxxx-x after qualification.

1. Specifications. "Material Specification for PBX 9502 Molding Powder," Los Alamos Scientific Laboratory 13Y-188727;

"Material Specification for PBX 9503 Molding Powder," Los Alamos National Laboratory 13Y190273; and

"Material Specification for LX-17 Molding Powder," Lawrence Livermore Laboratory RM 255117.

2. Large-/Pilot Plant-Scale Preparations. Researchers at NAWC were also involved in the Navy's efforts to develop explosive compositions stable at temperatures above 500°C. Stott at the NAWC patented the preparation of one of the earliest high-temperature-stable formulations made with DATB, a 95/5 DATB/Viton-Chemlock formulation.[I-37]

The early (1961-1963) studies at LANL to develop a safe IHE formulation were concentrated on mixtures of DATB or TATB with HMX or RDX and Kel-F 820. By 1965, Benziger at LANL had made a DATB/Kel-F 827/Kel-F 800 85.4/7.3/7.3 formulation, pressed at 120°C and 0.69 GPa, and had compared slurry, Baker-Perkins, and roll-mill processes. This formulation was soon followed by an equivalent mixture made with TATB. The use of DATB was discontinued because the TATB-containing formulations could be pressed to higher densities, which could deliver better performance.

Some experimentation with processing equipment and methods led to formulation of TATB/Kel-F 827/Kel-F 800 90/5/5, prepared by the slurry method and pressed at 150°C and 138 MPa to a density of 1.915 g/cm^3 (98.5% of theoretical maximum density [TMD]). HMX was added to this composition, and the following formulations were produced and pressed for performance evaluations (see Section IV): TATB/HMX/Kel-F 63/27/10, 0/90/10, 18/72/10, 36/54/10, and 90/0/10. Sensitivity and explosive power of the PBXs could be varied over a considerable range by varying the HMX/TATB ratio.

In the meantime, formulation studies continued on TATB/binder compositions. In 1976, Benziger obtained a patent on an "Insensitive Explosive Composition of Halogenated Copolymer and Triaminotrinitrobenzene," a molding powder of TATB and Kel-F, in which the binder can vary from 5 to 10%.[I-38] The 95/5 TATB/binder formulation (X-0290) was chosen for production, based on exhaustive testing (see below) and on the fact that earlier studies had indicated that less binder could be used successfully. This formulation became PBX 9502. Benzinger found that good-quality molding powder (~1-mm size dense, uniform granules) can be produced at low solvent levels. The solvent-extraction slurry method produces such a powder. In 1977, Cady and Caley at LLL issued a report detailing the properties of Kel-F 800.[I-39]

From the many TATB-containing formulations developed in the 1960s, LANL's B. Craig selected the following for characterization studies:

Formulation	wt%
TATB/Kel-F 800	85/15
TATB/Kel-F 800	90/10
TATB/Elwax 460/B^2-170 wax	90/5/5
TATB/Elwax 460/B^2-170 wax	94/3/3
TATB/PS/DOP	94/4.5/1.5
TATB/PS/DOP	92/6/2
TATB/Estane	90/10
TATB/Estane	94/6
TATB/Estane (bimodal TATB)	94/6

In 1970, a TATB-containing propellant formulation, TKA-1, was developed for use in Plowshare-type devices (TKA-1 - TATB/$KClO_4$/Astrel 360 48/42/10). Burning-rate modifiers were needed to improve the burning rate of this formulation. The explosive 2,6-bis(picrylamino)-3,5-dinitropyridine (PYX), developed by Coburn at LANL, was tried in the composition

$PYX/KClO_4$, but it proved to be too sensitive for the intended application. In 1973, Urizar, also at LANL, formulated a 50/50 mixture of TATB/PYX, density (ρ)= 1.760 g/cm^3 (4.9% voids); and he found that this mixture was pressable (PYX alone cannot be pressed) and had better performance than TATB alone. He carried out other studies to sensitize TATB-containing formulations without plasticizers, such as $TATB/KClO_4$, TATB/TNT for casting, and TATB/HMX/Estane.

Urizar's study of castable compositions was expanded to include TATB/RDX formulations. Binder content was reduced substantially by decreasing the particle size of the RDX component, thus making the formulations easier to initiate.

In 1974, Quong at LLNL demonstrated the feasibility of a TATB/oxidizer system, in which the individual components are separately insensitive to impact. He incorporated an energetic oxidizer into the insensitive TATB matrix.[I-40]

The Livermore TATB/HMX/binder formulations, designated RX-26-xx, were developed to give an energy near that of Composition B.[I-41] They were produced and characterized at MHSMP.[I-42] TATB/HMX/binder formulations, using high density fluoropolymer and fluoroplasticizer, were more recently reported to have ~30% higher energy by von Holtz, Scribner, Moody, and McGuire at LLNL in 1990.[I-43]

Humphrey, Rizzo, and Hallam at LLNL developed the formulations TATB/Kel-F 800 92.5/7.5 (RX-03-BB, now LX-17) and TATB/phenoxy 92.5/7.5 (RX-03-CK) in th late 1970s. Their efforts included development of a low- or no-growth TATB-containing formulation.[I-44] By 1980, Hornig and McGuire at LLL had developed three TATB/HMX/binder compositions in an effort to balance sensitivity and safety.[I-45] Their test results are described hereafter in the appropriate sections.

About 1980, Rivera at LANL began a study to develop a booster formulation from TATB/HMX/binder mixtures. This study led to the production of PBX 9503, an 80/15/5 wt% mixture of TATB/HMX/Kel-F by Torres and Sanchez, also at LANL. Another formulation, X-0450, TATB/HMX/Estane 60.9/35.0/4.1, was developed because it showed similar corner-turning performance at cold (-54°C) and at ambient temperatures (See Section IV).

In 1980, Urizar at LANL developed X-0407, TATB/PETN/Kel-F 800/Dye 69.8/25.0/5.0/0.2, for use as a booster explosive that would closely match the output energy of PBX 9502. Anderson and Ringbloom of NSWC formulated a cook-off-resistant booster explosive for use in munitions aboard Navy vessels and aircraft; the TATB/RDX/binder composition selected for additional development was PBXW-7, TATB/RDX/polytetrafluoroethylene (PTFE) 60/35/5 .[I-46]

It became evident during attempts to fabricate components with TATB-containing explosives that the explosive part expanded on heating. The problem was traced to crystal properties and the coefficient of thermal expansion of TATB (See Section III). By the late 1980s, both LANL and LLNL were pursuing routes they hoped would reduce "growth": LANL by compounding formulations with different binders and different ratios of TATB/binder; LLNL by annealing TATB to change its "crystallinity."

Other temperature-dependent properties, such as density, mechanical initiation, and compatibility, to name a few, were also studied in depth.

3. Processing. Formulating explosive mixtures into homogeneous lots required control of numerous variables, such as particle size/surface area, moisture content/drying temperature, and impurities. Even the use of scrap and machining wastes from earlier PBX productions was studied in detail. Specification 13Y-188727 allows the use of a maximum of 50% recycled scrap. Control measures are applied to the same processing methods used to obtain TATB, but additional problems arise from the use of PBXing additives, such as binders, and surfactants. Especially difficult is pressing PBXs to shape. Larger-particle size, that is larger-crystal size, TATB is easier to press. The slurry process now used to produce PBX 9502 was developed cooperatively by Rivera at LANL, Osborn at MHSMP, and Brumley at Holston.

These controls are essential to obtain structurally, that is, mechanically stable materials and components. Surface-active agents were incorporated because they were thought to improve physical properties. The moisture content was of some concern because of possible compatibility problems during storage of fabricated parts.

MHSMP personnel studied processing of Livermore explosives by aqueous and nonaqueous direct and reverse slurry methods with and without wetting agents (pretreatment). Osborn and others concluded that the direct slurry method was preferable for large-scale production; addition of wetting agents in the aqueous reverse-slurry process had less effect on properties than did the water temperature. Scale-up of RX-03-AU/X-0290 from 30-ℓ to 100-gal lots for 1.8-kg batches was difficult when using fine, wet-aminated TATB. Only one batch, made by a nonaqueous process that uses heptane/methyl ethyl ketone (MEK) solvent and untreated TATB achieved the required physical properties.[I-47 to I-50] Pruneda, McGuire, and Clements in 1990 at LANL reported on effects of processing parameters on mechanical properties of TATB/Kraton G-1650 formulations.[I-51] Duncan at MHSMP states that formulating decreases the mean particle size and chloride content of TATB and increases re-entrant pore volume and specific surface area. Pressing and compacting reduce particle size, thus increasing pore volume and surface area.[I-52]

a. Particle Size/Surface Area. The specifications require particle-size limits for molding powders and lots for specific applications of explosives; surface area is inversely proportional to particle size. A particle-size specification was developed at LANL in 1977, after much experimentation and testing. Specific particle sizes can be achieved by varying the processing method and by sieving. Duncan at MHSMP carried out several sieving studies on TATB and TATB-containing mixtures.[I-53] He investigated particle characteristics for TATB before and after formulating and after pressing into PBX 9502.

b. Drying/Moisture. In 1976, Colmenares and McDavid at LLL measured total moisture content and water vapor pressure for TATB/Kel-F 90/10, TATB/Estane 94/6, and TATB/Viton A 91/9. The total moisture content of the samples was <0.0021, 0.0102, and 0.0165 wt%, respectively.[I-54]

Studies were carried out by Stull and Ashcraft at MHSMP on the effect of drying temperature on moisture content in LX-17 and PBX 9502.[I-55,I-56] Results are listed in Table I-2.

In 1983 Ward, Felver, and Pyper at LLNL reported on a proton nuclear magnetic resonance (NMR) method to determine moisture in TATB, LX-17, and PBX 9502.[I-57] Their results are included in Table I-2.

TABLE I-2. Average % Moisture Content of IHEs at Various Drying Temperatures

Formulation and Process	Temp. (°C)	Drying time (h)					
		0	24	48	72	96	108
LX-17-1	90	0.077	0.037	0.032	0.0250	0.008	--
	100	0.68	0.031	0.043	0.016	0.008	--
	120	0.090	0.008	0.004	<0.004	<0.004	--
LX-17	90	0.066	0.028	0.020	0.018	0.012	--
	100	0.096	0.029	0.042	0.020	0.011	--
	120	0.084	0.011	0.006	<0.004	<0.004	--
PBX 9502	70	0.32	0.05	0.03	--	--	0.02
NMR average		0.35					
NMR tablet		0.04					
NMR tablet	70/168 h						0.19
TATB NMR		0.37					

*c. **Pressing and Machining.*** Effective pressing conditions depend on the constituents, for example, the softening temperature or melting point of the binder. The final density, particle size, and particle-size distribution depend also on the number of pressing cycles. Results of early LANL pressing studies with 41.28-mm (1-5/8-in.) pellets are listed in Table I-3:

TABLE I-3. Pressing Conditions for TATB Formulations

Formulation	Pressure (MPa)	Temperature (°C)		Final Density (g/cm^3)	%TMD
TATB/Kel-F	69	100		1.866	
		120		1.863	
		150		1.873	
	110	100		1.877	
		120		1.890	
		150		1.893	
		one 5-min cycle			
TATB/HMX/Kel-F	110	120			96-97
TATB/Elwax/Wax	13.8	100			
X-0272	138	90		1.843	98.7
		100		1.843	98.7
		120		1.840	98.5
	207	90		1.846	98.8
		100		1.847	98.9
		120		1.845	98.8
		effect of number of cycles			
X-0272	138	100	1	1.833	98.1
			2	1.838	98.4
			3	1.843	98.7
			5	1.844	98.7
		two 1-min cycles			
X-0407	200	84	2	1.870	98.6

Comparison of isostatic and mechanical pressing methods showed that less fracturing of TATB particles occurred during isostatic pressing.[I-58] Pressing studies and production work were carried out at MHSMP, mainly by Crutchmer and Harrell.[I-59,I-60] The effects of pressing on mechanical properties of TATB and its mixtures are described in Section III.

Hatler at LANL did pressing and growth studies on PBX 9502 ($\rho = 1.899$ g/cm^3). He found that the PBX 9502 needed to be cycled over the full temperature range of -54 to +60°C before significant irreversible growth occurs.

Machining is the final step in the production process for IHE components. High-speed machining tests were performed routinely. For example, no hazards were found on X-0407, a formulation containing 25% PETN.

C. References for Section I

I-1. C. L. Jackson and J. F. Wing, "LIX. On Tribromotrinitrobenzol," *Amer. Chem. J.* **10**, 283 (1888).

I-2. C. L. Jackson and J. F. Wing, "LIII. On the Action of Nitric Acid on Symmetrical Trichlorobenzene," *Amer. Chem. J.* **9**, 348 (1887).

I-3. A. W. Palmer, "I. A Note Upon the Reduction of Triaminotrinitrobenzene," *Amer. Chem. J.* **14**, 377 (1892).

I-4. B. Flürscheim and E. L. Holmes, "CCCXCIX. Pentanitroaniline," *Chem. Soc.* (London) 1928, 3041.

I-5. B. Flürscheim and E. L. Holmes, "L. Hexaminobenzene," *Chem. Soc.* (London) 1929, 330.

I-6. H. J. Backer and Sj. van der Baan, "Plane Radiary Compounds. Hexavalent Amides of Hexaminobenzene," *Recl. Trav. Chim. Pays-Bas* **56**, 1175 (1937).

I-7. F. Taylor, Jr., "Synthesis of New High Explosives II. Derivatives of 2,3,5-Tribromo-2,4, 6-Trinitrobenzene," U.S. Naval Ordnance Laboratory report NAVORD 4405 (1956).

I-8. M. E. Hill and F. Taylor, Jr., "Nitration of 1,3,5-Trihalobenzenes," *J. Org. Chem.* **25**, 1037 (1960).

I-9. L. A. Kaplan and F. Taylor, Jr., "Preparation of 1,3,5-Triamino-2,4,6-Trinitrobenzene," USP 3,002,998 (filed 1959, issued 1961).

I-10. M. Blais, M. Worman, V. I. Siele, and H. J. Matsuguma, "Preparation of Thermally Stable Explosives: 2,4,6-Trinitrobenzene Derivatives," Picatinny Arsenal technical report PA-TR-2524 (1958).

I-11. G. P. Sharnin, I. E. Moisak, and S. P. Smirnov, Transactions of the Kirov Institute of Chemical Technology (Kazan) **3**, 39 (1960), Ref. in A. P. Glazkova and Yu A.

Kazarova, "Self-Inhibition During TATB Combustion," Fiz. Goreniya Vzryva (trans. Combust. Explos. Shock Waves **28**, no. 6, p. 37 [1992]).

I-12. D. M. O'Keefe and F. T. Gurule, "The Synthesis of Symmetrical Trichlorotrinitrobenzene. Part I - Nitrations with Alkali Metal Nitrates," Sandia National Laboratories report SAND74-0112 (1977). "Part II - Nitrations with Nitric Acid; Synthesis of By-Products," Sandia National Laboratories report SAND78-1001 (1978).

I-13. Rockwell International Corporation, Rocketdyne Division, Canoga Park, Calif. "TATB Research Process Studies," Final Report, August 1975–March 1976," report UCRL-13681.

I-14. N. N. Ogimachi, "Researching an Alternate Synthesis of Triaminotrinitrobenzene," Lawrence Livermore Laboratory report UCRL-13808 (1978).

I-15. A. T. Nielsen, R. L. Atkins, and W. P. Norris, "Oxidation of Poly(Nitro)Anilines to Poly(Nitro)Benzenes. Synthesis of Hexanitrobenzene and Pentanitrobenzene," *J. Org. Chem.* **44**, 1181 (1979).

I-16. D. G. Ott and T. M. Benziger, "Preparation of 1,3,5-Triamino-2,4,6-Trinitrobenzene from 3,5-Dichloroanisole," *J. Energ. Mater.* **5**, 343 (1987), and USP 4,997,987 (filed 1990, issued 1991).

I-17. L. A. Kaplan and F. Taylor, Jr., "High Temperature Stable Explosives. I. Process Development Study of 1,3,5-Triamino-2,4,6-Trinitrobenzene," U.S. Naval Ordnance Laboratory report NAVORD-6017 (1958).

I-18. T. M. Benziger and R. K. Rohwer, "Pilot Plant Production of Triaminotrinitrobenzene (TATB)," Los Alamos Scientific Laboratory report LA-3632 (1966).

I-19. F. I. Honea, "TATB Process Development and Pilot Production Summary," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-73-16 (1973).

I-20. V. H. Evans, W. T. Quinlan, C. L. Schaffer, and Z. L. Estes, "Toluene Recycle in the Synthesis of TATB," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-76-5 (1975).

I-21. W. T. Quinlin, Z. L. Estes, V. H. Evans, and C. L. Schaffer, "Pilot Scale Synthesis of TATB," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-76-20 (1976).

I-22. V. H. Evans, "Optimization of TATB Processing," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-77-2 (1977).

I-23. H. D. Johnson, A. G. Osborn, and T. L. Stallings, "TATB PBX Formulations," Mason & Hanger, Silas Mason, Company, Inc., Pantex Plant report MHSMP-76-5 (1975).

I-24. T. M. Benziger, "Method for the Production of High-Purity Triaminotrinitrobenzene," USP 4,032,377 (filed 1976, issued 1977).

I-25. T. M. Benziger and R. K. Davey, "Amination of Trichloro-Trinitrobenzene," Los Alamos Scientific Laboratory report LA-UR-78-2131 (1978).

I-26. T. M. Benziger, "Development of TATB," *Symposium on Processing Explosives, Propellants, and Ingredients*, American Defense Preparedness Association (Albuquerque, N.M., 1979).

I-27. T. M. Benziger, "Properties and Applications of TATB," Los Alamos Scientific Laboratory report LA-UR-80-1934 (1980); and American Defense Preparedness Association, *Pyrotechnics and Explosives Applications Meeting*, Crane, Indiana, 1980.

I-28. T. M. Benziger, "Manufacture of Triaminotrinitrobenzene," Los Alamos Scientific Laboratory report LA-UR-81-992, and *International Annual Conference of ICT*, (Karlsruhe, Federal Republic of Germany, July 1981).

I-29. T. M. Benziger, "Method of Making Fine-Grained Triaminotrinitrobenzene," USP 4,481,371 (filed 1983, issued 1984).

I-30. J. R. Kolb and R. G. Garza, "The Sublimation of 1,3,5-Triamino-2,4,6-Trinitrobenzene (TATB)," Lawrence Livermore Laboratory report UCRL-85971 Preprint (1981).

I-31 D. W. Firsich, "Energetic Materials Separations and Specific Polymorph Preparations Via Thermal Gradients Sublimation," *Joint Symposium on Compatibility of Plastics/Materials with Explosives, Propellants, Pyrotechnics, Ingredients*, American Defense Preparedness Association (Lake Ozark, Missouri, 1983.)

I-32. R. Thorpe and W. R. Fairheller, "Development of Processes for Reliable Detonator Grade Very Fine Secondary Explosive Powders," Monsanto Research Corporation, Mound Laboratory report MLM-3503 (1988).

I-33. D. W. Firsich, R. Thorpe, and L. A. Cox, "TATB Purification and Particle Size Modification: An Evaluation of Processing Options," EG&G Mound Applied Technologies report MLM-3629 (1990).

I-34. R. J. Copeland, "The Effect of Drying Conditions on the Moisture Content of Water-Aminated, Dry-Aminated, and Emulsion-Aminated TATB," Mason & Hanger, Silas Mason, Company, Inc., Pantex Plant report MHSMP-82-40 (1982).

I-35. T. W. Stull and J. Sandoval, "Moisture Retardation of Micronized TATB Pellets Through Parylene Coating," Mason & Hanger, Silas Mason, Company, Inc., Pantex Plant report MHSMP-80-43 (1980).

I-36. H. H. Cady, "Growth and Defects of Explosives Crystals," *Proceedings, Structure and Properties of Energetic Materials*, Boston, Massachusetts, 1992, D. H. Liebenberg, R. W. Armstrong, and J. J. Gilman, Eds (Materials Research Society, Pittsburgh, Pennsylvania, 1994) p. 243.

I-37. B. A. Stott and D. A. Sbrocca, "Plastic-Bonded Explosive Compositions and the Preparation Thereof," USP 3,728,170 (filed 1962, issued 1973).

I-38. T. M. Benziger, "Insensitive Explosive Composition of Halogenated Copolymer and Triaminotrinitrobenzene," USP 3,985,595 (filed 1974, issued 1976).

I-39. W. E. Cady and L. E. Caley, "Properties of Kel-F 800 Polymer," Lawrence Livermore Laboratory report UCRL-52301 (1977).

I-40. R. Quong, "N-Component Explosive Systems: Feasibility Study," Lawrence Livermore Laboratory report UCID-16529 (1974).

I-41. J. S. Hallam, "TATB Formulation Study," Lawrence Livermore Laboratory report UCID-17087 (1976).

I-42. T. L. Stallings, "HMX/TATB/Binder Development," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-81-26 (1981).

I-43. E. von Holtz, K., Scribner C. Moody, and R. McGuire, "The Search for High-Energy Low-Vulnerability Explosives," *Twenty-First International Annual Conference of ICT*, Karlsruhe, Federal Republic of Germany, 1990, pp. 12/1 to 12/9.

I-44. J. R. Humphrey and H. F. Rizzo, "A New TATB Plastic-Bonded Explosive," Lawrence Livermore Laboratory report Preprint UCRL-82675 Revision 1 (1979).

I-45. H. C. Hornig and R. R. McGuire, "Preliminary Development and Characterization of a TATB/HMX Plastic-Bonded Explosive," Lawrence Livermore Laboratory report UCID-18534 (1980).

I-46. E. W. Anderson and V. D. Ringbloom, "PBXW-7, A New, Cook-Off-Resistant Booster Explosive," *Minutes of the Ninteenth Explosive Safety Seminar* (Los Angeles, California, 1980) Vol. I, p. 727.

I-47. A. G. Osborn and R. W. Ashcraft, "Comparison of Small-Scale RX-03-EY Processing Methods," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-90-42 (1990) (report UCNI).

I-48. A. G. Osborn and T. L. Stallings, "TATB PBX Processing Experiments - RX-03-AU/X-0290," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-76-30 (1976).

I-49. T. L. Stallings, A. G. Osborn, and C. L. Brasher, "Direct Slurry Process for Formulating RX-26-AF," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-84-05 (1984) (report UCNI).

I-50. A. G. Osborn, J. A. Crutchmer, N. O. Rhoton, and C. L. Brasher, "Evaluation of Ultrafine TATB Processing Variables," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-85-27 (1985).

I-51. C. O. Pruneda, R. R. McGuire, and R. E. Clements, "Development of a High-Tensile Strain Plastic-Bonded Explosive," Lawrence Livermore National Laboratory report UCRL-10299 (1990); and *Twenty-First International Annual Conference of ITC* (Karlsruhe, Federal Republic of Germany, 1990) pp. 99/1 to 99/9.

I-52. A. A. Duncan, "The Effects of PBX 9502 Processing on Dry Aminated TATB Powder Characteristics," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-92-03 (1992) (report UCNI).

I-53. A. A. Duncan, "TATB Powder Characteristics of Holston-Formulated PBX 9502," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-91-18 (1991) (report UCNI).

I-54. C. Colmenares and L. C. McDavid, "Equilibrium Water Vapor Pressure and Total Moisture Content Measurements on TATB," Lawrence Livermore Laboratory report UCID-17049 (1976).

I-55. T. W. Stull and R. W. Ashcraft, "Drying Studies of LX-17 at 90, 100, and 120°C," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-83-39 (1983) (report UCNI).

I-56. T. W. Stull, "Available Moisture in PBX 9502 at 70°C," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-84-08 (1984) (report UCNI).

I-57. R. L. Ward, T. Felver, and J. W. Pyper, "Bound and Free Moisture in Explosives and Plastics," *Joint Symposium on Compatibility of Plastics/Materials with Explosives, Propellants, Pyrotechnics, Ingredients,* American Defense Preparedness Association (Lake Ozark, Missouri, 1983).

I-58. A. A. Duncan, "TATB Powder Characteristics of Mechanically and Isostatically Pressed PBX 9502," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-91-36 (1991).

I-59. J. A. Crutchmer, "Mechanical Pressing Study Of Several Explosives," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-89-17 (1989) (report UCNI).

I-60. J. D. Harrell, "A Study for Pressing LX-17 Explosive," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-82-45 (1982).

II. ANALYSES

A. Introduction

The development of analytical and assay methods for TATB—its starting materials, impurities, and admixtures—proved difficult because of sample insolubility. As synthesis and scale-up efforts were carried out, analytical methods were developed for chlorine-containing and organic soluble impurities. About 1970, Benziger found that the most convenient measure of the impurities in TATB production was chlorine content from NH_4Cl and 1-chloro-3,5-dinitro-2,4,6-triaminobenzene, and the amination byproducts. He measured total chlorine present after combustion of the sample. Inorganic chlorine was determined separately by heating (to sublime the NH_4Cl), then washing with HNO_3 dilute (dil.), and analyzing for Cl^-. The NH_4Cl level in TATB (as % Cl) was ~0.3%.

B. Analytical Methods

Schwartz at LANL concentrated early analytical work on isolation of 12 possible chlorine-containing aromatic impurities from TATB's starting materials. He used thin-layer chromatography (TLC), liquid chromatography, and infrared (IR) spectroscopy to identify and quantify these and other impurities.[II-1] He also developed a wet gravimetric procedure to analyze X-0219. Butyl acetate was saturated with HMX and TATB, then this mixture was filtered and used to dissolve Kel-F in a weighed sample. The weight loss represented the Kel-F content. DMSO was added to the residue to dissolve the HMX, leaving only TATB to be weighed.

New and novel analysis methods for TATB and TATB-containing mixtures were developed as suppliers of starting materials, production processes, and admixtures changed. In 1962, Glover of the NOL used a spectrophotometric method, with concentrated H_2SO_4 as solvent for TATB, to identify four impurities, NH_4Cl, TCTNB, and the mono- and diamino derivatives of TCTNB.[II-2] Over the next several years, Yasuda at LANL developed a two-dimensional TLC method to identify 12 chloro-aromatic impurities in TATB.[II-3] He determined that DMSO dissolved 70 ppm TATB at ambient temperature and used an H_2SO_4/DMSO mixture as solvent to purify TATB. Yasuda found that methanesulfonic acid could solubilize 800 ppm of TATB, so he tried the H_2SO_4/methanesulfonic acid system. Impurities in TCTNB were determined by Yasuda by gas chromatography (GC).[II-4,II-5]

Also in 1973, Schwartz and Mortensen of LANL developed a method for analysis of TCTNB by using the Parr bomb to decompose the compound, washing the sample and performing titrimetric and atomic absorption spectroscopic analyses. The main impurities found from TCTNB amination were dinitrotrichlorobenzene (DNT3CB) and dinitrotetrachlorobenzene (DNT4CB). Recrystallization of TCTNB removed the DNT3CB impurity only. They were able to isolate and purify six chloro-aromatic impurities of TATB. The compounds were:

1. 1-Amino-3,4,5-trichloro-2,6-dinitrobenzene;
2. 1-Amino-2,4,6-trichloro-3,5-dinitrobenzene;
3. 1-Amino-2,3,5-trichloro-4,6-dinitrobenzene;
4. 1,3-Diamino-5,6-dichloro-2,4-dinitrobenzene;
5. 1,3-Diamino-5-chloro-4,6-dinitrobenzene; and
6. 1,3,5-Triamino-2,4-dinitrobenzene.

These and other impurities were isolated and purified by TLC in order to investigate their properties, so a way might be found for a suitable assay method. Other purification methods were discussed in Section I.

Impurities resulting from Benziger's nitration step at LANL were:

1. Mononitrotrichlorobenzene (MNTCB);
2. Trichlorodinitrobenzene (T3);
3. TCTNB; and
4. Tetrachlorotrinitrobenzene (T4).

The samples were dissolved in chloroform and analyzed by GC.

Inorganic impurities, including metals, were isolated by ashing the sample in a muffle furnace and analyzing the residue by emission spectrography. For example, Mortensen's analyses of TATB and X-0290 in 1976 identified the inorganic elements listed in Table II-1 as impurities.

TABLE II-1. Inorganic Impurities in TATB and X-0290

TATB		X-0290	
Element	**ppm**	**Element**	**ppm**
Fe, Si	>1	Fe	50
Na, Cr, Ni	1.0	Al, Si, Ca	>10
Mg, Al, Ca	0.5	Cr	10
Cu, Zn, Mo	0.5	Na, Mg, Zn	5
B, Ti, Mn, Pb	0.1	W	2
V, Co, Sr	<0.1	Ni, Cu, Pb, B	1
Ag, Sn, Ba	<0.1	Ba, Be, Ti, V	<1
		Mn, Co, Sr, Mo	<1
		Ag, Sn	<1

The analytical technology was transferred to Pantex in mid-1970. As a means for analysis of residual chloride, Faubion of MHSMP employed base hydrolysis to digest TATB.[II-6] He determined the hydrolysis constants at 50, 75, and 96°C as 3.24×10^{-6}/h, 2.22×10^{-5}/h, and 2.05×10^{-4}/h, respectively. Kohn at MHSMP used a wet-analytical method to determine inorganic chlorides in TATB;[II-7] he found inorganic chloride content to be high in proportion to aromatic chlorine content. McDougall and Jacobs, both of MHSMP, produced and identified TATB-related species, attempting assay and determination of chloride content by IR spectroscopy and TLC.[II-8] They gave total chlorine content for triaminodinitrochlorobenzene as 14.64%, and for triaminodinitrobenzene as 0.27%.

Selig and others at LLL reported on a variety of analytical methods developed for TATB-containing formulations, for example NMR and spectrophotometric methods.[II-9 to II-15] Rigdon, Stephens, and Harrar, also at LLNL, used a Kjeldahl-type apparatus, in 1980, to determine 0.1 mg to 2.0 mg of TATB with precision and an accuracy of 0.25 to 0.5%. The sample was dissolved in a DMSO/NaOH mixture, then amino or nitro groups were measured by controlled-potential coulometry.[II-16]

In 1983, Kayser at NSWC published results from their high-performance liquid chromotography (HPLC) method for polynitro compounds. NMR, TLC, and melting-point data are also compiled in this document.[II-17]

In the mid-1980s, Harris at LANL developed and patented a spot test for TATB suitable as a routine qualitative field test.[II-18] Baytos, also at LANL, adapted Harris' procedure for use in a portable testing kit.[II-19]

Most of the analytical work was transferred from LANL and LLNL to MHSMP by the late 1970s. Save for a few exceptions, the pertinent MHSMP reports are listed in the Bibliography. In the early 1980s, Sandoval proved a titrimetric moisture determination in TATB[I-20]; Worley used x-ray fluorescence spectrometry to determine the existence of elements with atomic numbers 9 to 30 in TATB[II-21]; and in 1984, Teter synthesized and identified the major impurities in TATB - TCTNB, T_3, T_4, and 1,3,4,5-tetrachloro-2-nitroaniline.[II-22] In 1992 Schaffer developed an HPLC method with a 2-ppm limit for detecting TATB in soil and water.[II-23]

A listing of the organic impurities identified appears as Appendix A.

C. References for Section II

II-1. M. Schwartz, "The Los Alamos Specification Analysis of TATB and Analytical Developments Since Then," Los Alamos Scientific Laboratory report LA-UR-78-2450 (1978).

II-2. D. J. Glover, "Heat-Resistant Explosives XII. Quantitative Analysis of 1,3,5-Triamino-2,4,6-Trinitrobenzene," Naval Ordnance Laboratory report NOL-62-76 (1962).

II-3. S. K. Yasuda, "Identification of 1,3,5-Triamino-2,4,6-Trinitrobenzene Impurities by Two-Dimensional Thin-Layer Chromatography," *J. Chromatogr.* **71**, 481 (1972).

II-4. S. K. Yasuda, "Determination of Impurities in 1,3,5-Trichlorobenzene," *J. Chromatogr.* **75**, 39 (1973).

II-5. S. K. Yasuda, "Simultaneous Determination of 1,3-Dinitro-2,4,6-Trichlorobenzene and 1,3-Dinitro-2,4,5,6-Tetrachlorobenzene in 1,3,5-Trichloro-2,4,6-Trinitrobenzene," *J. Chromatogr.* **76**, 331 (1973).

II-6. B. D. Faubion, "Chemical Analysis of TATB," Mason & Hanger, Silas Mason Company, Pantex Plant report MHSMP-75-5 (1975).

II-7. E. Kohn, "Determination of Inorganic Chlorides in TATB," Mason & Hanger, Silas Mason Company, Pantex Plant report MHSMP-75-5 (1975).

II-8. C. S. MacDougall and B. J. Jacobs, "Production and Identification of TATB-Related Species," Mason & Hanger, Silas Mason Company, Pantex Plant report MHSMP-76-30 (1976).

II-9. W. Selig, "Some Analytical Methods for Explosives and Explosive Simulants, Part V," Lawrence Livermore Laboratory report UCRL-7873 Pt. V (1976).

II-10. W. Selig, "The Photometric Determination of 1,3,5-Triamino-2,4,6-Trinitrobenzene (TATB) in Dimethylsulfoxide (DMSO)," Lawrence Livermore Laboratory report UCID-17542 (1977).

II-11. W. Selig, "Spectrophotometric Determination of Some Bifunctional Polynitroaromatic Compounds With Ethylenediamine," *Mikrochim. Acta* **1**, 435 (1978).

II-12. W. Selig, G. L. Crossman and C. L. Schaffer, "The Analysis of 1,3,5-Triamino-2,4,6-Trinitrobenzene/Phenoxy Composites," Lawrence Livermore Laboratory report UCID-18084 (1979).

II-13. W. Selig, G. L. Crossman, and M. C. Waggoner, "Procedure for the Analysis of RX-03-EJ (LX-17)," Lawrence Livermore Laboratory report UCID-19033 (1981).

II-14. G. L. Crossman and W. Selig, "Analysis of Composites Containing 1,3,5,7-Tetranitro-1,3,5,7-Tetrazacyclooctane, 1,3,5-Triamino-2,4,6-Trinitrobenzene, and Benzotrifuroxan," Lawrence Livermore Laboratory report UCID-15644-80-1, p. 26 (1980).

II-15. J. A. Happe and W. Selig, "NMR Method for the Determination of NH_4 in 1,3,5-Triamino-2,4,6-Trinitrobenzene (TATB)," Lawrence Livermore Laboratory report UCID-17756 (1978).

II-16. L. P. Rigdon, F. B. Stephens, and J. E. Harrar, "Precise Assay of TATB by the Determination of Total Amino and Nitro Functional Groups," *Propellants, Explos., Pyrotech.* **8**, 206 (1983).

II-17. E. G. Kayser, "Analysis Methods for Explosive Materials - I. Polynitro Compounds," *J. Energ. Mater.* **1**, 251 (1983).

II-18. B. E. Harris, "TATB - Strong Basic Reactions Provide Soluble Derivatives for a Simple, Qualitative High Explosive Spot Test," *J. Energ. Mater.* **3**, 81 (1985), and USP 4,618,452 (filed 1984, issued 1986).

II-19. J. F. Baytos, Field Spot-Test Kit for Explosives, Los Alamos National Laboratory report LA-12071-MS (1991).

II-20. J. Sandoval, "Titrimetric Determination of Water in TATB Using Karl Fischer Reagent," Mason & Hanger, Silas Mason Company, Inc, Pantex Plant report MHSMP-80-59 (1980).

II-21. R. D. Worley, "Qualitative Analysis of TATB for Elements in the Range of Atomic Numbers $9 \le Z \le 30$ Using X-Ray Fluorescence Spectrometry," Mason & Hanger, Silas Mason Company, Inc, Pantex Plant report MHSMP-81-52 (1981).

II-22. A. C. Teter, "Synthesis and Isolation of Byproduct Impurities in TATB," Mason & Hanger, Silas Mason Company, Inc, Pantex Plant report MHSMP-84-16 (1984) (report UCNI).

II-23. C. L. Schaffer, "Analysis of Soil and Water for TATB Content," Mason & Hanger, Silas Mason Company, Inc, Pantex Plant report MHSMP-92-40 (1992).

III. PROPERTIES

A. Introduction

As mentioned previously, properties were measured as they were needed to handle the IHEs safely and to characterize their performance. Sometimes new test methods had to be developed or new instruments and equipment came on the market. Results from characterization and performance tests of TATB and its mixtures were found to vary with TATB particle size, pressing conditions, impurity content, and initial test temperatures; that is, lot-to-lot variations happen within the specifications. Here only representative data are given, so no lot or batch numbers are listed.

B. Chemical and Physical Properties

1. TATB

a. Crystal and Molecular Structure. TATB crystal structure, as determined by Cady and Larson at LANL in 1962, is triclinic, space group P_1 or $P_{\bar{1}}$, cell dimensions are:

$a = 9.010$ Å, $b = 9.028$ Å, $c = 6.812$ Å, and
$\alpha = 108.59°$, $\beta = 91.82°$, $\gamma = 119.97°$.[III-1]

Strong hydrogen bonding is indicated by the lack of a distinct melting point and by the almost total insolubility of TATB in common solvents. The only suitable solvent seems to be concentrated sulfuric acid (H_2SO_4). The inorganic impurity NH_4Cl is trapped within the TATB crystal as discrete crystals (Refs. I-36, III-1).

This structure is similar to that of graphite, which indicates anisotropy for all directionally dependent properties. This effect is particularly obvious in thermal expansion and thermal cycling. Kolb and Rizzo at LLNL verified the results of Cady and Larson and determined additional crystalline forms of TATB; the monoclinic and triclinic$_2$.[III-2] These unit-cell dimensions are:

Monoclinic: $a = 13.386$ Å, $b = 9.039$ Å, $c = 8.388$ Å, and $\alpha = 90°$, $\beta = 118.75°$, $\gamma = 90°$; and
Triclinic$_2$: $a = 4.599$ Å, $b = 6.541$ Å, $c = 7.983$ Å, and $\alpha = 103.81°$, $\beta = 92.87°$, $\gamma = 106.95°$.

They compared TATB's crystal structure to those of graphite and boron nitride, and they measured all linear and volume thermal expansion coefficients at various temperatures (See Section III.D.1.b.).

Cady also studied the effect of manufacturing processes on the microstructure of TATB. Wet-aminated TATB (using a toluene and water mixture before adding ammonia) has lower chlorine content and forms smaller, more perfect crystals than does TATB produced by the dry amination method (dry toluene and anhydrous ammonia). Very small TATB particles (crystallites) of 0.2 microns can be produced by crash precipitation.[III-3] The preferred orientation in pressing is related to the anisotropy of the TATB crystal and carries over into pressing of TATB mixtures, such as X-0219.

Surface and morphological studies on single TATB crystals were reported by Land, Foltz, and Siekhaus at LLNL at the Tenth International Detonation Symposium in 1993.[III-4] They verified the lattice spacings using atomic force microscopy (AFM), which provided better resolution than SEM. AFM provides direct real-space images of most samples without modification.

Molecular structure as expressed by electronic levels and the length and strength of the bonds is another characteristic that defines TATB's extraordinary stability. Therefore, in the early 1980s, Sharma, Garrett, Owens, and Vogel of ARDC; Towns of LLNL; and Rogers, Peebles, Rye, Houston, and Binkley of SNLA used different, and sometimes newly developed, spectral methods to determine these fundamental parameters.[III-5 to III-7] Surface studies using x-ray photoelectron spectroscopy (XPS) and other modern tools were reported by Pu and Wittberg of MLM in 1989, and by Beard and Sharma of NSWC in 1993.[III-8, III-9] Effects of impact, heat, and radiation on the stability of TATB and its mixtures will be discussed in Section IV.

b. Density (g/cm3).

1.915 (pressed, 22°C)
1.915 ±0.006 by flotation with $Ba(ClO_4)_2$ (Cady, LANL, 1973)
1.925 (99.4% of TMD) by He gas pycnometry (Cady, LANL, 1980)
1.935 by He gas pycnometer (Ref. III-3)
1.937 ±0.004 by x-ray crystallography (Cady, LANL, 1981)

c. Heat of Sublimation (kcal/mol).

40.21[III-10]
43.1[III-11]

d. Melting Point (°C). In 1961, studies by Urizar at LANL indicated that TATB sublimed at ≥300°C and decomposed without melting at 325 to 350°C, leaving a solid residue; TATB was not fusible. Others determined melting points at:

330 (Ref. I-12)
360, $\rho = 1.934$ g/cm^3, (Ref. I-7)
>370 by Thomas Hoover Capillary Melting Point Apparatus with 2°/min heating rate (Ref. II-17)

e. Optical Effects. TATB is yellow and turns to shades of green when exposed to radiation from visible, ultraviolet (UV), electromagnetic, gamma, or ^{60}Co sources. Cady studied this phenomenon in 1961 at Los Alamos and concluded that the green color of TATB was caused by formation of an electronically excited state rather than by a new chemical species. The color varied from yellow-green to deep green to nearly black or brown-green. TATB turned dark yellow-brown on exposure to elevated temperatures.

The refractive indices were measured by immersion as X = 1.45, Y and Z >2.11.

f. Phase Diagrams. Faubion and Quinlin studied the phase diagrams of TCTNB and DNTCB; these two compounds seem to form a eutectic with a melting point of 110°C (Fig. III-1).[III-12]

Cady, in 1979, at LASL, developed phase diagrams for the systems T3/T4 and T3/TCTNB, knowing the phase transition data would help Benziger improve the amination of TCTNB to TATB (Figs. III-2 and III-3).

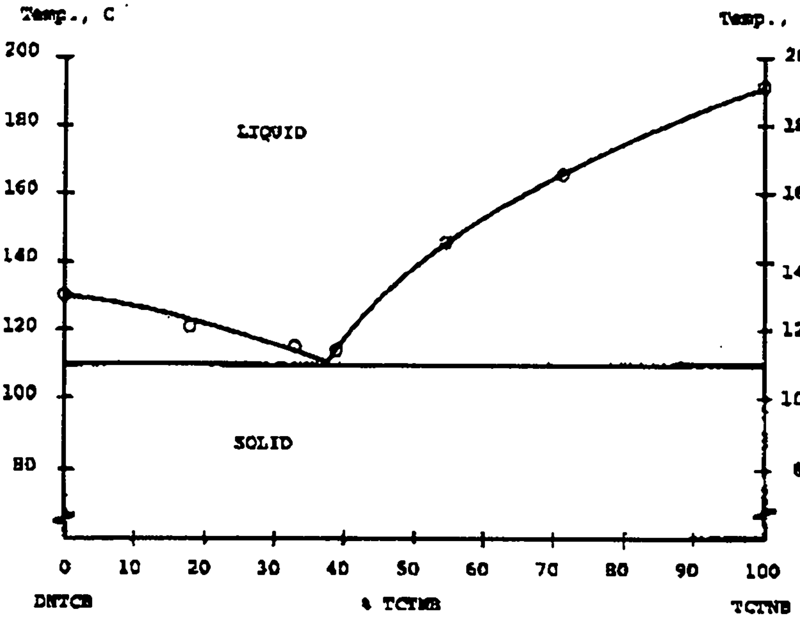

Fig. III-1. Approximate phase diagram of TCTNB/DNTCB.

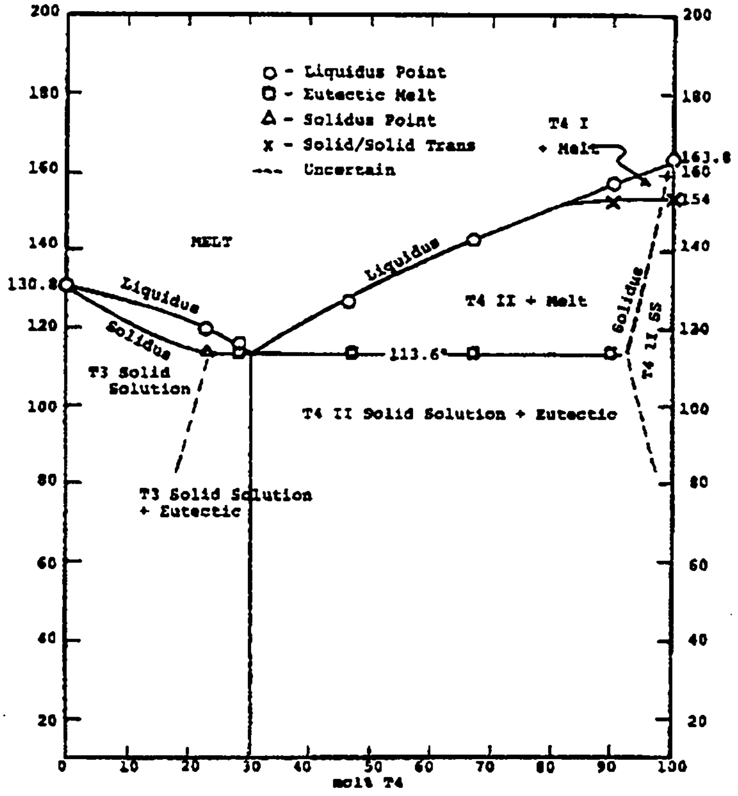

Fig. III-2. Phase diagram of the system T3/T4.

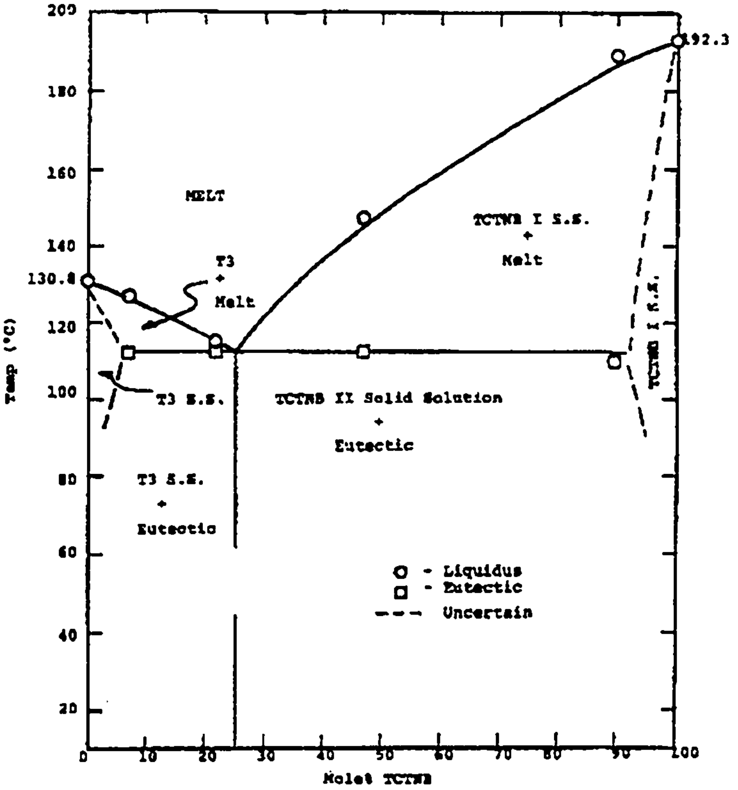

Fig. III-3. Phase diagram of the system T3/TCTNB.

The phase diagrams show two stable polymorphs for TCTNB and T4. The second polymorph for T3 is not shown in Figures III-2 and III-3, because it is apparently metastable at all temperatures, and it forms solid solutions with T4 on recrystallization from the melt. These solid solutions transform slowly to the stable form.

g. Solubility. Jackson and Wing recognized TATB's peculiar solubility characteristics (Ref. I-1). Selig at LLL established solubility parameters for TATB in the 1970s. He found an almost exponential solubility increase for TATB in H_2SO_4:H_2O mixtures with increasing H_2SO_4 content, shown in Table III-1.[III-13]

TABLE III-1. Solubility of TATB in Sulfuric Acid:Water Mixtures

H_2SO_4:H_2O	Acid (vol %)	Maximum amount dissolved (g TATB/100 ml)
1:1	50	>0.02
2:1	66.7	<0.02
4:1	80	~0.24
5.67:1	85	~0.32
7:1	87.5	>1.28
9:1	90	~3.84
concentrated	100	>24.0

Selig also developed a method to estimate low levels of solubility of TATB in various solvents by measuring absorbance of the solution with a Beckman spectrophotometer.[III-14] Solubilities >20% wt/vol were found for concentrated H_2SO_4, chlorosulfonic acid ($ClSO_3H$), fluorosulfonic acid (FSO_3H), and trifluoromethylsulfonic acid (F_3CSO_3H). Solubilities in ppm ranged from 1 for acetic acid to 820 for methanesulfonic acid.

h. Sound Velocity. In the early 1970s, Marsh at LASL and Nidick at LLL reported measured sound velocities for pressed DATB ($\rho = 1.78$ g/cm^3) and pressed TATB ($\rho = 1.87$ g/cm^3). The data are included in Table III-2. Olinger and Cady of LASL reported on hydrostatic compression to 10 GPa, unreacted Hugoniot and thermodynamic properties of TATB at the Sixth Symposium on Detonation in 1976.[III-15] The pressing method has a pronounced effect on sound speed. These sound speed measurements and those of other researchers are listed in Table III-2.

TABLE III-2. Sound Velocities of DATB and TATB (km/s)

Bulk:	DATB	– 2.40 ±0.06
	TATB	– 1.46 ±0.05; 1.43 (Ref. III-1)
Longitudinal:	DATB	– 2.99 ±0.05
	TATB	– 1.98 ±0.03; 2.00 parallel to pressing direction
		2.55 perpendicular to pressing direction (Ref. III-15)
		1.91, 1.83
		2.050[III-16]
Shear:	DATB	– 1.55 ±0.02
	TATB	– 1.16 ±0.02
		1.18 parallel to pressing direction (Ref. III-15)
		1.08, 1.10

i. Vapor Pressure v_p ($\times 10^7$torr at °C).

0.733, 0.746 at 129.3 (LANL)
1.83, 1.93 at 136.2 (LANL)
10.3, 9.42, 9.73 at 150 (LANL)
32.2, 32.3 at 161.4 (LANL)
45.8 at 166.4 (LANL)
167.0 at 177.3 by the Langmuir method (Ref. III-8)
10 ±0.2 at 150 by the Knudsen method (Ref. III-9)
240 ±0.2 at 175 by the Knudsen method (Ref. III-9)
2100 ±0.1 at 200 by the Knudsen method (Ref. III-9)

2. TATB Formulations.

a. Density. In the late 1970s, Cady and Mortensen at LANL studied the pressed densities of TATB mixtures at different temperatures, because density affects mechanical and initiation properties. Results of density changes are listed in Table III-3, and other temperature effects are presented later in this report.

TABLE III-3. Density Changes of TATB Formulations as Function of Treatment

HE and treatment	Density (g/cm³) and Temp. (°C) T1	ρ	T2	ρ	Density Meas. Method
X-0219 pressed/machined	18.5	1.910	68.2	1.890	flotation
X-0290 pressed/machined	21.8	1.880	69.4	1.863	flotation
X-0291 pressed/machined	18.9	1.884	69.3	1.871	flotation
X-0291 after CTE measurements	21	1.911	–54	1.929	flotation
from -54 to +70°C			70	1.888	flotation
PBX 9502 T cycl 20 times for 24 h	21	1.883	–54	1.901	flotation
			70	1.868	flotation
After CTE measurements from	21	1.891	–54	1.907	flotation
–54 to 70°C			70	1.871	flotation
Molding powder	22	1.930			gas pycnometry
Pressed	22	1.888			gas pycnometry

Improvements in computer technology led to development of a nondestructive method to determine densities of high explosives (HEs). Computer tomography was used by Fugelso at LANL in 1981, at LLNL and MHSMP a few years later by Martz, Schneberk, Roberson, Azevedo, and Lynch, respectively.[III-17,III-18]

b. ***Heat of Sublimation (kcal/mol).*** RX-03-BB 41.1 (Ref. III-11)

c. ***Heat of Vaporization.*** Colmenares and McDavid (LLNL) measured moisture content, heats of vaporization, permeability, solubilities, and volumetric changes of three TATB/binder formulations from 23 to 92°C (Ref. I-54). They found that water transport in the samples was controlled by the permeation characteristics of the binder and that the Clausius-Clapeyron equation was applicable below 60°C.

Heat of Vaporization H (kcal/mol).

TATB/Kel-F 90/10	4.0 ± 0.9
TATB/Estane 94/6	6.7 ± 0.7
TATB/Viton 91/9	5.6 ± 1.2

d. ***Sound Velocity.*** Sutherland and Kennedy at SNLA reported on measured acoustic phase velocity and acoustic attenuation of X-0219 as a function of temperature at 0.5 and 1.0 MHz in 1975.[III-19] Nidick's previously unpublished values from LLL are listed in Table III-4 with those of other researchers.

TABLE III-4. Measured Sound Velocities of TATB Formulations (km/s)

PBX 9502 –	longitudinal: 2.74[III-20] shear: 1.38 (Ref. III-20) bulk: 2.20 (value suspect because of TATB anisotropy (Ref. III-20)
RX-03-AU –	longitudinal: 2.73, 2.06 (LLNL) shear: 1.22, 115 (LLNL)
RX-03-BB –	longitudinal: 2.81[III-21] shear: 1.37 (Ref. III-21)
X-0219 –	longitudinal: 2.57 (LLNL) shear: 1.32 (LLNL)

*e. **Surface properties.*** Surface-active agents, also called coupling or wetting agents, were tried in order to improve physical and mechanical properties of TATB formulations, HE/filler bonding, and the particle size of slurried TATB. In 1976, Benziger at LASL found that DAPON-M prepolymer in small amounts (0.15%) acted as a satisfactory wetting agent with X-0290. He determined critical surface tension, using the American Society for Testing & Materials (ASTM) D-2578-67 method, as 45 dyn/cm for TATB and 27 dyn/cm for Kel-F 800.

Later surface studies established the critical surface tension of TATB and various binders. Results compare well with Benziger's data. In 1983, Rivera and Matuszak, also at LANL established experimentally the surface tension/dewetting of TATB and various solid binders by measuring the force of dewetting; a critical surface tension γ_{SL} was then calculated.[III-22] These results agree well with those reported by Bower, Kolb, and Pruneda of LLNL in 1980.[III-23] The data are summarized in Table III-5.

TABLE III-5. Surface Properties of Selected Explosives and Binders

Material	Force of Dewetting (dyn/cm)	Surface Tension γ (dyn/cm)
TATB	36.5, 36.1	--
Kraton G	23.3, 25.7	1.9
Estane 5703	30.1	0.5
Kel-F 800	32.0, 32.7	1.4
Viton A	29.7	0.4
Polystyrene	32.0	0.3
Phenoxy PKHJ	30.5	0.6
P-DNPA	25.9	1.2
Nitrocellulose (NC)	29.1	0.8
RX-03-BB	34.5	
RX-03-DI	36.2	
RX-03-DK	36.2	

C. Mechanical Properties of TATB and Its Formulations

Mechanical properties are important for fabrication, machining, and pressing operations; they also affect safety and sensitivity (See Section IV). The properties of concern here—tensile and compressive - stress, strain, creep, strength, and failure—were evaluated for TATB and many of its formulations. Properties of the binder have considerable effect too.

Also discussed here is the "growth" effect of TATB. Volume expansion of TATB on heating or thermal cycling ("growth") affects mechanical properties (Ref. III-2). Such growth of TATB causes problems that must be addressed in the design of components that incorporate TATB, to withstand extreme environments.

1. Compressive and Tensile Properties and Growth Effects. Tests were conducted before and after thermal cycling, which caused measurable growth, to establish the maximum service temperature for TATB and its formulations. Strength measurements were carried out on the following explosives: TATB, LX-17, LX-17-1, PBX 9502, RX-03-AU, RX-03-BB, RX-03-DI, RX-03-DU, RX-03-DY, RX-03-EY, RX-26-AF, TATB/HMX/Estane mixtures, TATB/HMX/Kel-F mixtures, TATB/TNT/Al mixtures, X-0219, X-0253, X-0272, X-0407, X-0433, and X-0450 at temperatures from -54 to 110°C (Refs. I-47 to I-53).[III-24 to III-38] As expected, strength decreases with increasing temperature. The data are tabulated in Appendix B, Table B-1.

In 1973, measurements were taken by Urizar at LASL on the effects of temperature cycling from –54 to +74°C on growth of X-0219. The cycles were programmed at temperature rate changes of 11°C/h from ~4.5 h at ambient temperature to 74°C for ~11.5 h to -54°C for ~7 h and at return to ambient temperature. The results are summarized in Table III-6.

TABLE III-6. Growth Of X-0219 After Thermal Cycling at –54 to +74°C

Number of Cycles (24 h)	Density (g/cm^3)	Length (mm)	Cumulative Growth (mm)
0	1.921	72.66	--
1		72.75	0.0978
5		72.90	0.127
8		72.94	0.287
14	1.903	72.98	0.323

Urizar, Schwartz, and DuBois at LASL concluded from these and from earlier data:

1. Growth appears to be anisotropic, because it is three to seven times greater in the axial direction of a cylindrical charge than in the transverse direction;
2. TATB alone has about the same growth characteristics as X-0219, which indicates that the binder is not responsible for the irreversible growth;
3. Growth was independent of density of X-0219 over the density range 1.90 to 1.92 g/cm^3;
4. X-0219 charges pressed at 150°C seemed to grow slightly less than those pressed at 120°C; and
5. Charges pressed to densities above 1.925 g/cm^3 grew more than those pressed to lower densities, and the greatest growth in hydrostatically pressed charges occurred in areas of greatest material motion during pressing.

Growth (from thermal cycling) and particle sizes of the pressed and machined explosives had some effects on mechanical properties and sensitivity. Thermal cycling of parts made from TATB-containing formulations resulted in dimensional growth of these parts, more so for units made from PBXs containing wet-aminated TATB than for those with dry-aminated material. Some growth can be compensated for by making allowances or adjustments in the design. Both LANL and LLNL undertook extensive studies to ameleorate the growth problem by modifying production, processing, and pressing parameters and by changing the amount and kind of binder.

In 1979, Rizzo, Humphrey, and Kolb at LLL determined that repeated thermal cycling causes permanent volume expansion of the PBX with resultant debonding of the Kel-F binder. Binders with high glass transition temperatures (T_g) reduced growth dramatically.[III-39]

Johnson at MHSMP studied the effect of thermal cycling (–54 to +74°C) on dimensional changes in LX-17-1.[III-40,III-41] The measurements, taken after 30 cycles, are listed in Table III-7.

In 1987, Freer at LANL noted significant growth when PBX 9502 was cycled through the T_g of the binder. He developed X-0500, a mixture of 95.4 wt% TATB with 4.6 wt% polyvinylidene fluoride (PVF), coated and agglomerated to ~2- to 3-mm in diameter. The resultant particles were quite fragile. Other binders with T_gs in the temperature range -54 to 74°C are being investigated.

TABLE III-7. Density and Dimensional Changes on LX-17-1 After Thermal Cycling at –54 to +74°C

Sample	Density (g/cm^3)		Relative Dimensional Change (mm/m)		
Number	**Initial**	**Final**	**Height**	**Diameter**	**Average**
			1 cycle/day		
1	1.906	1.870	6.2	6.8	6.5
2	1.907	1.880	5.2	4.8	5.0
3	1.907	1.869	6.9	7.2	7.1
			3 cycles/day		
1	1.909	1.867	7.2	7.3	7.3
2	1.915	1.878	6.3	6.2	6.3
3	1.910	1.872	6.5	6.5	6.5
			5 cycles/day		
1	1.909	1.871	6.5	6.7	6.6
2	1.913	1.880	5.6	5.8	5.7
3	1.909	1.875	6.1	6.3	6.2

Similar studies have been reported by LLNL researchers Rizzo, Humphrey, and Kolb in 1979 (Ref. III-39) and by Pruneda, McGuire, and Clements in 1990 (Ref. I-51).

Flowers and Colville at MHSMP are presently studying the possibility of reducing irreversible growth in LX-17 through annealing by isothermal aging.

Generally, formulations made with dry-aminated TATB showed less growth after thermal cycling than did the wet-aminated mixtures. Locke at MHSMP determined that reducing the amount of water used in the amination process of LX-17 did not lessen the problem of irreversible growth.[III-42]

2. Coefficient of Static Friction. The coefficient of static friction μ between explosive and machined surfaces is important for establishing safe handling procedures and for obtaining well-machined assemblies. The average μ, as determined by Anthony and Ashcraft at MHSMP in 1979, are listed below for PBX 9502 and RX-03-BB, sliding on dry and wet surfaces:[III-43]

	Dry			Wet		
	Aluminum	**Plexiglas**	**Steel**	**Aluminum**	**Plexiglas**	**Steel**
PBX 9502	0.237	0.246	0.165	0.642	0.827	0.238
RX-03-BB	0.253	0.206	0.156	0.534	0.513	0.21

During the 1980s, Stallings, Osborn, Schaffer, and Crutchmer at MHSMP tested various formulations to establish a relative friction threshold by determining the force needed for reaction to occur.[III-44] The maximum weight used was 5000 lbs. TATB, LX-17, PBX 9202, and PBX 9503 did not react at 5000 lb-f; thresholds for RX-26-AF ranged from 907 to 1867 lb-f; RX-26-AY 4000 lb-f; TATB/HMX/Kel-F 800 mixtures gave reactions in the range of 1966 to 2698 lb-f; X-0450 reacted at 5000 lb-f; X-0407 threshold force ranged from 846 to 4694 lb-f, depending on the manufacturing process. After aging for 18 months at 70°C, RX-26-AF required 1380 ± 163 lb-f to react. In this test PBXW-7 had a 50% point of 980 lb-f.

D. Thermal Properties

1. TATB.

a. Burning Rate. TATB would not sustain self-deflagration at pressures of ≤10.34 MPa in a test carried out by Boggs, Price, Zurn, Atwood, and Eisel at NSWC.[III-45] At pressures of 13.8 to 103 MPa, the self-deflagration rate is an order of magnitude lower than that for HMX.

b. Coefficient of Thermal Expansion (CTE) (10^{-6}mm/mm-°C). The anisotropic, linear thermal expansion of TATB, mostly along the c-axis of the crystal, causes irreversible growth in pressed TATB and its mixtures (References III-2 and III-39). The relative expansion along the c axis was found to be about 40 times that along the a axis and 12 times that along the b axis. The volumetric expansion is approximately three times that of the linear expansion.

Crystal Form	Measurement	Temperature Range	Linear Expansion
Triclinic	x-ray diffraction	214 to 377	101
Monoclinic	x-ray diffraction	216 to 380	95
Powdered compact, $\rho = 1.866$ g/cm^3	dilatometer	223 to 343	50
Single crystal		0 to −10	66
		40 to 70	125
Micronized		−50 to −10	110
		40 to 70	142

c. Differential Thermal Analysis (DTA) and Pyrolysis. In the 1960s, thermal response of TATB was determined by Rogers at LASL through DTA and pyrolysis measurements. The DTA exotherm starts at 310°C and onset of decomposition is shown in Fig. III-4.

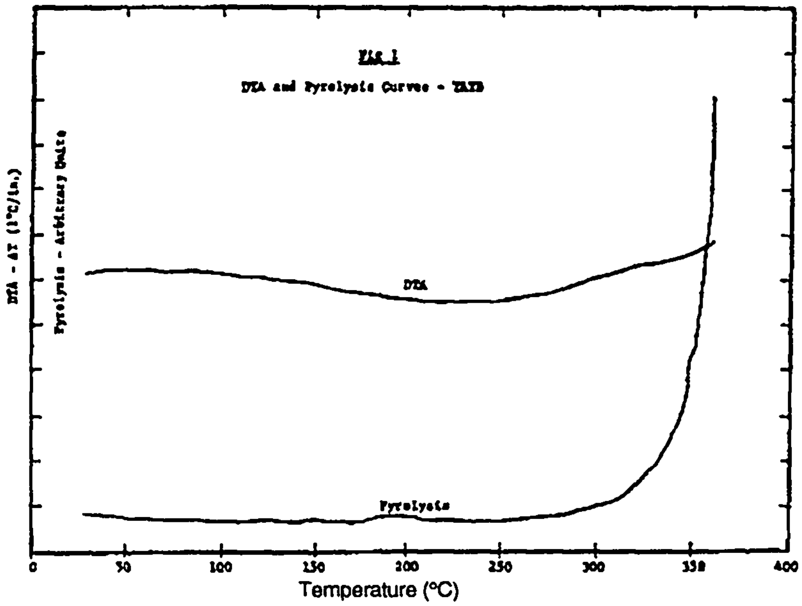

Fig. III-4. DTA and pyrolysis curves for TATB.

d. Heat Capacity/Specific Heat C_p (cal/g-°C).

$0.215 + 1.32 \times 10^{-3}T - 2.0 \times 10^{-6}T^2$ (LANL)
$0.243 + 0.00063T$ (37-137°C) [III-46]
0.26 (20°C)[III-47]
0.293 (50°C) (LLNL)
0.336 (100°C) (LLNL)
0.402 (200°C) (LLNL)
0.429 (275°C) (LLNL)
0.43 (350°C) (Ref. III-47)

e. Heat of Detonation H_d (cal/g)

1018 ± 10[III-48]
1076[III-49]

f. Heat of Formation H_f (kcal/mol)

–33.4[III-50]

g. Thermal Conductivity (10^{-4} cal/s-cm-°C)

10.55, $\rho = 1.8268$ g/cm^3 (Ref. III-48)
11.1, $\rho = 1.849$ g/cm^3 (Ref. III-48)
13.0, $\rho = 1.892$ g/cm^3 (LANL)
19.1 (20°C)[III-51]
12.4 (100°C) (LLNL)
9.12 (100°C) (LLNL)
6.09 (150°C) (LLNL)
14.2 (160°C) (Ref. III-51)
pressed into cylinder: 12.80, $\rho = 1.891$ g/cm^3 at 38°C (Ref. III-46)

h. Thermal Stability/Decomposition. Rice and Simpson (LLNL) in 1990 compiled a detailed, annotated bibliography on the unusual thermal stability of TATB; the topics include structure and physical properties, DTA, time to explosion, shock response, and theoretical aspects.[III-52]

In 1983, Catalano, Crawford, and Rolon at LLNL published studies of confined and unconfined thermal decomposition of TATB.[III-53 to III-55] They obtained an overall equation for thermal decomposition of a TATB sample exploding at 312°C as:

$$\begin{aligned} C_6H_6N_6O_6 \rightarrow\ & 0.94\ N_2 + 0.01\ H_2O + 0.59\ CO_2 + 1.29\ CO \\ & + 0.17\ H_2 + 0.18\ C_2N_2 + 0.83\ HCN + 0.37\ NO \\ & + \text{solid containing C, H, N, and O.} \end{aligned}$$

In the mid-1970s, Bailey at SNLA and Rogers and Janney at LASL established the Arrhenius kinetic parameters for thermal decomposition.[III-56 to III-58] Dubois at LASL noted in 1980 that the induction time to thermal decomposition is very long for pure TATB, as it is for all pure explosives:

$$\log \text{induction time (h)} = 18.562 + 1045 \times 1/T\ (\text{K}).$$

In 1982, Rogers, Janney, and Ebinger studied thermal decomposition by the kinetic isotope effect.[III-59] The Arrhenius kinetics constants for several types of TATB are summarized in Table III-8.

TABLE III-8. Arrhenius Kinetic Constants for TATB

Type of TATB	E (kcal/mole)	Z (s^{-1})
	by the ASTM E698 method	
ultrafine	48.6	1.68×10^{14}
	46.9	4.10×10^{13}
	by isothermal DSC	
unconfined	50 to 79 (305 to 357°C)	
ultrafine	59.4	3.79×10^{18}
	56.6	4.87×10^{18}
	in Al cell	
deuterated	59.9	3.18×10^{19}
Holston	49.3	4.9×10^{15}
	54.9	6.08×10^{17}

i. Critical temperature T_c. The critical temperature of TATB was determined by several different methods.

Faubion at MHSMP reported on thermal stability of TATB and its formulations through one-dimensional time-to-explosion (ODTX), Henkin, and DSC tests, and kinetic effects.[III-60] His results are included in Tables III-9 and III-10.

TABLE III-9. Critical Temperature of TATB Measured by Various Methods

Type of TATB	Pressed thickness (mm)	T_c (°C)	Test and Reference
Recrystallized from DPE	0.65	354	Henkin (LANL)
Cordova	0.67	355	Henkin (LANL)
Hercules	0.63	358	Henkin (LANL)
Recrystallized from DMSO	0.68	345	Henkin (LANL)
Rocketdyne	0.55	357	Henkin (LANL)
Recrystallized from H_2SO_4	0.61	354	Henkin (LANL)
TATB		352	Henkin (LANL)
TATB-d_6	0.61	366	Henkin (LANL)
TATB		312	(Gilding metal) (Ref. III-56)
TATB	0.66	331 to 332	(Al cell) (Refs. III-56 to III-58)
Recrystallized from DMSO	~0.8	345 to 355	(Al cell) (Ref. III-58)
Cordova	~0.8	345 to 355	(Al cell) (Ref. III-58)
TATB		256	(ODTX, $\rho = 0.284$ cm) (Ref. III-47)[III-61]
TATB		230	(ODTX, $\rho = 0.635$ cm) (Ref. III-47)

TABLE III-10. Temperature (°C) and Time (s) to Explosion (ODTX).

Temperature	Time	Tester
215	22,680	(MHSMP)
216	21,744	(MHSMP)
215	24,624	(MHSMP)

*ii. **Temperature and time to explosion.*** A heavily confined heating test, called the One-Dimensional Time to Explosion (ODTX) test, was developed by McGuire at LLL. This test permitted determination of thermal decomposition rates and times to explosion. Description of the test and results were presented at the Sixth Detonation Symposium in 1976. Predictive and theoretical models were also developed (Refs. III-47,III-61).[III-62] At LANL accelerating-rate calorimetry (ARC) was used to determine thermal stability of TATB. The capabilities were transferred to MHSMP.

Myers at MHSMP obtained reproduceable Henkin times to explosion for various lots of TATB at 368°C. He used aluminum blasting caps and Lee plugs in these tests, and sample size was 80 mg.[III-63]

Type of TATB	Particle Size %<20 µm	Particle Size %<44 µm	Total Cl (%)	Time to explosion(s)	Averages From Number of Samples	Averages From Number of Tests
Pantex	13	43	0.68	149	3	4
Cordova	19	39	0.63	133	2	4
Teledyne	94	16	3.45	39	1	4

*iii. **Vacuum thermal stability (VTS)/chemical reactivity test (CRT).*** The thermal stability and decomposition products of TATB are determined in two tests. The CRT is used predominantly at LLNL. It identifies certain specific gases evolved (N_2, NO, CO, N_2O, CO_2), and results are generally reported as the sum of these individual volumes. The VTS test is used mainly at LANL and determines only total gases evolved. Results are reported as cm^3/g of gas per unit time at °C; only total gases evolved are listed here.[III-64 to III-66] Results of both the CRT and the VTS tests for TATB are listed in Table III-11.

TABLE III-11. VTS/CRT Results for TATB

Gas Evolution ($cm^3/g/h/°C$)	Test Used	
0.36/48 h/100°C	CRT	
6.0/2 h/260°C	CRT (ρ =1.934)	
11.5/0.5 h/300°C	CRT	
0.0-0.5/48 h/120°C	VTS	
0.2/48 h/150°C	VTS	
0.3/168 h/150°C	VTS	
0.3/48 h/175°C	VTS	
0.4/168 h/175°C	VTS	
0.3/48 h/200°C	VTS	
0.9/168 h/200°C	VTS	
1.0/48 h/200°C	VTS	DMSO Recrystallized
4.7/168 h/200°C	VTS	DMSO Recrystallized
0.5/48 h/200°C	VTS	
2.3/48 h/220°C	VTS	
18.9/34 h/240°C	VTS	
0.0/2 h/200°C	VTS	Fine
0.2/2 h/225°C	VTS	
1.1/2 h/250°C	VTS	
1.8/2 h/275°C	VTS	
19.8/2 h/300°C	VTS	
92.8/1 h/320°C	VTS	

In a 200°C VTS test at LASL in 1975, Benziger noted that water-aminated TATB evolved 1.5 cm^3/g of gas in 21 days whereas production-grade (in this case, dry-aminated) TATB evolved 4.1 cm^3/g during the same time period. Apparently, the occluded NH_4Cl in dry-aminated TATB was the culprit.

2. TATB Formulations

a. Coefficient of Thermal Expansion CTE. Stull and Ashcraft at MHSMP determined the CTE in cores from pressed and machined, temperature-cycled LX-17-1 parts.[III-67] The CTE decreased as parts were thermally aged and/or cycled and increased with increasing temperature. Lot number and sample orientation had no significant effect on the CTE. These and other measurements are summarized as Table III-12.

TABLE III-12. Coefficients of Linear and Volume Thermal Expansion for TATB Formulations (10^{-6}/°C)

	Linear
LX-17-1 (temperature cycled, averages of several measurements)	53.4 (no cycling)
	53.8 (horizontal orientation)
	52.4 (vertical orientation)
	38.5 (-50°C)
	45.8 (15°C)
	58.5 (35°C)
	70.9 (70°C)
TATB/Kel-F 92.5/7.5	50–65 (-50 to +75°C) (Ref. III-2)
TATB/TNT/Al 40/40/20	44 (LANL)
X-0219	75 (LANL)
X-0407	53.8 (-54 to +24°C, $\rho = 1.852$ g/cm^3) (LANL)
	61.6 (-54 to +24°C, $\rho = 1.857$ g/cm^3) (LANL)
	94.3 (24 to 74 °C, $\rho = 1.852$ g/cm^3) (LANL)
	108.3 (24 to 74 °C, $\rho = 1.857$ g/cm^3) (LANL)
	Volume
X-0219	185 (0 to 65°C) (LANL)
	quadratic fit
X-0407	$(57.2 + 0.0191T)$ $(\rho = 1.852)$
	$(65.3 + 0.0202T)$ $(\rho = 1.857)$

*b. **Differential Thermal Analysis (DTA) and Pyrolysis.*** Janney and Rogers (LANL) also carried out numerous DTA and pyrolysis tests. A representative pyrolysis curve is shown for PBX 9502 in Figure III-5, which demonstrated graphically the effects of heating. Results of DTAs are listed in Table III-13.

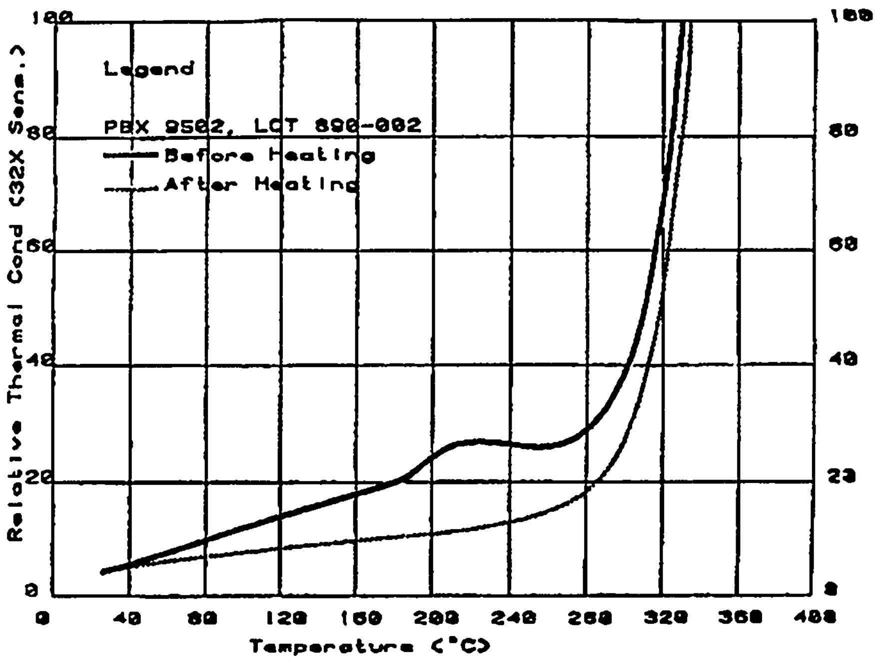

Fig. III-5. Pyrogram of PBX 9502 before and after heating.

TABLE III-13. Onset of Exothermic Decomposition of TATB Formulations from DTA

Explosive	Onset of Exotherm (°C)
TATB/Kel-F 800 90/10	~310
TATB/HMX/Kel-F 800 40/50/10	280
TATB/TNT/Al 40/40/20	270
X-0219	330
TATB/AN 1/9 molar ratio	275, maximum 310
	370, maximum 395
TATB/AN 1/3 molar ratio	260, maximum 295
	370, maximum 395

c. Heat Capacity/Specific Heat C_p (cal/g-°C)

PBX 9502	0.239 (2°C)[III-68]
	0.287 (100°C)(Ref.III-68)
RX-03-BB	0.272 (50°C) (LLNL)
	0.306 (100°C) (LLNL)
	0.366 (200°C) (LLNL)
	0.404 (275°C) (LLNL)
X-0219	0.222 + 0.00070T, ρ = 1.907 at +50 to 275°C (Ref. III-46)
X-0290	0.249 + 0.00059T, ρ = 1.900 at +37 to 177°C (Ref. III-46)

d. Heat of Detonation H_d (cal/g)

RX-36-AA	1291 ± 13	(Ref. III-48)
RX-36-AF	1267 ± 13	(Ref. III-48)
X-0407	~1200 calc.	(LANL)

e. Heat of Fusion (cal/g)

PBX 9502	50 (420°C)	(Ref. III-68)

f. Slow Cook-Off Test at MHSMP

Booster/HE	Confinement	Time to Reaction(s)	Reaction Temperature (°C)
LX-10/LX-17-0	Confined	10,320	362*
LX-10/LX-17-0	Unconfined	9,420	348*
LX-07/PBX 9502	Confined	9,660	365*

*No detonation

g. Thermal Conductivity (10^{-4} cal/s-cm-°C)

PBX 9502	13.20, $\rho = 1.893$ g/cm^3 at 38°C (Ref. III-46)
RX-03-AU	12.3, $\rho = 1.89$ g/cm^3 (MHSMP)
RX-03-BB	12.05, $\rho = 1.893$ g/cm^3 (MHSMP)
	18.0, $\rho = 1.88$ g/cm^3 at 40°C[III-69]
	12.5 (50°C) (LLNL)
	11.5, $\rho = 1.88$ g/cm^3 at 100°C (Ref. III-69)
	9.53 (100°C) (LLNL).
	15.0, $\rho = 1.88$ g/cm^3 at 140°C (Ref. III-69)
	5.86 (150°C) (LLNL).
	14.2, $\rho = 1.88$ g/cm^3 at 160°C (Ref. III-69)
TATB/Kel-F 800 90/10	13, $\rho = 1.92$ g/cm^3 (LANL)
X-0219	13.23, $\rho = 1.907$ g/cm^3 at 45°C (Ref. III-46)
X-0290	13.2, $\rho = 1.893$ g/cm^3 (LANL)
X-0329	14.0, $\rho = 1.876$ g/cm^3 (LANL)
X-0407	12.0, $\rho = 1.85$ g/cm^3 (LANL)

h. Thermal Diffusivity (cm^2/s). Thermal diffusivities of RX-03-BB, $\rho = 1.88$ g/cm^3, ranged from 0.00406 at 20°C to 0.00215 at 160°C (Ref. III-69).

i. Thermal Stability/Decomposition. In the mid-1970s, Selig at LLL used electron spectroscopy for chemical analysis (ESCA) to examine surface and bulk decomposition due to aging of TATB-containing formulations (Ref. II-9). He determined the intensity ratio of the lines resulting from the amino nitrogen and the nitro nitrogen at the surface and at ~1-mm depth. There was no significant difference between bulk and surface samples, indicating that initially no decomposition had occurred. After four months of aging, the surfaces of the samples showed considerable decomposition that was limited to a depth of <1 mm. Depletion of nitrogen indicated formation of decomposition products.

In 1980, Jaeger at LASL used the EXPLO computer code to predict the critical temperature of PBX 9502, using the Arrhenius kinetics model (Ref. III-68). He conducted one-dimensional heating experiments to establish critical thermal parameters and noticed a memory effect on reheated samples.

Scocypec and Erickson at SNLA reported at the Ninth Detonation Symposium in 1989 on developing a method to use thin-film samples with time-of-flight mass spectrometry (TOFMS) and time-resolved infrared spectral photography (TRISP).[III-70] These experiments, to study slow and rapid thermal and isothermal decomposition as well as isothermal aging, were continued by Erickson, Scocypec, Trott, and Renlund at SNLA.[III-71,III-72] Using thin-film samples and multiple diagnostics, explosives were heated in partial confinement by 5 to 10°C/s, and gas evolution was monitored with TRISP. Unconfined samples were heated to 500°C within 40 μs and gas evolution was monitored with TOFMS. Spectra from TRISP indicated that hydrogen cyanide may be a major decomposition product of TATB. Spectra from both experiments showed that very little water was evolved. Unconfined TATB gave primarily low-molecular decomposition within 20 μs of heating to 500°C.

Propagation of decomposition reactions and transition to ignition, initiation, and detonation will be discussed in Section IV.

Arrhenius kinetic constants for TATB formulations are listed in Table III-14.

TABLE III-14. Arrhenius Kinetic Constants for TATB Formulations

Explosive		E (kcal/mole)	Z (s^{-1})	Reference
		For Liquid-Phase Decomposition		
RX-26-AF		54.2	9.2×10^{18}	III-60
		By ASTM E698 Method		
PBX 9502		51.3	1.02×10^{15}	III-56
RX-03-EX		47.7	5.35×10^{13}	III-73
RX-03-EY		50.0	3.39×10^{14}	III-73
RX-26-AF		52.2	2.35×10^{15}	III-56
		By DSC		
LX-17-0		56.4	3.79×10^{17}	III-59
LX-17-1		50.9	4.22×10^{15}	III-59
PBX 9502		56.1	2.96×10^{17}	III-59
		59.9	3.18×10^{19}	III-68
RX-03-EY,	first exotherm	51.1	3.59×10^{16}	III-73
	second exotherm	49.5	1.39×10^{15}	III-73
X-0407		35	4.407×10^{14}	LANL

i. Critical temperatures T_c. Critical temperatures for TATB formulations have been determined with the Henkin test. Results are listed in Table III-15.

TABLE III-15. Critical Temperatures of TATB Formulations

Explosive	Henkin Critical Temperature (°C)	Reference
PBX 9502	349	LANL
	344.3	III-74
PBX 9502 B180-02	349	LANL
PBX 9502-13 Holston (0.65-mm thick)	356	LANL
RX-26-AF	223.6	III-44
TATB/HMX/Kel-F 70/25/5	253	III-44
TATB/AN 1/9 molar ratio	314	LANL
TATB/AN 1/3 molar ratio	302	LANL
X-0407 BI 84-08 (0.635-mm thick)	178	LANL

ii. Temperature and time to explosion. Janney at LANL developed a large-scale time-to-explosion (LSTX) apparatus using a 6.5-cm-radius hemisphere contained in a mantle for heating. All samples burned and left residues. Results from thermocouple readings are included in the listing in Appendix B, Table B-2 along with ARC and ODTX measurements by Rodin from MHSMP.[III-75] The time to explosion is shorter at higher temperatures and longer aging times.

iii. Vacuum thermal stability (VTS)/Chemical reactivity test (CRT). Another means for determining thermal stability is to measure gas evolution at set temperatures for a certain time period. Such data reflect stability and compatibility during aging of materials in close contact with one another. The CRT, which is run mainly at LLNL and MHSMP, can measure the amounts of individual gases evolved. The VTS, which is run at LANL, gives only total gas. Only the amounts of total gases evolved are listed here. Chemical reactivity and explosivity tend to increase with increasing temperature.

Loughran, Wewerka, Rogers, and Berlin at LASL conducted such experiments with TATB and selected metals.[III-76] Aluminum had little effect; but copper, iron, and brass increased the gas evolution substantially.

Pane, Seaton, and Hornig at LLNL investigated the thermal decomposition behavior of three TATB/HMX/binder formulations by determining gas evolution using CRT and dimensional and weight changes (Ref. III-66). Results on other formulations were reported from MHSMP (Ref. III-73). All these results are listed in Appendix B, Table B-3.

The VTS results for X-0219 were reported by Baytos at LANL in 1991 (Ref. III-64), and are reported in Table III-16 with other LANL results.

TABLE III-16. VTS Results for LANL TATB Formulations

Formulation	Time (h)	Temperature (°C)	Total gases (ml/g)
TATB/Kel-F 800 90/10	48	150	0.05
TATB/HMX/Kel-F 800 70/20/10	48	150	0.14
TATB/HMX/Estane 2/95/3	48	120	0.2
40/50/10	48	120	0.1
—	48	150	0.2
X-0219	48	200	0.4
	48	220	2.9
	24	240	18.8
X-0407	48	100	0.2
	48	120	13.1
X-0433	22	120	0.013
X-0458	48	120	0.3

E. References for Section III

III-1. H. H. Cady and A. C. Larson, "The Crystal Structure of 1,3,5-Triamino-2,4,6-Trinitrobenzene," *Acta Crystallogr.* **18**, 485 (1965).

III-2. J. R. Kolb and H. F. Rizzo, "Growth of 1,3,5-Triamino-2,4,6-Trinitrobenzene (TATB)," *Propellants Explos.* **4**, 10 (1979).

III-3. H. H. Cady, "Microstructural Differences in TATB that Result from Manufacturing Techniques," *Seventeenth International Annual Conference of ICT* (Karlsruhe, Federal Republic of Germany) 1986, p. 53-1 to 53-13.

III-4. T. A. Land, M. F. Foltz, and W. J. Siekhaus, "Nanometer-Scale Surface Structure and Morphology of High Explosives Determined by Atomic Force Microscopy," *Paper Summaries, Tenth International Detonation Symposium* (Boston, Massachussetts, 1993), Naval Surface Weapons Center report NSWCDD/MP-92/456, p. 225.

III-5. J., W. Sharma, L. Garrett, F. J. Owens, and V. L. Vogel, "X-Ray Photoelectron Study of Electronic Structure and Ultraviolet and Isothermal Decomposition of 1,3,5-Triamino-2,4,6-Trinitrobenzene," *J. Phys. Chem.* **86**, 1657 (1982).

III-6. T. G. Towns, "Vibrational Spectrum of 1,3,5-Triamino-2,4,6-Trinitrobenzene," *Spectrochim. Acta* **39A**, 801 (1983).

III-7. J. W. Rogers, Jr., H. C. Peebles, R. R. Rye, J. E. Houston, and J. S. Binkley, A Carbon Auger Line Shape Study of Nitroaromatic Explosives, *J. Chem. Phys.* **80**, 4513 (1984).

III-8 S. W. Pu and T. N. Wittberg, "Surface Characterization of 1,3,5-Triamino-2,4,6-Trinitro Benzene by X-Ray Photoelectron Spectroscopy and Fourier Transform Nuclear Magnetic Resonance," *J. Mater. Sci.* **24**, 1533 (1989)

III-9 B. C. Beard and J. Sharma, "Surface Chemical Characterization Method Applied in Energetic Materials," *Structure and Properties of Energetic Materials,* (Boston Massachusetts, 1992), D. H. Liebenberg, R. W. Armstrong, and J. J. Gilman, Eds (Materials Research Society, Pittsburgh, Pennsylvania, 1993) p. 257 .

III-10. J. M. Rosen and C. Dickinson, "Vapor Pressures and Heats of Sublimation of Some High Melting Organic Explosives," *J. Chem. Eng. Data* **14**, 120 (1969).

III-11 R. G. Garza, "A Thermogravimetric Study of TATB and Two TATB-Based Explosives," Lawrence Livermore Laboratory report UCRL-82723 Preprint (1979).

III-12. B. D. Faubion and W. T. Quinlin, "Optical Thermal Analysis of Explosives," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-73-19 (1973).

III-13 W. Selig, "Some Analytical Methods for Explosives and Other Organic Materials, Part VI," Lawrence Livermore Laboratory report UCRL-7873 Part VI (1980).

III-14. W. Selig, "Estimation of the Solubility of 1,3,5-Triamino-2,4,6-Trinitrobenzene (TATB)," Lawrence Livermore Laboratory report UCID-17412 (1977).

III-15. B. Olinger and H. C. Cady, "The Hydrostatic Compression of Explosives and Detonation Products to 10 GPa (100 kbars) and their Calculated Shock Compression: Results for PETN, TATB, CO_2 and H_2O," *Proceedings, Sixth Symposium (International) on Detonation* (Coronado, California, 1976), Office of Naval Research—Department of the Navy report ACR-221, p. 700.

III-16. N. L. Coleburn and T. P. Liddiard, Jr., "Hugoniot Equations of State of Several Unreacted Explosives," *J. Chem. Phys.* **44**, 1929 (1966).

III-17. E. Fugelso, J. D. Jacobson, R. R. Karpp, and R. Jensen, "Radiographic Study of Impact in Polymer-Bonded Explosives," Los Alamos National Laboratory report LA-UR-81-3024 (1981), and *Shock Waves in Condensed Matter—1981*, W. J. Nellis, L. Seaman, and R. A. Graham, Eds (American Institute of Physics, New York, 1982) p. 607.

III-18. H. E. Martz, D. J. Schneberk, G. P. Roberson, S. G. Azevedo, and S. K. Lynch, "Computerized Tomography of High Explosives," Lawrence Livermore National Laboratory report UCRL-102345 Preprint (1990).

III-19 H. J. Sutherland and J. E. Kennedy, "Acoustic Characterization of Two Unreacted Explosives," *J. Appl. Phys.* **46**, 2439 (1975).

III-20. B. Olinger and J. W. Hopson, "Dynamic Properties of Some Explosives and Explosive Simulants," *International Symposium on High Dynamic Pressures* (Paris, France, 1978) p. 9.

III-21. G. H. Bloom, "Gruneisen Parameter Measurements for High Explosives," *Shock Waves in Condensed Matter—1981,* W. J. Nellis, L. Seaman, and R. A. Graham, Eds (American Institute of Physics, New York, 1982), p. 588.

III-22. T. Rivera and M. L. Matuszak, "Surface Properties of Potential Plastic-Bonded Explosives (PBX)," *J. Colloid Interface Sci.* **93**, 105 (1983).

III-23. J. K. Bower, J. R. Kolb, and C. O. Pruneda, "Polymeric Coatings Effect on Energy and Sensitivity of High Explosives," Lawrence Livermore Laboratory report UCRL-83602 Preprint; and *Ind. Eng. Chem. Prod. Res. Dev.* **19**, 326 (1980).

III-24 R. D. Breithaupt, "Mechanical Properties of Thermally Aged RX-03-BB Explosive," Lawrence Livermore Laboratory report UCID-17871 (1978).

III-25. H. D. Johnson, "Evaluation of Mechanical Property Test Program for LX-17-0," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-83-31 (1983).

III-26. H. D. Johnson, "Mechanical Properties of Thermally-Cycled LX-17-0 and RX-03-DI Plastic Bonded Explosives," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-84-23 (1984) (report UCNI).

III-27. A. G. Osborn, "Evaluation of LX-17 Made from Water-Aminated TATB," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-82-38 (1982).

III-28. A. G. Osborn and R. W. Ashcraft, "The Effect of TATB Particle Size on LX-17 Properties," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-87-20 (1987).

III-29. H. D. Johnson, "PBX 9502 Creep and Stress Relaxation Physical Properties Progress Report," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-87-03 (1987) (report UCNI).

III-30. A. G. Osborn, "Characterization of RX-03-EY Lot No. 87275-250D-01," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-90-43 (1990) (report UCNI).

III-31. A. G. Osborn and T. L. Stallings, "Formulation and Evaluation of RX-03-DY Made from Water-Aminated TATB," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-83-04 (1983).

III-32. T. L. Stallings, "Characterization of a Lot of X-0433," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-92-35 (1992) (report UCNI).

III-33. T. L. Stallings, "Characterization of X-0450," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-90-23 (1990) (report UCNI).

III-34. T. L. Stallings, "Evaluation of TATB/HMX/Estane Mixtures," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-86-35 (1986) (report UCNI).

III-35. H. D. Johnson, "Mechanical Properties of RX-26-AF," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-86-04 (1986) (report UCNI).

III-36. T. L. Stallings, A. G. Osborn, and C. Brasher, "The Effect of HMX Particle Size on RX-26-AF Properties," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-85-13 (1985) (report UCNI).

III-37. T. L. Stallings, A. G. Osborn, H. D. Johnson, A. A. Duncan, and C. L. Schaffer, "Evaluation of Low Chlorine TATB from a Production Source," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-81-34 (1981).

III-38. A. G. Osborn, A. A. Duncan, T. L. Stallings, and H. D. Johnson, "Effect of Particle Size on Strength of Low Chlorine TATB Formulations," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-81-04 (1981).

III-39. H. F. Rizzo, J. R. Humphrey, and J. R. Kolb, "Growth of 1,3,5-Triamino-2,4,6-Trinitrobenzene (TATB). II. Control of Growth by Use of High T_g Polymeric Binders," Lawrence Livermore Laboratory report UCRL-52662 (1979).

III-40. H. D. Johnson, "Thermal Growth and Mechanical Properties of RX-03-BB," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-76-17 (1976).

III-41. H. D. Johnson, "LX-17 Growth (Expansion) Test Parameter Study," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-87-29 (1987) (report UCNI).

III-42. J. G. Locke, "The Effect of Damp Amination on Irreversible Growth of LX-17-1," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-90-15 (1990) (report UCNI).

III-43. J. R. Anthony and R. W. Ashcraft, "Coefficient of Static Friction Between Explosives and Machine Surfaces," Mason & Hanger, Silas Mason, Company, Inc., Pantex Plant report MHSMP-79-11 (1979).

III-44. T. L.Stallings, A. G. Osborn, C. L. Schaffer, and J. A. Crutchmer, "HMX/TATB/Binder Development," Mason & Hanger, Silas Mason, Company, Inc., Pantex Plant report MHSMP-81-26 (1981).

III-45. T. L. Boggs, C. F. Price, D. E. Zurn, A. I. Atwood, and J. L. Eisel, "Self-Deflagration Rates of 1,3,5-Triamino-2,4,6-Trinitrobenzene (TATB)," *Seventeenth JANNAF Combustion Meeting*, Vol. 2, p. 557 (1980).

III-46. J. R. Baytos, "Specific Heat and Thermal Conductivity of Explosives, Mixtures, and Plastic-Bonded Explosives Determined Experimentally," Los Alamos Scientific Laboratory report LA-8034-MS (1979).

III-47. R. R. McGuire and C. M. Tarver, "Chemical Decomposition Models for the Thermal Explosion of Confined HMX, TATB, RDX, and TNT Explosives," *Proceedings, Seventh Symposium (International) on Detonation* (Annapolis, Maryland, 1981), Naval Surface Weapons Center report NSWC MP 82-334, p. 56.

III-48. D. L. Ornellas, "Calorimetric Determinations of the Heat and Products of Detonation for Explosives: October 1961 to April 1982," Lawrence Livermore Laboratory report UCRL-52821 (1982).

III-49 R. M. Doherty J. M. Short, and J. J. Kamlet, "Improved Prediction of Cylinder Test Energies," *Combust. Flame* **76**, 297 (1989).

III-50. P. E. Rouse, Jr., "Enthalpies of Formation and Calculated Detonation Properties of Some Thermally Stable Explosives," *J. Chem. Eng. Data* **21**, 16 (1976).

III-51. B. D. Faubion, "Thermal Conductivity of TATB and TATB Blends by Differential Scanning Calorimetry," Mason & Hanger, Silas Mason, Company, Inc., Pantex Plant report MHSMP-76-30 (1976).

III-52. S. F. Rice and R. L. Simpson, "The Unusual Stability of TATB: A Review of the Scientific Literature," Lawrence Livermore National Laboratory report UCRL-LR-103683 (1990).

III-53. E. Catalano and P. C. Crawford, "An Enthalpic Study of the Thermal Decomposition of Unconfined Triaminotrinitrobenzene," *Thermochim. Acta* **61**, 23 (1983).

III-54. E. Catalano and C. E. Rolon, "A Study of the Thermal Decomposition of Confined Triaminotrinitrobenzene. The Gaseous Products and Kinetics of Evolution," *Thermochim. Acta* **61**, 37 (1983).

III-55. E. Catalano and C. E. Rolon, "On the Solid State Products of the Thermal Decomposition of Confined and Unconfined Triaminotrinitrobenzene," *Thermochim. Acta* **61**, 53 (1983).

III-56. R. N. Rogers, "Thermochemistry of Explosives," *Thermochim. Acta* **11**, 131 (1975).

III-57. P. B.Bailey, "On The Problem of Thermal Instability of Explosive Materials," *Combust. Flame* **23**, 329 (1974).

III-58. J. L. Janney and R. N. Rogers, "The Thermal Decomposition Kinetics of 1,3,5-Triamino-2,4,6-Trinitrobenzene," *International Annual Conference of ICT*, (Karlsruhe, Federal Republic of Germany, 1980) p. 411.

III-59. R. N. Rogers, J. L. Janney, and M. H. Ebinger, "Kinetic-Isotope Effects in Thermal Explosions," *Thermochim. Acta* **59**, p, 287 (1982).

III-60. B. D. Faubion, "Thermal Stability, Part I: Non-Isothermal Decomposition of HMX Based Explosives, MHSMP-84-33 (1984); Part II: Isothermal Decomposition of HMX Based Explosives, MHSMP-84-50 (1984); Part III: Large-Scale ODTX Test, MHSMP-85-44 (1985); Part IV: Non-Isothermal Decomposition of TATB Based Explosives, MHSMP-85-43 (1985); and Part V: Isothermal Decomposition of TATB Based Explosives," Mason & Hanger, Silas Mason, Company, Inc., Pantex Plant report MHSMP-87-24 (1987) (reports UCNI).

III-61. E. Catalano, R. McGuire, E. Lee, E. Wrenn, D. Ornellas, and J. Walton, "The Thermal Decomposition and Reaction of Confined Explosives," Lawrence Livermore Laboratory report UCRL-78245 Preprint; and *Proceedings, Sixth Symposium (International) on Detonation* (Coronado, California, 1976), Office of Naval Research—Department of the Navy report ACR-221, p. 214.

III-62. C. M Tarver., R. R. McGuire, E. L. Lee, E. W. Wrenn, and K. R. Brein, "The Thermal Decomposition of Explosives With Full Containment in One-Dimensional Geometries," *Seventeenth Symposium (International) on Combustion* (The Combustion Institute Pittsburgh, Pennsylvania, 1978), p. 1407.

III-63. L. C. Myers, "Henkin Time to Explosion for TATB - Part I," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-77-18 (1977).

III-64. J. F. Baytos, "High-Temperature Vacuum Thermal Stability Tests of Explosives," Los Alamos Scientific Laboratory report LA-5829-MS (1975).

III-65. J. F. Baytos, "Vacuum Thermal Stability of Explosives Monitored Electronically," Los Alamos National Laboratory report LA-12173-MS (1991).

III-66. A. J. Pane, D. L. Seaton and H. C. Hornig, "Thermal Decomposition of Safe, High Energy Explosives," Lawrence Livermore National Laboratory report UCID-19762 (1983).

III-67. T. W. Stull and R. W. Ashcraft, "Coefficient of Thermal Expansion of LX-17-1," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-89-13 (1989) (report UCNI).

III-68. D. L. Jaeger, "Thermal Response of Spherical Explosive Charges Subjected to External Heating," Los Alamos Scientific Laboratory report LA-8332 (1980).

III-69. R. J. Cornell and G. L. Johnson, "Measuring Thermal Diffusivities of High Explosives by the Flash Method," Lawrence Livermore Laboratory report UCRL-52565 (1978).

III-70. R. D. Skocypec and K, L, Erickson, "Time-Resolved Mass Spectrometry Technique For Studying Fast Transient CHNO Explosive Decomposition Kinetics," *Proceedings, Ninth Symposium (International) on Detonation* (Portland, Oregon, 1989), Office of the Chief of Naval Research report OCNR 113291-7, Vol. II, p. 1140.

III-71. K. L. Erickson, R. D. Skocypec, W. M. Trott, and A. M. Renlund, "Development of Thin-Film Samples for Examining Condensed-Phase Chemical Mechanisms Affecting Combustion of Energetic Materials," *Proceedings, Fifteenth International Pyrotechnics Seminar* 1990, p. 239.

III-72. K. L. Erickson, W. M. Trott, and A. M. Renlund, "Use of Thin-Film Samples to Study Thermal Decomposition Chemistry of Explosives," *Eighteenth International Pyrotechnic Seminar* (1992) p. 241, and *Paper Summaries, Tenth Symposium International on Detonation* (Boston, Massachusetts, 1993), Naval Surface Weapons Center report NSWCDD/MP-92/456, p. 480.

III-73. W. A. Rodin, "Differential Scanning Calorimetric Determination of Kinetic Constants of TATB/Kraton G Formulations," Mason & Hanger, Silas Mason, Company, Inc., Pantex Plant report MHSMP-90-45 (1990) (report UCNI).

III-74. B. D. Faubion, "Henkin One-Shot Test - A Statistical Approach for Estimating Critical Temperatures," Mason & Hanger, Silas Mason, Company, Inc., Pantex Plant report MHSMP-83-19 (1987).

III-75. W. A. Rodin, "Examination of PETN/TATB Explosive Thermal Stability Via Accelerating Rate Calorimetry," Mason & Hanger, Silas Mason, Company, Inc., Pantex Plant report MHSMP-92-23 (1992) (report UCNI).

III-76. E. D. Loughran, E. M. Wewerka, R. N. Rogers, and J. K. Berlin, "The Influence of Metals on the Thermal Decomposition of s-Triaminotrinitrobenzene (TATB)," Los Alamos Scientific Laboratory report LA-6873-MS (1977).

IV. PERFORMANCE

A. Introduction

TATB and mixtures containing TATB behave like other HEs in performance, safety, and sensitivity tests, but to a much lesser extent. Many types of tests were conducted to quantify both performance and sensitivity or insensitivity of TATB-containing HE formulations. These tests were designed to also provide safety and lot-qualification information. For example, by 1986 the Air Force had developed a testing program specifically for full-scale systems containing IHEs.[IV-1] Initial, small-scale tests of an IHE are conducted for thermal stability, shock sensitivity, and initiability; then the following full-scale tests are done:

1. Sympathetic detonation;
2. Fast cook-off (bonfire);
3. Slow cook-off;
4. Sled impact;
5. Bullet impact;
6. Fuel fire; and
7. Arena performance.

Again, we assume that the user of this compilation is familiar with the test methods mentioned. Most of the sensitivity tests used for TATB were described in 1976 by Dobratz, Finger, Green, Humphrey, McGuire, and Rizzo at LLL.[IV-2] In 1992, Colville at MHSMP compiled the raw data for PBX 9501 and PBX 9502, LX-10 and LX-17 from detonation velocity, corner turning, onionskin, and gap tests.[IV-3]

Early (1961) Becker-Kistiakowski-Wilson EOS (BKW) calculations by Mader at LASL on formulations of HMX with DATB or TATB at 98% TMD gave the following C-J pressures:

Composition (wt%)		**C-J Pressure (kbar)**
DATB/HMX	10/90	357
	20/80	345
	25/75	340
	40/60	326
TATB/HMX	10/90	359
	20/80	352
	25/75	352
	40/60	340

The higher C-J pressures calculated and higher pressing densities achieved (see Section I.B.3.c.) caused researchers at Los Alamos to concentrate their efforts on TATB-containing formulations for use as insensitive production explosives.

In 1977, Davis at LASL summarized the sensitivity characteristics of TATB-containing HEs.[IV-4] A variety of safety tests is required to establish the relative sensitivity of an explosive, and results from any single test can be misleading. At that time at LASL the tests deemed sufficient to define safety and sensitivity were DTA, pyrolysis, drop-weight impact, gap, Susan, and skid. The safety tests required in the DOE Safety Manual to qualify HEs as IHEs and HE subassemblies as IHE assemblies are (as of 1991) drop-weight impact, friction, spark, ignition and unconfined burning, card gap, detonation (cap), cook-off, spigot, skid, Susan, bonfire, and bullet impact.[IV-5] Other tests, such as booster and thermal ignition tests, have been done since the early 1970s to establish initiability and initiation processes of TATB and its mixtures.

The safety and performance studies use booster, detonator, and electrically or explosively driven flyer plate, or wedge experiments in various geometries with differing materials. Measurements were done with Fabry-Pérot interferometry, Lagrange gauges, manganin gauges, particle-velocity gauges, and/or streak cameras, as appropriate. Manufacturing and fabrication methods, test temperatures, input pressures, and pulse lengths generated by the type of shock—prompt, short, sustained, to name the most common—affect the ease of initiation. Data are provided by the following tests:

aquarium - determine shock pressure and time to onset of decomposition, and detonation velocity;
booster - determine amount and kind of donor HE and configuration needed for initiation of main-charge HE;
corner turning/divergence - determine material variable (density or percent voids) and test variable (pressure-pulse intensity and duration) to measure distance from entrance surface to perpendicular emergence of the detonation wave;
failure diameter - establish safe operating and performance limits;
minimum priming - establish safe operating limits;
plate dent - establish safe operating and performance limits;
flyer plate/gun/wedge - provide quantitative data on the relationship between shock pressure and duration on the time and distance to detonation, leading to Hugoniot and $p^2 \tau$ parameters for initiation, decomposition kinetics and rates; and
gap - determine critical card gap or pressure for initiation of detonation.

B. Shock Initiation and Detonation

In 1976, Walker and Wasley at LLL developed a model for shock initiation of chemical explosives based on decomposition kinetics of free radicals and initiation of chain reactions.[IV-6] Shock initiation events of TATB formulations have been modeled successfully since then by several researchers at DOE Laboratories.[IV-7 to IV-16]

Shock initiation of TATB formulations presents special problems because of TATB's stability, that is, lack of response to external stimuli. Numerous tests and theories have been advanced to help researchers understand and interpret the processes involved in shock initiation of explosives.

The threat of accidental or sympathetic detonation is always a safety concern when working with HEs, even IHEs. TNT is considered the standard for establishing safety parameters for building design and distances in case of accidental detonations of HEs. Demerson and Ashcraft at MHSMP used air-blast data to determine the TNT equivalency for PBX 9502.[IV-17] They determined that the TNT equivalency of PBX 9502 is not constant, but is a function of scaled distance, and that the equivalency numbers of PBX 9502 are, based on impulse, <100% of TNT over the given range; that is, PBX 9502 generally yielded slightly less output than did TNT over the scaled distance of 0 to 20 ft.

Recent breakthroughs have shown how TATB formulations can be accidentally initiated. For example, at LANL in 1993, Ferm and Hull designed an experiment to detect shock-to-detonation transition (SDT) in PBX 9502.[IV-18,IV-19] They observed the transition of a Mach reflection into a detonation, because a high-pressure Mach stem propagated into unshocked explosive and caused initiation. Such an initiation mechanism can reduce the distance to detonation drastically for HE charges with high-impedance boundaries. These researchers supported their experiments with calculational models.

This effect was also reported by Tarver, Cook, Urtiew, and Tao of LLNL at the Tenth Detonation Symposium in 1993. They observed effects of diverging, multiple shocks and Mach-stem interactions on reaction rates in LX-17.[IV-20] They also concluded that two (or perhaps more) colliding shocks in reacting LX-17 can accelerate the local reaction rate and result in formation of a detonation wave.

As a safety measure, explosives can be desensitized by preshocking them. Mulford, Sheffield, and Alcon at LANL reported the results of light gas-gun experiments at pressures to 10.5 GPa in 1993.[IV-21] They used magnetic impulse and velocity gauges in their experiments to measure particle velocity in the Lagrangian frame. Figure IV-1 shows gauge records for TATB of a 3.7 GPa precursor shock followed by a 7.95-GPa second shock. The Hugoniot of PBX 9502 seems to show a discontinuity at ~7.5 GPa.

Campbell, Flaugh, Popolato, and Ramsay at LANL summarized preparative methods and safety test results of PBX 9502 and of other TATB formulations containing various amounts of HMX in 1981; and in 1989 Akst also at LANL, summarized cylinder and detonation data from LLNL, MHSMP, and LANL.[IV-22,IV-23]

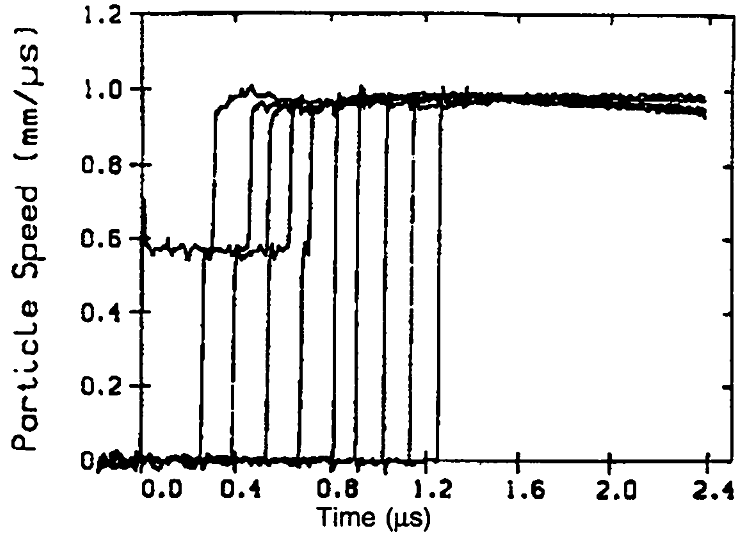

Fig. IV-1. Material velocity gauge records for doubly shocked PBX 9502, a 3.7 GPa preshock followed by a second shock at 7.95 GPa.

1. Summary of Detonation Properties. A summary of detonation properties is provided in Table IV-1. Campbell at LANL presented detonation velocities for TATB/HMX/Kel- F 800 formulations as percent TATB content in Fig. IV-2 and diameter effects in Fig. IV-3 for various formulations.

TABLE IV-1. Summary of Detonation Properties

	Density ρ		$P_{C\text{-}J}$	Detonation Velocity		$T_{C\text{-}J}$	
Explosive	**(g/cm^3)**	**%TMD**	**(kbar)**	**D (km/s)**	**γ**	**(°C)**	**Ref.**
LX-17	1.903		275	7.596			IV-24
	1.903		250	7.596			IV-25
	1.90		290				IV-26
PBX 9502	1.895			7.706			IV-27
	1.894		285	7.707	2.95		IV-28
	1.892			7.695			IV-29
	1.89		289	7.89			IV-23
PBX 9503	1.875			7.840			IV-29
RX-26-AF	1.836		325	8.239			IV-25
RX-36-AA	1.843	96.4		8.41	3.07	2857	IV-30
RX-36-AB	1.855	96.6		8.15	3.06	2857	IV-30
RX-36-AC	1.817	95.3		8.72	3.09	2857	IV-30
RX-36-AD	1.829	95.2		8.04	3.15	2502	IV-30
RX-36-AF	1.840	95.9		8.30	3.17	2477	IV-30
RX-36-AG	1.838	96.3		7.89	2.98	3247	IV-30
TATB	1.88			7.756		2732	III-49
	1.876			7.663			LANL
	1.854		291	7.93			IV-23
	1.847		259	7.66			III-16
	1.800			7.552			IV-28
	1.80		265	7.472			IV-24
wet	1.84			7.4-7.6			IV-30
TATB/Kel-F 800/827 90/5/5							
	1.916		270	7.518			LANL
TATB/Kel-F 95/5 and BKW							
	1.917		297	7.810	2.937		LANL
TATB/Al/Kel-F 77/18/5							
	2.016		280-290	7.474			LANL
			293 calc.				LANL
X-0219	1.915			7.627			IV-27
X-0272	1.845			8.800			LANL
	1.844			8.791			LANL
	1.840			8.780			LANL
X-0407	1.866			7.773			IV-28
	1.858		310	7.794			LANL

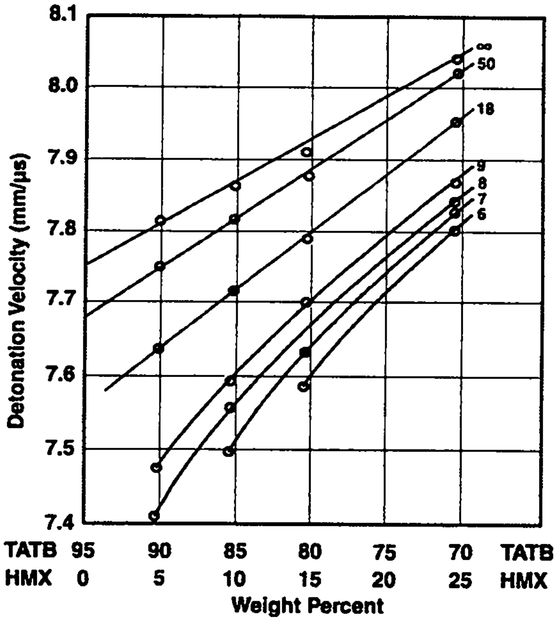

Fig. IV-2. Change in detonation velocity with change in TATB/HMX ratios for some TATB/HMX/Kel-F 800 formulations.

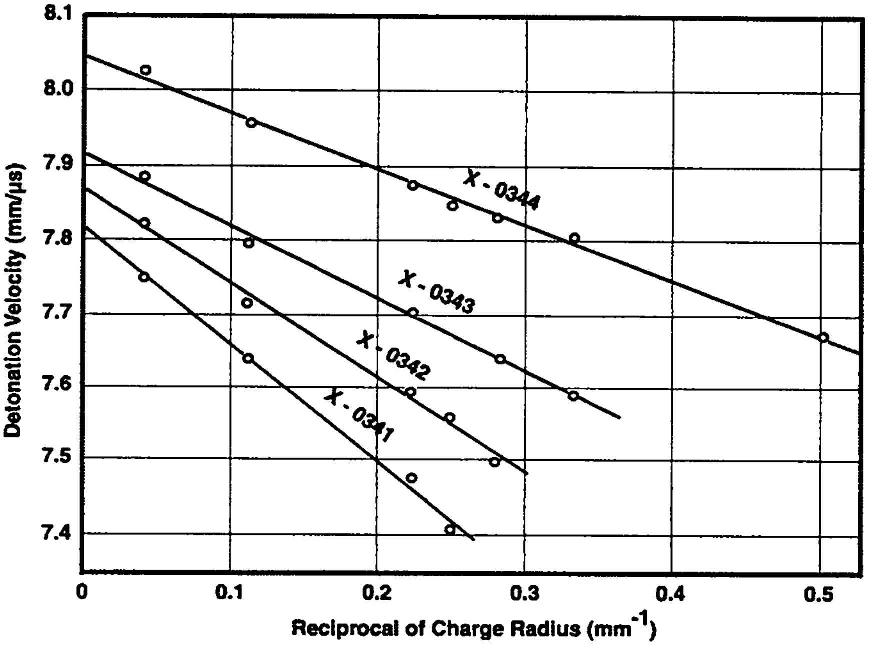

Fig. IV-3. Effect of charge diameter on detonation velocity of some TATB/HMX/Kel-F 800 formulations.

2. Aquarium Test. Results from aquarium tests aid in the understanding of shock decomposition and shock initiation processes. In the early 1980s, Goldstein at LANL performed aquarium tests on PBX 9502 at temperatures from –55 to +75°C and charge diameters from 25.4 to 108 mm. Test media were water and ethanol. Results indicate that the detonation velocity decreased from 7.74 km/s at 14°C to 7.59 km/s at –44°C, but the difference lessens with charge diameters much larger (~10 times) than TATB's failure diameter. The performance of PBX 9502 is adversely affected by firing at other than ambient temperature, and the lowered energy release persists long after passage of the detonation front. Shock-wave data were compiled by Mader, Johnson, and Crane at LANL in 1981.[IV-31]

Liddiard, Forbes, Watt, Baker, Sharma, and Beard at the NSWC reported on a method to recover shocked HE samples after preignition reactions subsequent to aquarium testing.[IV-32] A Teflon sample holder kept the 30-mg, 5-mm-diam by 1-mm-thick samples contained and uncontaminated after exposures up to 3 GPa and pulse widths of a few microseconds. Recovered TATB samples showed submicron-size ragged holes and fine deposits of furoxan and furazan derivatives of TATB.

3. Booster Tests. In the early 1970s, Urizar at LANL began to test initiation systems with TATB-containing formulations, using a setup similar to the plate-dent test. The subject of these studies was X-0219 at 1.920 g/cm^3 density; the booster explosive used was PBX 9501 at ~1.84 g/cm^3 density. Dimensions of the cylindrical boosters were varied: diameter from 25.4 to 15.24 mm in 2.54-mm increments and height from 25.4 to 6.35 mm in 6.35-mm increments, correspondingly. The acceptor charge was 50.8-mm diam by 50.8-mm high. A "maximum dent" was obtained from a 50.8-mm diam by 50.8-mm high booster of PBX 9404. Results are shown in Table IV-2.

TABLE IV-2. Initiation Study of X-0219 With Booster PBX 9501 (ρ = 1.84 g/cm^3)

Booster				
Diameter (mm)	**Height (mm)**	**Weight (g)**	**Result**	**Dent (mm)**
50.8	50.8	190 PBX 9404	event	9.73
25.4	25.4	23.7	event	7.62
25.4	19.05	17.8	event	7.49
25.4	12.7	11.9	event	8.18
25.4	6.35	5.9	event	8.46
22.86	25.4	19.2	event	8.46
22.86	6.35	4.8	event	8.15
20.32	25.4	15.2	event	6.17
20.32	19.05	11.4	event	8.15
20.32	12.7	7.6	event	5.41
20.32	6.35	3.8	event	5.84
17.78	25.4	11.6	event (C on plate)	3.73
17.78	12.7	5.8	event (C on plate)	4.32
17.78	6.35	2.9	event	5.26
15.24	25.4	8.5	no event	0.56
15.24	6.35	2.1	event (C on plate)	3.76

These data suggest that boosters smaller than the failure diameter of TATB (~17 mm) should not be used, but a properly designed 10-g PBX 9501 booster appears sufficient to detonate X-0219 in this configuration. Among the phenomena affecting initiation of TATB formulations might be low-order detonation, buildup or decay of detonation upon reflection at the plate, wave-shaping, and nonaxial initiation. DATB/Kel-F 800 90/10 and PYX were found unsuitable as boosters. Changing the configuration to hemispherical boosters for these HEs did not improve their performance. Dents of <7.62 mm indicate marginal or failed initiation.

Urizar also demonstrated that TATB pellets that could be intiated by flying plates could be used as boosters (at proper density and geometry) to initiate X-0219. He expanded his intiation studies to include the use of 1E30 detonators to initiate X-0290 and various grades of TATB. Tests indicate that superfine TATB will not detonate with one 1E30 detonator at densities above 1.75 g/cm^3. Low-temperature (-78°C) tests using superfine TATB cylinders of 25-mm diam by 25-mm high with densities of 1.703, 1.752, and 1.800 g/cm^3 were detonated successfully with three 1E30 detonators.

In 1973, Urizar successfully initiated X-0219 charges ($\rho = 1.92$ g/cm^3) of 50.8-mm diam by 50.8 mm high with 50.8-mm-diam by 25.4-mm-high booster pellets of superfine TATB ($\rho = 1.7$ g/cm^3), giving plate dents of ~9.91 mm. Twenty five-and-four-tenths millimeter diam by 25.4-mm-high pellets of production TATB ($\rho = 1.7$ g/cm^3) gave only marginal initiation of the X-0219 with a dent of 6.63 mm.

In the 1980s, Bahl, Bloom, Erickson, Honodel, Lee, McGuire, Sanders, Slettevold, Tarver, von Holle, and Weingart at LLNL, and Duncan at MHSMP studied effects of booster material and test configuration, of TATB particle size and temperature on shock initiation and divergence, using hemispherical boosters or thin flyers.[IV-33 to IV-35] They determined that:

1. The initiation threshold is higher, even marginal, at -54°C than at ambient;
2. The effect of particle size is greater at lower densities;
3. Thermal cycling causes cracking of the HE near the booster;
4. Large changes in the average pore diameter produce only modest changes in the shock-initiation threshold; and
5. Shock pressure increases as particle size decreases.

Their results agree with the conclusions reached at LANL for similar tests with X-0219 and PBX 9502.

4. Corner-Turning/Divergence. Experiments were conducted at LANL by Hatler, Ramsay, Seitz, and Wackerle to determine distance to breakout of detonation, that is, corner-turning, and to study effects of temperature on this phenomenon. This characteristic is called divergence at LLNL, where this work was done predominantly by Jackson, Weingart, and Green. This phenomenon is generated by flying plates; and input shocks can be short, long, or sustained.

Early in the 1970s Leeman at SNLA, Todd at LASL, Jackson, and Weingart at LLL successfully initiated DATB and TATB cylindrical charges with electrically driven foils (also called flyers, flying plates, or slappers). By 1973, both Todd and Leeman had successfully initiated DATB charges with flying foils. At Livermore large-area foils at ~5.5 km/s flyer velocity initiated high-density pressed X-0219.

Jackson and Weingart summarized their thin-flyer-plate initiation studies of TATB-containing mixtures in 1976, and concluded that:

1. Divergence is improved by decreasing the HE density, amount of binder, or HE particle size; and by increasing the flyer velocity or the environmental temperature;
2. Divergence is inhibited at lower temperatures (-50°C) in some compositions;
3. Sensitivity is increased by decreasing the HE density, amount of binder, or HE particle size.[IV-36 to IV-38]

During the late 1970s Seitz at LASL and West at MHSMP compared short-shock wedge, onion skin, and corner-turning test results for two lots of PBX 9502 at -55, -18, and +20°C. One lot contained a small number of fine particles; the other, recycled material with a higher percentage of fines. The two formulations have nominally identical Pop plots, but they respond quite differently in performance tests. The larger percentage of fines results in a lessened temperature dependence. Distances to detonation and breakout distances are longer at lower temperatures. Results from the onionskin test relate the spreading angle to specific surface area of the TATB powder. This test is therefore very useful as a qualification test for production lots of TATB.

In 1987, Tang at LANL, using results from onionskin tests with low-density superfine and ultrafine TATB as boosters, determined that initiation of TATB PBXs could be enhanced by lowering the density and decreasing the grain size of the TATB.[IV-39] He arrived at this conclusion by numerical simulation using a reactive-burn model in a hydrodynamic code.

Comparable results from corner-turning tests were obtained after the capability was established at MHSMP for routine testing of TATB, its formulations, and production lots.[IV-40 to IV-47] The LLNL snowball divergence tests were run by Kramer, Osborn, Stallings, and others at MHSMP. They found that temperature, particle size (milling/grinding time), and polysaccharide content can have a significant effect on corner turning. Some of the results are summarized in Appendix B, Table B-4.

Cox and Campbell at LANL reported in 1981 that high densities and low temperatures have significant effects on corner-turning radius and distance, as well as on the volume of the dark (largely undetonated) region of PBX 9502.[IV-48] For example, a 1% change in density may cause a 61% change in corner-turning distance. Lowering the temperature by 130°C (from +75 to -55°C) can cause a 44% increase in corner-turning distance. The results are given in Appendix B, Table B-5.

Bahl, Breithaupt, Tarver, and von Holle at LLNL presented their results on the successful initiation and divergence of LX-17 at ambient (+20°C) and cold (-54°C) temperatures at the Ninth Symposium on Detonation in 1989 (Ref. IV-24).

5. Detonation Reaction Zone, Failure Diameter, Diameter Effect and DDT. Craig's results on wedge tests at LASL are summarized in Table IV-3 as parameters from fit to x - t data, where $x = U_{s0}t \pm 1/2bt^2$. Driving systems were plane-wave lenses.

TABLE IV-3. Wedge-Test Data

		Initial Shock Parameters				Coordinates for High-Order Detonation	
Explosive	Density (g/cm^3)	P_0 (kbar)	U_{p0} (km/s)	U_{s0} (km/s)	1/2b (km/s^2)	x* (mm)	t* (μs)
PBX 9502	1.894	8.76	1.01	4.58		19.1	5.43
	1.885	27.4	2.02	7.19		0.68	0.104
at 23°C	1.875	8.89	1.02	4.62		19.6	4.01
at 75°C	1.875	8.93	1.06	4.55		9.99	2.04
at 250°C	1.875	5.44	0.806	3.95		4.73	1.11
TATB	1.876	67.4	0.858	4.186	0.049	«12.65	«2.92
	1.876	94.2	1.063	4.723	0.111	≥12.74	≥2.44
	1.876	130.3	1.340	5.184	0.425	5.80	1.02
	1.876	162.2	1.471	5.879	0.684	3.23	0.52
TATB/HMX/Kel-F 40/50/10 wt%							
	1.912	39.0	0.554	3.683	0.035	>12.7	>3.32
	1.912	63.0	0.811	4.062	0.061	8.476	1.946
	1.912	71.5	0.883	4.237	0.436	4.18	0.86
X-0290	1.898	12.3	1.24	5.24		12.78	2.243

Failure-diameter studies by Campbell and Engelke at LASL in 1974 are shown in Fig. IV-4 and Table IV-4 (Ref. IV-27). In 1982, Hallam at LLNL reported failure diameters and detonation velocities for LX-17 at different temperatures; the data are included in Table IV-4 with other previously unpublished data.

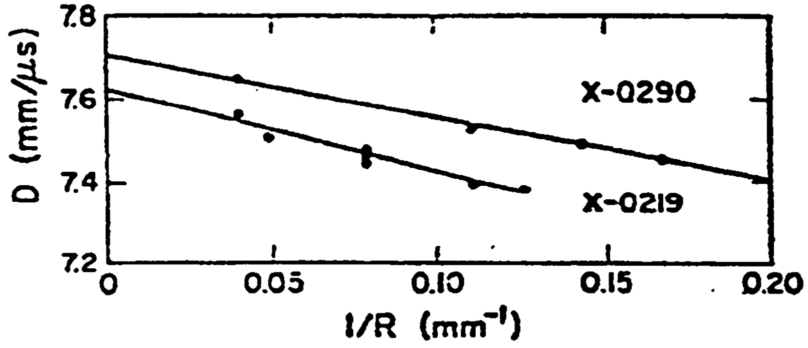

Fig. IV-4. Diameter-effect curves for X-0290 ($\rho = 1.895\ g/cm^3$) and X-0219 ($\rho = 1.915\ g/cm^3$).

TABLE IV-4. Detonation and Failure-Diameter Data

Explosive	Density		Detonation	Failure	Reaction	Temp
	(g/cm^3)	%Voids	Veloc. (km/s)	Diam (mm)	Zone (mm)	(°C)
LX-17			7.6 - 7.7	>11	~2	+22
			7.3 - 7.4	12 - 13		-56
LX-17	1.90				0.7	
PBX 9502	1.894	2.5	7.406	10.0		+24
			no detonation	8.0		+24
	1.892	2.6	no detonation			+75
	1.890	2.7	detonation	7.0		+75
	1.890	2.7	detonation	12		-55
			no detonation	≥4		240
	1.890	2.7	no detonation	11		-56
TATB/Elwax/B^{2}wax 90/5/5	1.74	0.7			5	
TATB/TNT/Al 40/40/20	1.90	0.7	detonation			
TATB (LANL superfine)	1.6 to 1.7			4.32 to 5.72		
	1.836	5.3	7.302	6		+24
X-0219	1.915	1.6	7.380	16		+24
			no detonation	14		+24
X-0290	1.895	2.4	7.706	9	3.3	

In 1978, Lee, Parker, and Weingart of LLL reported on measurement of the reaction-zone length of LX-17 ($\rho = 1.90$ g/cm^3). They obtained a reaction-zone length of 0.7 mm and C-J pressure of 29 GPa (Ref. IV-26). These values have been included in Tables IV-1 and IV-4. Erickson, Palmer, Parker, and Vantine of LLNL published free-surface velocity measurements for reacting RX-03-BB; their method permitted estimation of reaction-zone length.[IV-49]

In 1981, Mader, Shaw, and Ramsay reported from LANL on a theoretical and experimental study of the performance of X-0290 and PBX 9502 (Ref. IV-28). Performance parameters were calculated from BKW EOS and Forest Fire burn rates. Experiments were done to accomplish the following:

1. Determine the change of C-J pressure as a function of run distance to detonation;
2. Study the rate of energy delivered to a plate; and
3. Determine diverging detonations.

Representative data are included in Table IV-4; the Pop plot for PBX 9502 is shown in Fig. IV-5.

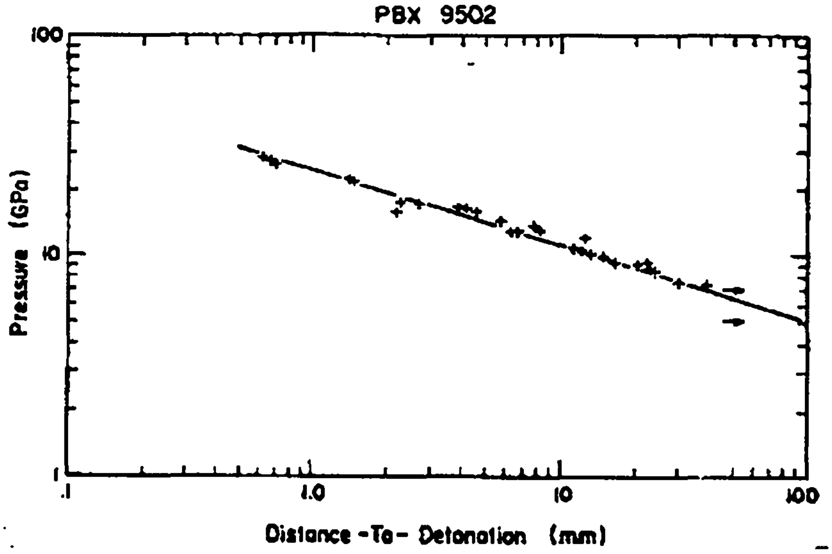

Fig. IV-5. The Pop plot for PBX 9502.

Campbell at LANL continued failure and reaction-zone studies and extended the range to high and low temperatures.[IV-50] Some of his unpublished results are also included in Table IV-4. Ramsay, also at LANL, extended Campbell's studies to confined PBX 9502, using the prism test.[IV-51] The failure diameter decreases with increasing impedance of the confining material, but it does not change with low-impedance (less than PBX 9502's) confinement. Very light confinement caused a larger-than-expected diameter decrease.

The most recent studies on the effect of temperature on failure thickness and DDT were reported by LANL's Asay and McAfee at the Tenth Detonation Symposium in 1993.[IV-52] The heavily confined sample of TATB was completely consumed by burning and combustion at the maximum test temperature of 240°C, but there was no evidence of detonation. Burning ceased, once confinement was lost. Failure thickness results for PBX 9502 are shown in Fig. IV-6 and are included in Table IV-4.

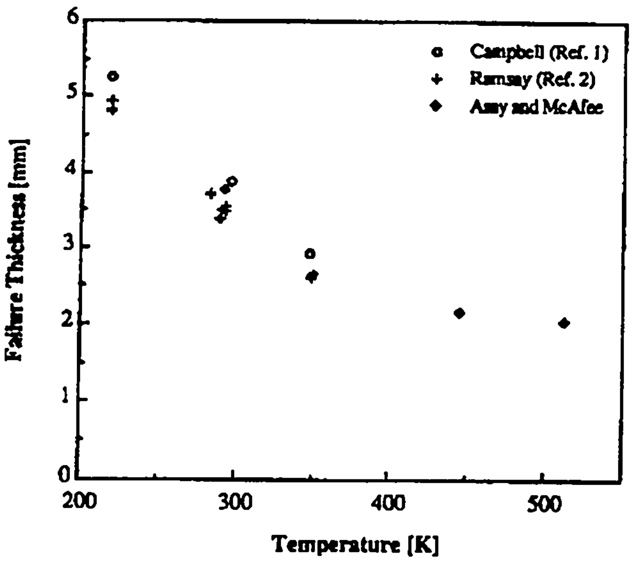

Fig. IV-6. Failure thickness or one-half failure diameter as a function of temperature.

At the Tenth Detonation Symposium in 1993, Cooper of SNLA reported the development of correlations between run distance and initial shock pressure, initial density, $p^2\tau$, critical energy fluence, or failure diameter.[IV-53] Correlations of run distance to detonation with critical energy fluence and failure diameter are shown in Figures IV-7 and IV-8.

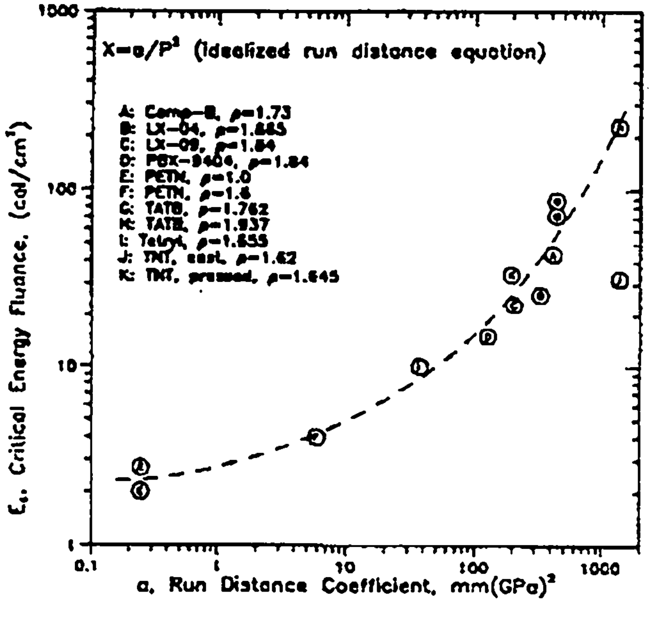

Fig. IV-7. Critical energy fluence correlated to run-distance coefficient for several explosives.

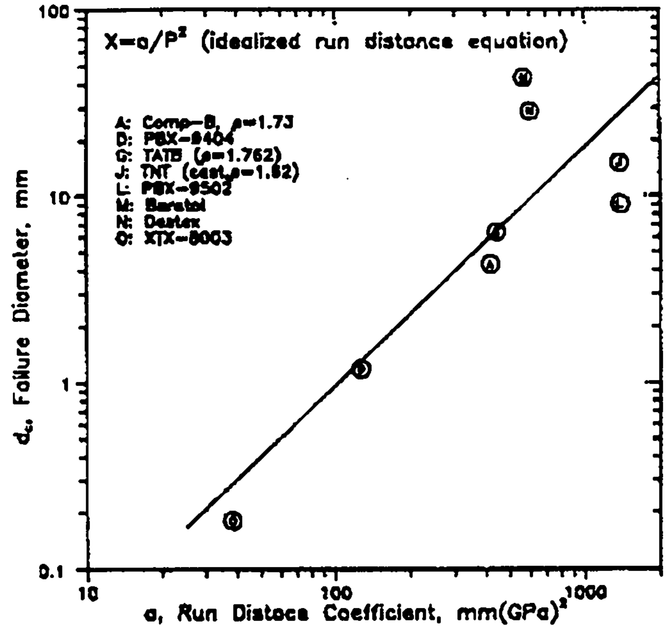

Fig. IV-8. Failure radius correlated to run-distance coefficient for several explosives.

Sheffield and Bloomquist at SNLA with Tarver at LLNL estimated an initial reaction rate for PBX 9502 of 80 ms^{-1}; the reaction rate decreases as the reaction proceeds.[IV-54] In 1993, Tarver, Ruggerio, Fried, and Calef at LLNL determined the rates of energy transfer among the internal states of large organic explosive molecules produced by exothermic decomposition processes.[IV-55] They noted complex Mach-stem interactions, and used the nonideal ZND model to identify four main regions within the chemical reaction zone.

6. Prompt and Short-Duration Shock Experiments. Distance to detonation is defined as the distance it takes for a nonreactive shock wave into the HE to turn into a detonation wave. At the Ninth Detonation Symposium in 1989, Lee, Tao, and Crouch of LLNL presented results on measurements of the distance to detonation for ultrafine TATB (pressed density 1.60 g/cm^3 [83% TMD]) and RX-26-AF (pressed density 1.84 g/cm^3 [99% TMD]) in the temperature region -80 to +80°C.[IV-56] They used an electric gun to make flyer plates, traveling down a 3-mm-long by 4-mm-diam barrel, strike the IHE targets at ~5.4 km/s. The flyer kinetic energy generated was ~2592 kJ/m^2. They saw no change in the distance-time trajectory with temperature; detonation velocity was 6.50 km/s for TATB and 7.80 km/s for RX-26-AF.

In 1978, Ramsey and Seitz of LANL reported distance and time to detonation, and Hugoniot data for TATB. Ramsay used standard grind TATB ($\rho = 1.806$ g/cm^3) with an explosive plane-wave booster system and input pressures of 3.34 to 9.42 GPa; Seitz used superfine TATB ($\rho = 1.801$ g/cm^3) with short-duration shocks generated with electrically driven flyers in explosive wedges. Experimental conditions and results of both experiments are tabulated in Table IV-5.

TABLE IV-5. Short-Shock Detonation and Hugoniot Experiments With TATB and PBX 9502

Explosive	Flyer Velocity (km/s)	Pulse Duration (ns)	Pressure (GPa)	Velocity Shock (km/s)	Velocity Particle (km/s)	Distance to Detonation (mm)	Time to Detonation (μs)
TATB standard grind			9.42	4.675	1.116	5.37	1.02
			7.95	4.465	0.985	6.54	1.33
			5.27	3.913	0.746	22.7	5.38
			3.34	3.125	0.575	>25.4	>8.0
TATB superfine	2.62	170	17.4	5.8	1.66	1.77	0.283
(averages)	3.26	74	22.9	6.2	2.04	1.23	0.222
PBX 9502, -55°C				8.2			71
23°C				8.2			29
75°C				8.2			14
252°C				8.2			2

In 1980, Lee, Honodel, and Weingart at LLNL described shock initiation experiments, using thin flyers and short-duration pulses.[IV-57] Shock initiation was accomplished with thin plastic flyer plates accelerated to 1 to 8 km/s by electrically exploded metal foils, using input pressures of 4 to 55 GPa and pulses of 8 to 500 ns duration. They found that their results agreed with those of Green at LLL, and of Craig, Ramsay, and Seitz at LASL. $P^2\tau$ varied from 5.8 to 23 GPa-μs.

In 1983 Dick at LANL reported on the short-pulse initiation of PBX 9502 with explosively driven Mg flyer plates; the thicker the plate, the shorter the run distance to detonation.[IV-58] Plate thickness was varied from 0.5 to 2 mm, and input pressure was 13.1 GPa. Results are listed in Table IV-6.

TABLE IV-6. Short-Shock Initiation Results for PBX 9502 With a Magnesium Flyer at 13.1 GPa Input Pressure

Flyer Thickness (mm)	Flyer Pulse Length (μs)	Distance to Detonation (mm)
0.5	0.135	no detonation
1.0	0.271	no detonation
1.6	0.433	26
2.0	0.541	12
thick	long	7.8

From the late 1970s through the 1980s, researchers at LANL and LLNL studied the detonation reaction zones of TATB and several TATB-containing formulations (using standard-grind, superfine-grind, or micronized TATB) by Fabry-Pérot interferometry and application of DAGMAR and HOM equations of state (Ref. IV-26).[IV-59 to IV-63] Analysis of the data showed initial reaction rates of ~100 μs^{-1} in detonating PBX 9502. The detonation-wave profiles were similar for the explosives tested. Sharply rising unreactive shocks were followed by decreasing particle velocities, pressures, densities, and internal energies; and interface velocities were not particularly sensitive to modest changes in reaction rates.

A theoretical and experimental study of the reaction rate of detonating PBX 9502 was described by Bdzil, Davis, and Critchfield of LANL at the Tenth Detonation Symposium.[IV-64] They used data from detonation-front curvature experiments (for example, rate sticks) and DSD (a two-dimensional reaction-zone analysis code) to determine a heat-release rate under detonation conditions. Tarver's ignition-and-growth-rate form was used in this work, because it provided a good fit to the data. At the level of 20%, the DSD-determined rate agrees with one published by Green, Tarver, and Erskine of LLNL (Ref. IV-25), which was calibrated to a series of experiments sampling different sets of conditions.

Many shock-initiation experiments also measured EOS and static, as well as dynamic Hugoniot parameters. In 1966, Craig performed experiments on the EOS of unreacted TATB/Kel-F mixtures at LASL. He estimated the EOS to be $U_s = 0.215 + 2.4283\ U_p$. A 25.4-mm-diam column of TATB/Dapon-M at $\rho = 1.805$ g/cm^3 would not sustain a detonation.

Coleburn and Liddiard of NOL published detonation, Hugoniot, and acoustic-velocity data in 1966 (Ref. III-16). Pastine and Bernecker of NOL developed a P, v, E, T equation of state for TATB and calculated shock Hugoniots in 1974.[IV-65]

During the 1970s, Anderson, Seitz, and Wackerle of LASL established Hugoniot data for TATB for the U_sU_p relationship, where U_S = shock velocity in km/s and U_P = particle velocity in km/s. Representative equations are:

Formulation	Density (g/cm^3)	Equation
TATB std grind	1.80	$U_s = 1.904 + 2.447U_p$
superfine	1.800	$U_s = 2.054 + 2.357U_p$

Later in the 1970s, Ramsay and Seitz developed Hugoniot parameters for standard grind and superfine TATB, respectively. The results are compiled in Table IV-7.

Kramer and Demerson at MHSMP conducted wedge tests on TATB before it had been dried and on RX-03-BB at ambient temperature and at 68°C.[IV-66] The results are included in Table IV-7.

During the early 1980s, Marsh at LANL compiled and published all EOS data determined at LANL up to that time.[IV-67]

TABLE IV-7. Hugoniot Parameters for TATB and RX-03-BB

Initial Density (g/cm^3)	Pressure (GPa)	Velocity U_S Shock (km/s)	 U_P Particle (km/s)	Distance to Detonation (mm)	Time to Detonation (µs)
		Standard-grind TATB using plane-wave booster			
1.806	9.42	4.675	1.116	5.37	1.02
1.806	7.95	4.465	0.985	6.54	1.33
1.806	5.12	3.770	0.752	19.6	4.82
1.806	3.34	3.215	0.575	>25.4	>8.0
		Superfine TATB using short-duration-shock flyer and wedge			
1.801	17.4	5.8	1.66	1.77	0.283
1.801	22.9	6.2	2.04	1.23	0.222
		Standard-grind undried TATB using wedge			
1.84	12.9			3.0	0.54-0.55
		Pure TATB using wedge			
1.842	9.0			6.9	1.40
1.842	11.8			3.8	0.72
		RX-03-BB at 68°C using wedge			
1.88	10.8			8.5	1.66
1.88	14.2			4.8	0.92

Dick at LANL found good agreement with earlier results when he compared Hugoniot curves generated from isothermal static compression measurements to 10 GPa with published data for Hugoniot curves generated from shock-wave experiments.[IV-68]

In 1985, Kerley at SNLA reported on a theoretical model for detonation properties, assuming steady-state detonation with chemical equilibrium behind the reaction zone.[IV-69] Then the EOS for the detonation products of CHNO explosives could be used to predict C-J velocities and pressures, release and reshock behavior, as well as the dependence of these properties on chemical composition and loading density.

In 1991, Tang at LANL modeled the behavior of PBX 9502, using special rate equations.[IV-70] The nonideal detonation was explained by a slow process following a fast one. Validity of the

EOS in the early phase of the detonation reflected the partially reacted state; these fast reactions were driven by reaction propagation and decomposition. The slower reactions probably reflected the formulation of large molecules.

During the late 1980s, Green, Tarver, Lee, Mitchell, and Erskine of LLNL conducted numerous experiments on shock compression of TATB-containing formulations, and they developed EOS parameters for LX-17 and RX-26-AF in the unreacted and reacted states (Ref. IV-25).[IV-71]

Dick, Forest, Ramsay, and Seitz in 1988 at LANL studied shock-initiation sensitivity, Hugoniot, and dynamic yield behavior of PBX 9502.[IV-72] They used explosively driven wedge tests and particle-velocity history measurements with electromagnetic gauges at a light-gas gun. Input pressures ranged from 0.5 to 25 GPa. The Hugoniot fits were given as

$$\begin{aligned}
U_s &= 1.857 + 3.15U_p, && U_p \leq 0.50 \text{ km/s,} \\
U_s &= 1.392201 + 5.153578U_p - 2.421567U_p^2 && \\
&\quad + 0.561615U_p^3, && 0.50 < U_p < 1.2 \text{ km/s,} \\
U_s &= 2.938 + 1.77U_p, && 1.2 \leq U_p \leq 2.3 \text{ km/s.}
\end{aligned}$$

Cooper of SNLA developed a correlation for estimating the P-U Hugoniot of an HE, using existing experimental data for pressure and particle velocity of detonation-reaction products of these HEs.[IV-73] Pressures ranged from 0.0015 to 81.8 GPa, particle velocities from 0.79 to 11.0 km/s, and densities from 1.133 to 7.47 g/cm^3 for the explosives studied.

7. Sustained shock experiments. In 1981, Anderson, Ginsberg, Seitz, and Wackerle at LANL reported on gas-gun experiments with superfine TATB ($\rho = 1.80$ g/cm^3), using embedded manganin gauges.[IV-74] They obtained a distance to detonation of ~10 mm with a 7.56-GPa input shock. Their explosively driven, streak-camera wedge experiments indicated distances to detonation of 5.6 to 0.5 mm for 10 to 28 GPa pressures.

8. Embedded-Gauge Studies. These studies were undertaken to evaluate stress, time, and particle velocity measurements of detonating TATB. In 1977, Barlett, Cochran, Erickson, Lee, and Weingart of LLL measured stress-time histories in TATB and PBX 9404, using a planar shock from a light gas gun and embedded manganin stress gauges.[IV-75] Input stresses were 2.4 GPa in PBX 9404 and 13 GPa in TATB. In TATB the stress grew at the shock front, whereas in PBX 9404 the stress at the shock front remained almost constant until just before detonation.

Lagrangian analysis was used at LLNL in the early 1980s to estimate detonation pressure in detonating TATB from measurement of stress and particle velocity.[IV-76] Nutt and Erickson of LLNL studied reactive flow in RX-26-AF, followed by development of a reactive-flow model with DYNA2D.[IV-77] The reaction built in two stages, using the JWL EOS for reactant gases. Nutt noted an energy release of 4.64 MJ/kg from an input pressure of 27 kbar.

Tarver, Parker, Palmer, Hayes, and Erickson of LLNL conducted experimental and calculational studies on reactive flow during shock initiation and detonation-wave propagation for PBX 9404, LX-17, and RX-26-AF.[IV-78,IV-79] They compared particle-velocity gauge, embedded manganin stress gauge, and Fabry-Pérot free surface measurement techniques. Their findings were consistent when compared through computational calculations based on the ZND-type ignition and growth model of detonation. They reported a reaction-zone length of ~2 mm and a detonation velocity of 7.596 m/s for LX-17. These data are included in Table IV-4.

In 1989 at LANL, Forest, Wackerle, Dick, Sheffield, and Pettit reported on the reaction rates of detonating PBX 9502 using magnetic impulse velocity gauges with Lagrangian evaluation of the data.[IV-80] In 1991, Tarver of LLNL reviewed embedded gauge and laser interferometry techniques.[IV-81]

9. Temperature Effects on Shock Initiation

a. Effects of Low Initial Temperatures. In 1983 Seitz and Wackerle reported on buildup to detonation studies of PBX 9502 and PBX 9503 at initial temperatures of -55°C and ambient.[IV-82] The miniwedge technique and plane-wave explosive booster systems were used for distances to detonation from ~1 to 10 mm. The increases in distance to detonation at the lower temperature were 50% for PBX 9502 and ~20% for PBX 9503.

In 1982, Honodel, Lee, Moody, and Weingart at LLNL reported the shock-initiation threshold of pure TATB as functions of density (1.5 to 1.9 g/cm^3) and of flyer-plate diameter (1.5 to 25 mm) at ambient temperature and at -54°C.[IV-83] They found the change in initiation threshold greater than would be expected from the increase in density on cooling to -54°C.

Using sustained and short-duration shocks and the explosive wedge technique, Seitz at LANL reported in 1984 on his study of the effects of both particle size and initial temperature on initiation of TATB and PBX 9502.[IV-84] Three different particle-size distributions in the range of 1 to 80 mm were studied for each material. Temperatures used for sustained-shock experiments were -55 and +20°C, and -55, -18, and +20°C for the short-duration shock experiments. Densities were 1.8 g/cm^3 for TATB and 1.89 g/cm^3 for PBX 9502. Flyer thicknesses were 0.33 mm for the TATB shots and ranged from 0.05 to 0.40 mm for PBX 9502. Input shock pressures were 17.9 GPa for TATB and ranged from 16 to 28 GPa for PBX 9502. In all cases, Seitz noted a linear relationship between distance to detonation and initial temperature, a much stronger relationship for PBX 9502 than for TATB; but the effect of particle size was comparable. In sustained-shock initiation, only very fine particle-size TATB showed a particle-size effect. With 0.13-mm-thick flyers, PBX 9502 showed a strong initial temperature and particle-size effect, the temperature effect being very dependent on the particle size; TATB showed a strong particle-size effect, but it was less influenced by initial temperature.

In 1989, Urtiew, Erickson, Aldis, and Tarver of LLNL reported on shock initiation studies of LX-17 at low and high initial temperatures (-54, +25, and +88°C) using flyer plates and embedded gauges with input shock pressures of 10 to 15 GPa.[IV-85] A reactive-flow model was used in the computational part of this study. Experimental and computational results showed that colder LX-17 had a smaller fraction of HE ignited in the hot spots created by shock compression. This in turn resulted in a smaller increase in the shock velocity and pressure than those measured for hotter LX-17. The growth of hot-spot reactions behind the shock front was also slower in cold LX-17, which resulted in a more gradual pressure rise behind the shock front than that measured for hotter LX-17. Transition to detonation in cold, ambient, and hot LX-17 occurred at approximately the same rate at all three initial temperatures; sufficient heat was transferred from the rapidly growing hot spots to the unreacted molecules in this transition region in order to overcome the 140°C temperature difference. These results are in general agreement with those reported by Lee, Tao, and Crouch of LLNL in their detonation-wave studies at -80°C and +80°C with TATB and RX-26-AF (Ref. IV-56).

b. Effects of High Initial Temperatures. In 1980, Scheloske, Green, and Weingart from LLL used electrically driven flyer plates to determine the shock sensitivity of TATB and RX-03-BB preheated to 250°C prior to impact.[IV-86] The flyer kinetic energy required to initiate pure TATB was reduced ~33% and for RX-03-BB ~50%.

In 1993, Urtiew, Cook, Maienschein, and Tarver of LLNL reported at the Tenth Detonation Symposium on the shock sensitivity of LX-17 at 250°C.[IV-87] They used flyer plates accelerated by a gas gun; the pressure pulse into the sample was 42 kbar at 0.9 km/s flyer velocity. Results for LX-17 and PBX 9502 at 250°C are:

IHE	**Flyer Velocity (km/s)**	**U_s (km/s)**	**P (GPa)**	**Distance to Detonation (mm)**
LX-17-1	0.74	2.68	2.5	>20
	0.81	2.7	3.0	12
	0.98	3.15	3.9	7.5
	1.295	3.5	6.5	3.3
PBX 9502	0.8	2.9	3.0	14.5
	0.885	3.0	4.0	12

Early in the 1990s, Wackerle and Dallman at LANL measured the shock initiation of PBX 9502 at ambient temperature, +75°C, and 250°C, using the wedge technique. They found that, combined with earlier measurements, the Hugoniot parameters could be defined over the temperature range -55 to +252°C. The least-squares fit to the shock-velocity/particle-velocity data results in Hugoniot curves of the following form:

$$U_s = 3.31 + 1.65U_p, \qquad (-55 \pm 4°C),$$
$$U_s = 2.54 + 1.97U_p, \qquad (+75 \pm 2°C),$$
$$U_s = 1.33 + 3.08U_p, \qquad (252 \pm 2°C).$$

Temperature comparisons of distances to detonation of PBX 9502 were reported by Dallman and Wackerle in 1993 at the Tenth Detonation Symposium.[IV-88] The distance to detonation for a given input pressure decreased approximately 50% as the temperature was raised from +20 to 75°C. These shock-sensitivity data for PBX 9502 at various initial temperatures are comparable to ambient-temperature data for LX-17 and PBX 9501. The data are shown in Fig. IV-9.

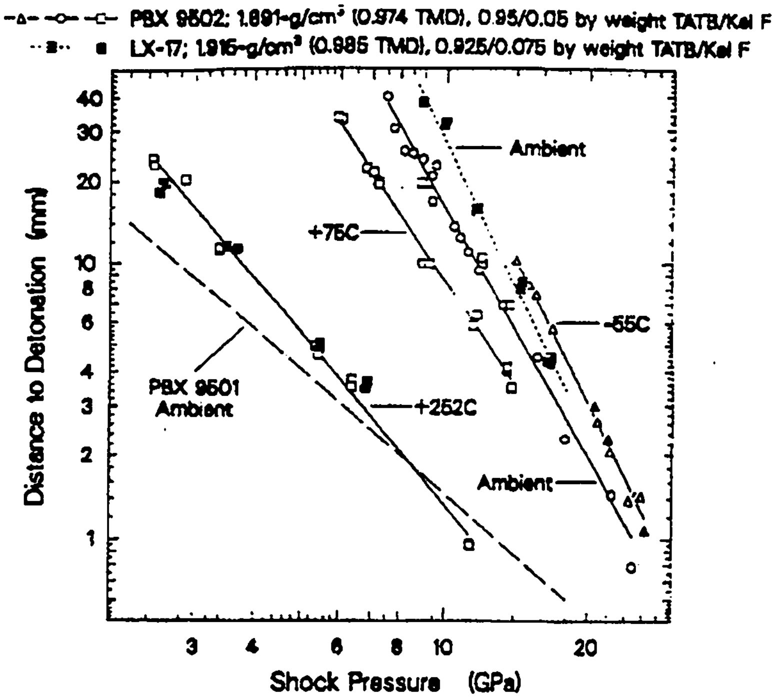

Fig. IV-9. Comparison of the temperature-dependent shock sensitivities of PBX 9502 and LX-17 with ambient PBX 9501.

10. Minimum-Priming Test. The minimum priming charge required to inititate an HE is an indication of the explosive's safety. The primer usually used is XTX-8003 (pentaerythritol tetranitrate [PETN]/Sylgard 80/20) at a density of 1.53 g/cm^3. In the LANL and MHSMP tests, results are given as 50% points for the amount of XTX used. Results are listed in Table IV-8.

TABLE IV-8. Results of Minimum-Priming Tests

Explosive	Density (g/cm^3)	Amount of XTX (g)	Amount of XTX (L_{95})	Result
TATB/HMX/Estane	2/95/3			
	1.840	0.023	±0.093	detonation
TATB/TNT/Al 40/40/20		>4.84		
TATB/Kel-F 800 90/10	1.920	4.835		no detonation
		5.012		no detonation
X-0219		15.3		no detonation
X-0272	1.842	0.0182		detonation
X-0351	1.890	1.53		detonation
X-0407	1.859	0.151		

11. Plate-Dent Test. This performance test was carried out by Craig and Urizar at LASL with 41.3-mm-diam samples. Results are listed in Table IV-9.

TABLE IV-9. Results of Plate-Dent Tests

HE Composition (wt%)	Density (g/cm³)	Temperature (°C)	Plate Dent (mm)	Estimated $P_{C\text{-}J}$ (kbar)
PBX 9502	1.889	25	7.50	--
	1.889	80	7.50	--
	1.885	-80	7.80	
PBX 9502/Al	2.016	--	6.63	231
TATB	1.753	--	4.42	245
TATB/HMX/Kel-F 90/0/10	1.915	--	7.95	
63/27/10	1.893	--	8.92	--
45/45/10	1.892	--	9.65	--
36/54/10	1.890	--	9.80	--
18/72/10	1.881	--	10.29	--
TATB/TNT/Al 40/40/20	1.90	99.3	6.78	--
X-0219	1.90	--	9.37	--
X-0290	1.893	--	7.80	
X-0296	1.827	--	7.41	258
X-0329	1.856	--	7.50	261
X-0345	1.832	--	7.37	256
X-0396	1.838	--	--	280
X-0407	1.858	--		310
X-0435	1.838	--	8.13	283

12. Cap Test. A test configuration was designed and used by Pantex personnel to initiate TATB and its mixtures with a No. 8 blasting cap. No detonations were observed in the many tests conducted. Tests with bulk powder and machining waste of PBX 9502 and LX-17 initiated brief burning reactions that died quickly.

13. Cylinder Test. Measuring expansion of a standard metal cylinder caused by a detonating explosive and its detonation-product gases provides performance data characteristic of the specific HE tested. A desirable formulation provides the highest delivered energy at lowest expansion volume in the divergent geometry of the cylinder test.

During 1972-1973, cylinder tests with TATB formulations were carried out at LASL. The results are reported here relative to those for PBX 9404 at cylinder expansions of 6 and 19 mm.

Formulation	Density (g/cm^3)	Velocity Ratio [V^2(HE)/V^2(PBX 9404)] at 6 mm	Velocity Ratio [V^2(HE)/V^2(PBX 9404)] at 19 mm
TATB/HMX/Kel-F 800 40/50/10	1.900	0.835	0.911
	1.900	0.836	0.851
TATB/Kel-F 800 90/10	1.921	0.673	0.689
	1.920	0.659	0.690
X-0272	1.839	1.003	1.021
	1.839	0.986	1.007
X-0407	1.855		1.67

Many cylinder shots were done at LLNL over the years. Representative data, compiled by McMurphy, are listed in Appendix B, Table B-6.[IV-89] Expansion data are scaled to a 25.4-mm (1-in.)-ID cylinder. In 1985, McGuire and Finger of LLNL determined the effect of detonation temperature on cylinder-test performance; the data are included in Table IV-9 (Ref. IV-30).

Doherty, Short, and Kamlet of NSWC in 1989 developed a correlation for estimating cylinder-test energies from expansion data. TATB and nitroguanidine (NQ) underperformed by ~15% relative to this equation (Ref. III-49). Their data are included in Table IV-1.

In 1991 the LLNL group of Simpson, Kury, Nichols III, Breithaupt, and Crawford reported on evaluation of IHE performance.[IV-90]

14. Other Energy Release Concepts and Calculations. Urizar and Rohwer at LASL established the $p^2\tau$ criterion for X-0219 at a density of 1.920 g/cm^3 in 1972. Tests showed a reaction at 90 kbar for 2.8 μs that consumed about half of the sample, and at 47 kbar for 10.5 μs that consumed about 3/4 of the sample ($p^2\tau$ = 23,000 $kbar^2$-μs). Christiansen and Taylor at LANL reported this result in 1973.[IV-91] They compared the $p^2\tau$ values of several explosives listed below. The constant $C = p^2\tau$ is characteristic for each HE, but it increases to a maximum as the reaction runs to completion. The value of C is also dependent on density, crystal size distribution, composition, and initial temperature.

Explosive	C (bar^2-s)
PBX 9404	540
Comp B-3	1,300
Cyclotol 75/25	1,600
TATB	23,000

The reaction is less violent for the less sensitive explosives, and therefore safer. Wackerle and Ramsay of LASL studied the $p^2\tau$ relationshop for X-0219 and, in 1974, suggested that spherical systems with short runs to detonation would make X-0219 easier to initiate.

In 1974, Walker, Wasley, Green, and Nidick, Jr. at LLNL set forth the critical energy concept for shock initiation to establish reliability and safety of the component.[IV-92] This concept is based on the assumption that a strong correlation exists between the shock initiation of an HE and a specific quantity of energy transmitted to the HE by a shock wave. They established a "critical energy fluence" or a $p^2\tau$ requirement for shock initiation. They determined that critical energy fluence E_c is related to $P^2\tau$; $E_c = \sim 950$ J/cm^2 for X-0219, $\rho = 1.93$ g/cm^3.

Lee, Honodel, and Weingart of LLL reported in 1980 on shock-initiation tests of TATB formulations conducted with input pressure pulses of 4 to 55 GPa (Ref. IV-57). Results indicated that the $P^2\tau$ relationship between initiating pressure and pulse duration was constant at high pressures and short pulse lengths. $P^2\tau$ varied from 5.8 to 23 GPa^2-µs.

Another concept of energy release was advanced by Hardesty and Kennedy at SNLA in 1977.[IV-93] Rather than expressing HE performance by relative ranking of cylinder-test results, they would determine the effective specific energy of an HE. Using the TIGER code, this energy could be determined, with the Gurney energy or velocity as an absolute indicator of an HE's metal accelerating ability.

15. Electrical and Friction Initiation. The possibility of accidental initiation by friction (See Thermal Ignition, Section IV-D), lightning or other electrical stimuli of HEs, and TATB specifically, was studied. Spark sensitivity and friction test methods are available for this purpose.[IV-94 to IV-96] TATB and its mixtures did not respond in these tests. Forbes at NSWC established the electrical breakdown voltage for pressed TATB as 5,750 V/mm.[IV-97]

In 1993, Kober, Copenhaver, and Ritchie at LANL presented a computer code that predicts the energetic properties of molecular HE crystals.[IV-98] Included in the code are the important contributions to crystalline energy—repulsion, dispersion and electrostatics.

C. Impact Tests

Urizar, Petersen, and Smith of LANL compiled sensitivity data obtained up to 1978 for LASL explosives.[IV-99] They describe the tests for which test results are compiled: minimum priming, wedge, and small- and large-scale gap tests.

1. Bullet Tests. Vulnerability of X-0219 in light and heavy confinement was tested with impacts from .50-cal. projectiles at velocities of ~850 to 922 m/s. The experiments were conducted by Hantel (LASL) in the early 1970s.[IV-100] The only reaction, burning, was caused at the highest velocity, 922 m/s, for the lightly cased explosive, whereas all heavily cased models burned at impact velocities around 850 m/s. Later tests by Upham with X-0290 produced similar results. Nor did .50-cal. bullet impact at 804 m/s cause any reaction in PBX 9502 heated to 80°C. Tests by Fletcher at LANL in the mid-1980s with TATB and LX-17 produced no detonations either. Tests with .30-cal. ammunition showed that the projectile lodged in the assembly at about 850 m/s and caused complete burning rather than pass through, as did the .50-cal. projectile that caused less burning. The burning reactions extinguished themselves in all test.

In the early 1980s, Sharp at MHSMP conducted .30-cal. rifle bullet tests on RX-26-AW/AX, RX-26-AY/AF, and RX-26-AF with HMX of different particle sizes [IV-101] Reactions occurred most often with the finest particle-size HMX. No detonations happened.

In 1982, Delistraty and Brandt at LLNL used a light gas gun to establish detonation parameters for LX-17 at a density of 1.90 g/cm^3.[IV-102] High-order diverging detonations were obtained with an 8-mm diam by a 19-mm steel rod at 5.67 km/s impact velocity and with a Ta plate of 24.2-mm diam at 6.53 km/s.

In 1993, Chidester and Green of LLNL reported on a method that allowed calculation of the frictional work on the IHE to accurately predict the reaction threshold for initiation in an accident scenario.[IV-103] Projectile impact tests produced a pressure of <3 kbar for 150 µs at the reaction threshold. The impacts failed to react LX-17 ($\rho = 1.9$ g/cm^3, 98% TMD), even when the IHE had been heated to 250°C.

2. Drop-Weight Impact Tests. In 1990, Storm, Stine, and Kramer at LANL compared LANL and NSWC results from drop-weight impact tests of many nitroaromatics, in the hope of finding a correlation with other sensitivity test results.[IV-104] They developed a "sensitivity index" based on oxygen balance (OB) to estimate sensitivities of closely related molecular species. Drop-weight impact tests are performed routinely on all new explosives. Maximum drop height at LLNL is 177 cm using a 2.5-kg weight, at LANL 320 cm using a 5-kg weight. Pure TATB gave no reactions in either machine. For mixtures, the amount of explosive more sensitive than TATB determined the drop height for reaction. Neither TATB nor X-0290 reacted in the drop-weight impact test at temperatures from 25 to 250°C. The test results are given in Appendix B, Tables B-7, and B-8. Drop height indicates a reaction, except for the "no go's" at 320 and 177 cm, respectively.

3. Large-Scale Impact Tests. The skid, sled, spigot, and Susan tests were developed to determine the likelihood of high-order detonation when a large HE-containing component or assembly is dropped or impacted accidentally. Reactions do occur, but the presence of TATB exerts a strong desensitizing influence.

In the skid test, spherical billets are swung pendulum-fashion at 14°- or 45°-angles to simulate a credible accident. Tests conducted at LASL during the late 1960s and early 1970s proved TATB unreactive, and formulations X-0219 and X-0272 showed only mild reactions. Results on TATB/HMX formulations showed that mixtures with more than 40% TATB did not react in the skid test.

In the spigot test, assemblies containing a booster explosive are dropped from a 46-m-high tower onto a steel pin. In the LANL studies, no reaction was observed and all PBX 9502, the test explosive, was recovered.

In the sled and Susan tests, which are horizontal impact tests, no reactions occurred at velocities below 152 m/s. Scheloske of LLL conducted Susan-like tests on RX-03-BB at 250°C; violent reactions occurred at impact velocites of ~700 m/s (Ref. IV-86). Weapon-like assemblies were tested at SNLA using PBX 9502. No reactions occurred at impact velocities of up to 610-m/s.

4. Gap Tests. Large- and small-scale gap sensitivity tests, developed and used at NOL since about 1960, were adapted for use at DOE installations. Price at NSWC studied this test method in depth over many years.[IV-105 to IV-107]

The small-scale gap test (SSGT) is run in a 12.7-mm geometry for sensitive explosives, but the large-scale gap test (LSGT) (38.1-mm geometry) provides more realistic results for less sensitive HEs. Because of TATB's extreme insensitivity, most of the gap tests on TATB formulations were run in the large-scale geometry, called standard at LANL, or in the special 25.4-mm geometry, developed at MHSMP to conserve material and to avoid effects from failure-diameter interference. Results are reported in Appendix B, Table B-9 as 50% probability of an event from large- and small-scale tests.

Results from 25.4-mm gap tests, studied by Urizar at LASL in the mid-1970s led to the following conclusions:

1. The sensitivity of TATB and its formulations with 5 to 10% Kel-F 800 binder is very strongly a function of the percentage of voids in the charges tested;

2. These formulations (X-0219, X-0290, X-0291) exhibit similar shock sensitivies at low void percentages (high % TMD), but the formulations with lower binder contents become relatively more sensitive at higher void levels; and
3. The superfine TATB (20 μ mean diam) does not appear to be more sensitive than regular production TATB (60 μ mean diam).

Price at NSWC concluded from a literature study and comparison with Seitz's data from shock-initiation experiments that coarse, porous HE appears more shock-sensitive than a fine HE in tests at relatively low pressures and long durations, where thresholds for ignition are measured (gap tests or thick-flyer impacts, Ref. IV-107). However, at relatively high pressures (sustained or short-duration shocks), fine HE seems more shock-sensitive than does coarse HE. Wedge tests are carried out at high pressure, therefore these tests show fine HE more shock-sensitive than coarse HE. A reversal of this relative rating is seen when a large range of pressures down to and including very low amplitudes is used, as was found for TNT, HNS, and TATB.

Liddiard, Forbes, and Price reported on shock initiation of HEs, including TATB in modified gap test (MGT) and underwater sensitivity test (UST) geometries[IV-108]. They compared their data with those from the LSGT and found that the most dominant effect on sensitivity was the method of preparation (cast or pressed, that is, % voids). They also found that TATB required the greatest shock for initiation of all the HEs tested.

Spivak, Betancourt, and O'Connor at NSWC developed a gap test that gives comparative data for IHEs. Their samples are for 0.5-in. diam by 0.5-in.-long IHE pressed into steel tubing, requiring only about 5 cm^3 of IHE.[IV-109] Results correlate well with the LSGT data.

D. Thermal Ignition

Summarized in this section will be the responses effected by thermal stimuli in TATB, its formulations, and fabricated HE charges. Such tests are essential to establish the safety of these materials and components in various environments. Together with other sensitivity parameters, we can obtain a good picture of the certification of TATB as an insensitive and safe production HE. While TATB and its mixtures show increased sensitivity at elevated temperatures (See cylinder- and gap-test results), they are many magnitudes less sensitive than HEs used in the past (for example, PBX 9404, Comp B).

LANL's Storm and Travis reviewed sensitivity data for TATB, and compared them with HMX's characteristics.[IV-110]

Laser ignition of TATB, using a pulsed, yttrium-aluminum-garnet neodymium-doped (YAG) laser, was achieved in 1988 by Dosser, Siwecki, Beckman, and Girmann at MLM. [IV-111]

1. Hot Spots.

a. Experimental. Numerous studies have been carried out in recent years on decomposition and initiation of TATB through shock loading, friction, underwater shock, or flyer-plate impact to study by various spectroscopic methods the molecular processes involved in subignition and thermal ignition. The early studies were carried out by Owens and Sharma at the ARDC in the mid-1970s, when they found evidence of shock-induced intra-molecular-bond breaking and production of radicals (The NO_2 group was severed from the molecule).[IV-112 to IV-115] In some cases, the bonds broken by shock were different from those broken in thermal decomposition.

These studies, related to electronic excitation, were continued and expanded at NSWC by Sharma with Beard, Coffey, Elban, Forbes, Glover, Hoffsommer, Liddiard, and Santiago into the 1990s.[IV-116 to IV-122] They identified reaction products that were more sensitive than the original sample. Sharma and coworkers at the NSWC reported in 1991 on work that demonstrated for the first time a linear correlation between shakeup spectra from XPS (energy transfer) and impact sensitivity of TATB.[IV-123 to IV-126] Demske at NSWC, Brazell, Farley, and Miller at LLNL, and Warnes at LANL reported on hot spots in TATB with a pulsed relativistic electron beam and on explosions that quickly quenched.[IV-127]

In the late 1980s, LANL scientists Greiner, Blais, Phillips, Johnson, and Fernandez, and Volk from ICT, developed a method to identify detonation products and determine their relative concentrations quantitatively for small samples.[IV-128,IV-129] Products could be measured at $\leq 1\ \mu$ after passage of the detonation wave; diamond was found in TATB/TNT soot.

At SNLA in 1988, Dodson, Venturini, and Rogers, Jr., subjected HEs to shock loading of 0.6 GPa.[IV-130] Only TATB showed signs of radical generation. Trott and Renlund of SNLA used pulsed-laser Raman scattering to study the NH_2 bond in TATB under shock loading. They found that hydrogen bonding is enhanced at modest dynamic pressures.[IV-131 to IV-134] This effect is reversed at elevated temperatures. Effects of temperatures to ~200°C and pressures to ~6 GPa were studied.

In 1993, Foltz at LLNL noted that pressure-dependent reaction propagation rates for TATB increased approximately linearly to about 20 GPa, then more rapidly (exponentially), showing further discontinuities at 30 and 40 GPa.[IV-135] The measurements were made in a diamond-anvil cell at 3 to 40 GPa. During the experiment, TATB changed color from the original yellow at ambient pressure to red, then to black above 30 GPa. And Fried and Ruggiero, also from LLNL, were able to estimate the phonon upconversion rate in TATB and other HEs from existing inelastic scattering data.[IV-136] They found that the estimated energy transfer rates in pure unreacted TATB were strongly correlated with impact sensitivity.

b. Modeling. The effect of hot spots on the shock-initiation behavior of TATB was modeled by Mader, Forest, Johnson, Kershner, and Tang at LANL and was interpreted with the aid of mercury-intrusion porosimetry by Lee, Bloom, von Holle, Weingart, Erickson, Sanders, Slettevold, and McGuire at LLNL (Ref. IV-34). These efforts were reported at the 8th Symposium on Detonation in 1985.[IV-137,IV-138]

At the Symposium in Beijing in 1987, Maiden from LLNL proposed a model of hot-spot formation to determine the minimal ignition properties of pyrotechnics and explosives.[IV-139] He assumed that sufficiently high pressure would lead to viscoplastic heating and pore motion, which then leads to ignition when the hot spot reaches the critical conditions predicted by thermal explosion theory. Ignition thresholds depend on $p^2\tau$. Experimental data used were pore-size distribution, viscosity, thermal conductivity, yield stress, pressure, and temperature. Viscosity and melting determined the rate of pore collapse. Heating rates were extremely fast, and ignition delays were short because of the high temperatures at the pore walls. His calculational results agreed well with results from flyer-plate experiments. $P^2\tau$ for TATB calculated to 627 $\text{kbar}^2\text{-}\mu\text{s}$. Cady concluded in 1992, based on experiments conducted earlier at LANL, that void collapse will produce hot spots leading to initiation (Ref. I-36).

Nichols, Tarver, and Chidester of LLNL reported at the Tenth Detonation Symposium in 1993 on modeling the SDT process, using the expanded heat transfer code TAPAZ2D.[IV-140] An unlimited number of chemical species and reactions relating to these species can now be included in the model, as data become available.

2. Confined and Unconfined Heating Tests. Donaldson and Lee at SNLA determined the times and temperatures to explosion for several HEs by heating them in cylindrical vessels.

Heating rates and confinement could be varied, so both burning and steady heating could be studied.[IV-141 to IV-143] The surface temperature at the time of explosion in a closed vessel was ~249°C with detonation for a HMX/TATB formulation, whereas it was ~316°C for a TATB mixture without HMX, but was accompanied by a nonviolent reaction. Both formulations burned in the unconfined tests but did not detonate. TATB mixtures emitted gases rapidly enough to rupture the stainless-steel confinement vessel, but only self-heating and exothermic decomposition were observed. Detonation, if initiated, failed to propagate. In 1991, Lundstrom at the NWC reported that a hot-spot variation of the Forest Fire burn model produced an unsteady reactive-flow field for PBX 9502 when impacted with flyer plates.[IV-143]

During the mid-1970s, Popolato, Ruminer, Vigil, Kernodle, and Jaeger at LANL conducted unconfined one-dimensional heating experiments in slab geometry on several HEs.[IV-145] The experimentally determined temperatures and times to ignition were reproduced computationally by solving a one-dimensional heat-conduction equation that contained a zero-order reaction-energy source term and a time-dependent temperature boundary condition. For PBX 9502 at a heating rate of 20°C/min, the temperature to ignition was 340°C and the time-to-ignition 18.5 min.

E. References for Section IV

IV-1. J. D. Corley, "Insensitive High Explosives Evaluation Techniques," *Minutes of the Twenty-Second Explosives Safety Seminar* (Anaheim, California, 1986) Vol. I, p. 41.

IV-2. B. M. Dobratz, M. Finger, L. G. Green, J. R. Humphrey, R. R. McGuire, and H. F. Rizzo, "The Sensitivity of Triaminobenzene (TATB) and TATB Formulations: Summary Report," Lawrence Livermore Laboratory report UCID-17808 (1978) (report U-NOFORN).

IV-3. J. C. Coleville, "LX-17 and LX-10 Test Data, PBX 9502 and PBX 9501 Test Data," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant reports SR-92-03 and SR-92-04 (1992).

IV-4. W. C. Davis, "Sensitivity of TATB Explosives," Los Alamos Scientific Laboratory report LA-6676-MS (1977).

IV-5. U.S. Department of Energy, Assistant Secretary for Environment, Safety, and Health, Office of Quality Programs, "DOE Explosives Safety Manual," report DOE/EV/06194 Revision 6 (1991).

IV-6. F. E. Walker, and R. J.Wasley, "A General Model for the Shock Initiation of Explosives," *Propellants Explos.* **1**, 73 (1976).

IV-7. S. Cochran, L. Erickson, R. Lee, and R. Weingart, "Shock Initiation of TATB," Lawrence Livermore Laboratory report UCRL-80441 Abstract (1978).

IV-8. E. L. Lee, S. G. Cochran, J. H. Chan, and C. M. Tarver, "Two-Dimensional Calculations of Detonation Processes in Condensed Explosives," *Am. Phys. Soc. Bull.* **24**, 722 (1979).

IV-9. J. J. Dick, "Buildup to Detonation in Solid High Explosives During Plane Shock Initiation: Some Comparisons," *Eighteenth Symposium (International) on Combustion* (The Combustion Institute, Philadelphia, Pennsylvania, 1981) p. 1623.

IV-10. C. L. Mader, "Initiation of Detonations," *Progress in Astronautics and Aeronautics*, Vol. 87, J. R. Bowen, N. Manson, A. K. Oppenheim, and R. I. Soloukhin, Eds (American Institute of Astronautics and Aeronautics, New York City, 1981) p. 468.

IV-11. C. M. Tarver and J. O. Hallquist, "Modeling Two-Dimensional Shock Initiation and Detonation Wave Phenomena in PBX 9404 and LX-17," Lawrence Livermore Laboratory report UCRL-84990 Preprint (1981).

IV-12. S. G. Cochran and C.M. Tarver, "Modeling Particle Size and Initial Temperature Effects on Shock Initiation of TATB-Based Explosives," *Shock Waves in Condensed Matter—1983*, J. R. Asay, R. A. Graham, G. K. Straub, Eds (Elsevier Science Publishers, New York, 1984) p. 593.

IV-13. C. M. Tarver, J. O. Hallquist, and L. M. Erickson, "Modeling Short Pulse Duration Shock Initiation of Solid Explosives," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSWC MP 86-194, p. 951.

IV-14. J. B. Bdzil and W. Fickett, "Detonation Shock Dynamics: A New Approach to Modeling Mult-Dimentsional Detonation Waves," *Proceedings, Ninth Symposium (International) on Detonation* (Portland, Oregon, 1989), Office of the Chief of Naval Research report, Vol. I, p. 730.

IV-15. C. M. Tarver, "Modeling Shock Initiation and Detonation Divergence Tests on TATB-Based Explosives," *Propellants, Explos., Pyrotech.* **15**, 132 (1990).

IV-16. C. L. Mader and J. D. Kershner, "Numerical Modeling of the Effect of Temperature and Particle Size on Shock Inititation Properties of HMX and TATB," *J. Energ. Mater.* **10**, 69 (1992).

IV-17 D. L. Demerson and R. W. Ashcraft, "TNT Equivalency of PBX 9502," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-83-53 (1983) (report UCNI).

IV-18. E. N. Ferm and L. M. Hull, "Reflected-Shock Initiation of Explosives," *Paper Summaries, Tenth International Detonation Symposium* (Boston, Massachusetts, 1993) Naval Surface Weapons Center report NSWCDD/MP-92/456, p. 394.

IV-19. L. M. Hull, "Mach Reflection of Spherical Detonation Waves," *Paper Summaries, Tenth International Detonation Symposium* (Boston, Massachusetts, 1993) Naval Surface Weapons Center report NSWCDD/MP-92/456, p. 87.

IV-20. C. M. Tarver, T. M. Cook, P. A. Urtiew, and W. C. Tao, "Multiple Shock Initiation of LX-17," *Paper Summaries, Tenth International Detonation Symposium* (Boston, Massachusetts, 1993), Naval Surface Weapons Center report NSWCDD/MP-92/456 p. 439.

IV-21. R. N. Mulford, S. A. Sheffield, and R. R. Alcon, "Intiation of Preshocked High Explosives PBX 9404, PBX 9502, and PBX 9501, Monitored With In-Material Magnetic Gauging," *High-Pressure Science and Technology—1993*, S. C. Schmidt, J. W. Shaner, G. A. Samara, and M. Ross, Eds (American Institute of Physics, New York, 1994), Part 2, p. 1405, and *Paper Summaries, Tenth International Detonation Symposium* (Boston, Massachusetts, 1993), Naval Surface Weapons Center report NSWCDD/MP-92/456, p. 415.

IV-22. A. W. Campbell, H. L. Flaugh, A. Popolato, and J. B. Ramsay, "Customized Explosives Based on Plastic-Bonded Mixtures to TATB and HMX," *Proceedings, Seventh Symposium (International) on Detonation* (Annapolis, Maryland, 1981), Naval Surface Weapons Center report NSWC MP 82-334, p. 566.

IV-23. I. B. Akst, "Heat of Detonation, the Cylinder Test, and Performance in Munitions," *Proceedings, Ninth Symposium (International) on Detonation* (Portland, Oregon, 1989), Office of the Chief of Naval Research report OCNR 113291-7, Vol. I, p.478.

IV-24. K. L. Bahl, R. D. Breithaupt, C. M. Tarver, and W. G. von Holle, "Fabry Pérot Velocimetry on Detonating LX-17 in Planar and Spherically Divergent Geometries," *Proceedings, Ninth Symposium (International) on Detonation* (Portland, Oregon, 1989), Office of the Chief of Naval Research report OCNR 113291-7, Vol. I, p. 133.

IV-25. L. G. Green, C. M. Tarver, and D. J. Erskine, "Reaction Zone Structure in Supracompressed Detonating Explosives," *Proceedings, Ninth (International) Detonation Symposium* (Portland, Oregon, 1989), Office of the Chief of Naval Research report OCNR 113291-7, Vol. I, p. 670.

IV-26. R. S. Lee, N. L. Parker, and R. C. Weingart, "Measurement of Reaction-Zone Width in TATB by Plate Jump-Off Experiments Using Visar," *Am. Phys. Soc. Bull.* **23**, 36 (1978).

IV-27. A. W. Campbell and R. Engelke, "The Diameter Effect in High-Density Heterogeneous Explosives," *Proceedings, Sixth Symposium (International) on Detonation* (Coronado, California, 1976), Office of Naval Research—Department of the Navy report ACR-221, p. 642.

IV-28. C. L. Mader, M. S. Shaw, and J. B. Ramsay, "PBX 9502 Performance," Los Alamos National Laboratory report LA-9053-MS (1981).

IV-29. W. L. Seitz, H. L. Stacy, and J. Wackerle, "Detonation Reaction Zone Studies on TATB Explosives," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSWC MP 86-194, p. 123.

IV-30. R. R. McGuire and M. Finger, "Composite Explosives for Metal Acceleration: The Effect of Detonation Temperature," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSW MP 86-194, p. 1018.

IV-31. C. L. Mader, J. Johnson, and S. L. Crane, "*Los Alamos Explosives Performance Data*," (University of California Press, Berkeley, California, 1982.)

IV-32. T. P. Liddiard, J. W. Forbes, J. W. Watt, R. N. Baker, J. Sharma, and B. C. Beard, "Recovery Technique For Shocked Explosive Samples," *Paper Summaries, Tenth International Detonation Symposium* (Boston, Massachusetts, 1993), Naval Surface Weapons Center report NSWCDD/MP-92-456, p. 508.

IV-33. K. Bahl, G. Bloom, L. Erickson, R. Lee, C. Tarver, W. von Holle, and R. Weingart, "Initiation Studies on LX-17 Explosive," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSWC MP 86-194, p. 1045.

IV-34. R. Lee, G. Bloom, W. von Holle, R. Weingart, L. Erickson, S. Sanders, C. Sletterveld, and R. McGuire, "The Relationship Between the Shock Sensitivity and the Solid Pore Sizes of TATB Powders Pressed to Various Densities," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSWC MP 86-194, p. 3.

IV-35. H. Bloom, A. Duncan, C. Honodel, R. Lee, W. von Holle, and R. Weingart, "Changes in the Particle Size Distribution of LX-17 Samples Induced by 3.5 to 11-GPa Planar Shock Waves," *Shock Waves in Condensed Matter—1987,* S. C. Schmidt and N. C. Holmes, Eds (Elsevier Science Publishers, 1988), p. 569.

IV-36. Jackson, R. K. and R. C. Weingart, "Detonation Properties of the Insensitive Explosive TATB," Lawrence Livermore Laboratory report UCRL-77755 Summary (1976).

IV-37. R. K. Jackson, L. G. Green, R. H. Barlett, W. W.Hofer, P. E. Kramer, R. S. Lee, E. J. Nidick, Jr., L. L. Shaw, and R. C. Weingart, "Initiation and Detonation Characteristics of TATB," *Proceedings, Sixth Symposium (International) on Detonation* (Coronado, California, 1976), Office of Naval Research—Department of the Navy report ACR-221, p. 756.

IV-38. R. C. Weingart, R. S. Lee, R. K. Jackson, and N. L. Parker, "Acceleration of Thin Flyers by Exploding Metal Foils: Application to Initiation Studies," *Proceedings, Sixth Symposium (International) on Detonation* (Coronado, California, 1976), Naval Surface Weapons Center report NSWC ACR-221, p. 653.

IV-39 P. K. Tang, "A Numerical Investigation of High Explosive Grain Size Effects on the Performance of Boosters," *Combust. Flame* **70**, 61 (1987), and *Proceedings, International Symposium on Pyrotechnics and Explosives,* Beijing, China, 1987 (China Academic Publishers, 1987) p. 687.

IV-40. R. W. Ashcraft and G. T. West, "Establishment of a Corner Turning Test Capability," Mason & Hanger, Silas Mason, Company, Inc., Pantex Plant report MHSMP-78-64 (1978).

IV-41. R. Avara, "PBX 9502 Corner Turning Test Fire and Data Analysis," Mason & Hanger, Silas Mason, Company, Inc., Pantex Plant report MHSMP-79-9 (1979).

IV-42. R. L. Stallings, A. G. Osborn, and G. T. West, "Corner Turning Characteristics of TATB/HMX/Kel-F Mixtures," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-83-03 (1983).

IV-43. T. L. Stallings, "TATB/HMX/Kel-F 800 Mixtures," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-84-13 (1984) (report UCNI).

IV-44. A. G. Osborn and R. W. Ashcraft, "Improving the Performance of Micronized TATB," Mason & Hanger, Silas Mason, Company, Inc., Pantex Plant report MHSMP-86-19 (1986) (report UCNI).

IV-45. A. G. Osborn, "Evaluating the Effect of Starting Material on the Firing Performance of Micronized TATB," Mason & Hanger, Silas Mason, Company, Inc., Pantex Plant report MHSMP-89-22 (1989) (report UCNI).

Iv-46. T. L. Stallings, "The Effect of HMX Particle Size on the Firing Performance of X-0433," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-90-09 (1990) (report UCNI).

IV-47. A. A. Duncan, "Correlation of TATB Powder Characteristics With the Corner Turning of PBX 9502," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-91-10 (1991) (report UCNI).

IV-48. M. Cox and A. W. Campbell, "Corner Turning in TATB," *Proceedings, Seventh Symposium (International) on Detonation* (Annapolis, Maryland, 1981), Naval Surface Weapons Center report NSWC MP 82-334, p. 624.

IV-49 L. M. Erickson, H. G. Palmer, N. L. Parker, and H. C. Vantine, "Free-Surface Velocity Measurements of Plates Driven by Reacting and Detonating RX-03-BB and PBX 9404," *Shock Waves in Condensed Matter—1981,* W. J. Nellis, L. Seaman, R. A. Graham, Eds, (American Institute of Physics, New York, 1982) p. 553.

IV-50. A. W. Campbell, "Diameter Effect and Failure Diameter of a TATB-Based Explosive," *Propellants, Explos., Pyrotech.*, **9**, 183 (1984).

IV-51. J. B. Ramsay, "Effect of Confinement on Failure in 95 TATB/5 Kel-F," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSWC MP 86-194, p. 372.

IV-52. B. W. Asay, and J. M. McAfee, "Temperature Effects on Failure Thickness and the Deflagration-to-Detonation Transition in PBX 9502," *Paper Summaries, Tenth International Detonation Symposium* (Boston, Massachusetts, 1993), Naval Surface Weapons Center report NSWCDD/MP-92/456, p. 60.

IV-53. P. W. Cooper, "A New Look at the Run Distance Correlation and its Relationship to Other Non-Steady-State Detonation Phenomena," *Paper Summaries, Tenth International Detonation Symposium* (Boston, Massachusetts, 1993), Naval Surface Weapons Center report NSWCDD/MP-92/456, p. 386.

IV-54. S. A. Sheffield, D. D. Bloomquist, and C. M. Tarver, "Subnanosecond Measurements of Detonation Fronts in Solid High Explosives," *J. Chem. Phys.* **80**, 3831 (1984).

IV-55. C. M. Tarver, A. J. Ruggerio, L. F. Fried, and D. F. Calef, "Energy Transfer in Detonation of Solid Explosives," *Paper Summaries, Tenth International Detonation Symposium* (Boston, Massachusetts, 1993), Naval Surface Weapons Center report NSWCDD/MP-92/456, p. 95.

IV-56. R. S. Lee, W. C. Tao, and L. D. Crouch, "Propagation of Detonation Waves from an Impact Region," *Proceedings, Ninth Symposium (International) on Detonation* (Portland, Oregon, 1989), Office of the Chief of Naval Research report OCNR 113291-7, Vol. 1, p. 798.

IV-57. R. S. Lee, C. A. Honodel, and R. C. Weingart, "Shock Initiation of TATB by Short-Duration Pulses," *Am. Phys. Soc. Bull.* **25**, 495 (1980).

IV-58. J. J. Dick, "Short Pulse Initiation of a Plastic-Bonded TATB Explosive," *J. Energ. Mater.* **5**, 267 (1987).

IV-59. W. L. Seitz, R. L. Rabie, and J. Wackerle, "Shock Initiation of Detonation Studies on PBX 9404 and Superfine TATB for Short Run Distances," *Am. Phys. Soc. Bull.* **24**, 722 (1979).

IV-60. M. J. Ginsberg and J. Wackerle, "Shock-Induced Decomposition of Triamino-Trinitrobenzene (TATB)," *Am. Phys. Soc. Bull.* **24**, 722 (1979).

IV-61. J. J. Dick and R. Engelke, "Reproducibility of Planewave Transit Times in Three Explosives During Initiation," *Am. Phys. Soc. Bull.* **24**, 722 (1979).

IV-62. W. L. Seitz, H. L. Stacy, R. Engelke, P. K. Tang, and J. Wackerle, "Detonation Reaction-Zone Structure of PBX 9502," *Proceedings, Ninth Symposium (International) on Detonation* (Portland, Oregon, 1989), Office of the Chief of Naval Research report OCNR 113219-7, Vol. I, p. 657.

IV-63. J. Wackerle, H. L. Stacy, and W. L. Seitz, "Velocimetry Studies on the Prompt Initiation of PBX 9502," *Paper Summaries, Tenth International Detonation Symposium* (Boston, Massachusetts, 1993), Naval Surface Weapons Center report NSWCDD/MP-92/456, p. 447.

IV-64. J. B. Bdzil, W. C. Davis, and R. R. Critchfield, "Detonation Shock Dynamics (DSD) Calibration for PBX 9502," *Paper Summaries, Tenth International Detonation Symposium* (Boston, Massachusetts, 1993), Naval Surface Weapons Center report NSWCDD/MP-92/456, p. 146, and *Phys. Fluids A* (to be published).

IV-65. D. J. Pastine and R. R. Bernecker, "P, v, E, T Equation of State for 1,3,5-Triamino-2,4,6-Trinitrobenzene," *J. Appl. Phys.* **45**, 4458 (1974).

IV-66. P. Kramer, and E. L. Demerson, "Performance and Sensitivity Testing of TATB," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant progress reports MHSMP-74-20, MHSMP-74-35 (1974), MHSMP-76-17, 76-30, 76-46, 77-52 (1976–1977), MHSMP-76-46 (1976), MHSMP-77-52 (1977), MHSMP-84-14 (1984), MHSMP-85-38 (1985).

IV-67. S. P. Marsh, Ed, *LASL Shock Hugoniot Data* (University of California Press, Berkeley, CA, 1980).

IV-68. J. J. Dick, "A Comparison of the Shock and Static Compression Curves for Four Solid Explosives," *J. Energ. Mater.* **1**, 275 (1983).

IV-69. G. I. Kerley, "Theoretical Equations of State for the Detonation Products of Explosives," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSWC MP 86-194, p. 540.

IV-70 P. K. Tang, "Modeling Hydrodynamic Behaviors in Detonation," *Propellants, Explos., Pyrotech.* **16**, 240 (1991).

IV-71. L. Green, E. Lee, A. Mitchell and C. Tarver, "The Supra-Compression of LX-07, LX-17, PBX 9404, and RX-26-AF and the Equations of State of the Detonation Products," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSWC MP 86-194, p. 587.

IV-72. J. J. Dick, C. A. Forest, J. B. Ramsay, and W. L. Seitz, "The Hugoniot and Shock Sensitivity of a Plastic-Bonded TATB Explosive PBX 9502," *J. Appl. Phys.* **63**, 4881 (1988).

IV-73. P. W. Cooper, "Shock Behavior of Explosives About the C-J Point," *Proceedings, Ninth Symposium (International) on Detonation* (Portland, Oregon, 1989), Office of the Chief of Naval Research report OCNR 113291-7, Vol. I p. 379.

IV-74. A. B. Anderson, M. J. Ginsberg, W. L. Seitz, and J. Wackerle, "Shock Initiation of Porous TATB," *Proceedings, Seventh Symposium (International) on Detonation* (Annapolis, Maryland, 1981), Naval Surface Weapons Center report NSWC MP 82-334, p. 385.

IV-75. R. Barlett, S. Cochran, L. Erickson, R. Lee, and R. Weingart, "Stress-Time Histories in Shock-Initiated TATB and PBX 9404 Explosives," *Am. Phys. Soc.Bull.* **22**, 36 (1977).

IV-76. W. D. Curtis, L. M. Erickson, R. S. Lee, and H. Vantine, "Stress and Particle Velocity Measurements on Detonating TATB," *Am. Phys. Soc. Bull.* **25**, p. 496 (1980).

IV-77. G. L. Nutt and L. M. Erickson, "Reactive Flow Lagrange Analysis in RX-26-AF," *Shock Waves in Condensed Matter—1983*, J. R. Asay, R. A. Graham, and G. K. Straub, Eds (Elsevier Science Publishers, 1984), p. 605.

IV-78. C. M. Tarver, N. L. Parker, H. G. Palmer, B. Hayes, and L. M. Erickson, "Reactive Flow Modeling of Recent Embedded Gauge and Metal Acceleration Experiments on Detonating PBX 9404 and LX-17," *J. Energ. Mater.* **1**, 213 (1983).

IV-79. C. M. Tarver. L. M. Erickson, and N. L. Parker, "Shock-Initiation, Detonation Wave Propagation and Metal Acceleration Measurements and Calculations for RX-26-AF," *Shock Waves in Condensed Matter—1983*, J. R. Asay, R. A. Graham, G. K, Straub, Eds (Elsevier Science Publishers, 1984), p. 609.

IV-80. C. A. Forest, J. Wackerle, J. J. Dick, S. A. Sheffield, and D. R. Pettit, "Lagrangian Analysis of MIV Gauge Experiments on PBX 9502 Using the Mass-Displacement Moment Function," *Proceedings, Ninth Symposium (International) on Detonation* (Portland, Oregon, 1989), Office of the Chief of Naval Research report OCNR 113291-7, Vol. I, p. 683.

IV-81. C. M. Tarver, "The Structure of Detonation Waves in Solids," *Shock Compression of Condensed Matter—1991*, S. C. Schmidt, R. D. Dick, J. W. Forbes, and D. G. Tasker, Eds (Elsevier Science Publishers, New York, 1992), p. 311.

IV-82. W. L. Seitz and J. Wackerle, "Prompt Initiation Studies of PBX 9502 and PBX 9503," Los Alamos National Laboratory report LA-UR-80-83 (1983).

IV-83. C.A. Honodel, R. S. Lee, G. W. Moody, and R. C. Weingart, "The Effect of Temperature on TATB Shock Initiation," *Am. Phys. Soc. Bull.* **27**, 485 (1982).

IV-84. W. L. Seitz, "Short-Duration Shock Initiation of Triaminotrinitrobenzene (TATB)," *Shock Waves in Condensed Matter—1983*, J. R. Asay, R. A. Graham, G. K. Straub, Eds (Elsevier Science Publishers, 1984), p. 531.

IV-85. P. A. Urtiew, L. M. Erickson, D. F. Aldis, and C. M. Tarver, "Shock Initiation of LX-17 as a Function of its Initial Temperature," *Proceedings, Ninth Symposium (International) on Detonation* (Portland, Oregon, 1989), Office of the Chief of Naval Research report OCNR 113291-7, Vol. I, p. 112.

IV-86. R. Scheloske, L. Green, and R. Weingart, "Sensitivity of Triaminotrinitrobenze (TATB) at Elevated Temperatures," Lawrence Livermore Laboratory report UCID-18336 (1980) (Distribution Limited).

IV-87. P. A. Urtiew, T. M. Cook, J. L. Maienschein, and C. M. Tarver, "Shock Sensitivity of IHE at Elevated Temperatures," *Paper Summaries, Tenth International Detonation Symposium* (Boston, Massachusetts, 1993), Naval Surface Weapons Center report NSWCDD/MP-92/456, p. 528; UCRL-JC-111337 Preprint.

IV-88. J. C. Dallman, and J. Wackerle, "Temperature-Dependent Shock Initiation of TATB-Based High Explosives," *Paper Summaries, Tenth International Detonation Symposium* (Boston, Massachusetts, 1993), Naval Surface Weapons Center report NSWCDD/MP-92/456, p. 322.

IV-89. F. McMurphy, "Cylinder Tests of HE Materials," Lawrence Livermore National Laboratory report M-118.

IV-90. R. L. Simpson, J. W. Kury, A. L. Nichols III, R. D. Breithaupt, and P. C. Crawford, "Performance Evaluation of Insensitive Explosives," Lawrence Livermore National Laboratory report UCRL-JC-106143 Preprint (1991), and *Proceedings of the Seventeenth Pyrotech Seminar*, Vol. 2, p. 824 (1991).

IV-91 D. E. Christiansen and J. W. Taylor, "HE Sensitivity Study," Los Alamos Scientific Laboratory report LA-5440-MS (1973).

IV-92. F. E. Walker, L. G. Green, and R. J. Wasley, "Critical Energy for Shock Initiation of Fuze-Train Explosives," Lawrence Livermore Laboratory report UCRL-75339 Preprint (1974).

IV-93. D. R. Hardesty and J. E. Kennedy, "Thermochemical Estimation of Explosive Energy Output," *Combust. Flame* **28**, 45 (1977).

IV-94. A. C. Campos, "Electrostatic Sensitivity of Secondary High Explosives," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-80-28 (1980).

IV-95. T. E. Larson, P. Dimas, and C. E. Hannaford, "Electrostatic Sensitivity Testing of Explosives at Los Alamos," *Proceedings, Ninth Symposium (International) on Detonation* (Portland, Oregon, 1989), Office of the Chief of Naval Research report OCNR 113291-7, Vol. II, p. 1076, and *Institute of Physics Conference Series* 118, p. 107 (1991).

IV-96. P. S. Wang and G. F. Hall, "Friction and Impact Sensitivities for High Explosives," *Minutes of the Twenty-Second Explosives Safety Seminar* (Anaheim, California, 1986), Vol. I, p. 417.

IV-97. J. W. Forbes, "Electrical Breakdown and Spark Initiation Studies of Secondary Explosives," *Am. Phys. Soc. Bull.* **25**, 496 (1980).

IV-98. E. M. Kober, A. S. Copenhaver, and J. P. Ritchie, "The Calculation of Electrostatic Interactions and Their Role in Determining the Energies and Geometries of Molecular HE Crystals, *Paper Summaries, Tenth International Detonation Symposium* (Boston, Massachusetts, 1993), Naval Surface Weapons Center report NSWCDD/MP-92/456, p. 271.

IV-99. M. J. Urizar, S. W. Peterson, and L. C. Smith, "Detonation Sensitivity Tests," Los Alamos Scientific Laboratory report LA-7193-MS (1978).

IV-100. L. W. Hantel, "Sensitivity of X-0219 to Bullet Impact," Los Alamos Scientific Laboratory report LA-5863-MS (1975).

IV-101. D. D. Sharp, "RX-26-AW/AX, RX-26-AY/AF, RX-26-AF Rifle Bullet Test," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant reports MHSMP-80-16 (1980), MHSMP-80-56 (1980), MHSMP-85-34 (1985) (report UCNI).

IV-102. J. Delistraty and H. Brandt, "Detonation Properties of 1,3,5-Triamino-2,4,6-Trinitrobenzene When Impacted by Hypervelocity Projectiles," *Propellants, Explos., Pyrotech.* **7**, 113 (1982).

IV-103. S. K. Chidester, and L. G. Green, "A Frictional Work Predictive Method for the Initiation of Solid High Explosives From Low-Pressure Impacts," *Paper Summaries, Tenth International Detonation Symposium* (Boston, Massachusetts, 1993), Naval Surface Weapons Center report NSWCDD/MP-92/456, p. 154.

IV-104. C. B. Storm, J. R. Stine, and J. F. Kramer, "Sensitivity Relationships in Energetic Materials," *Chemistry and Physics of Energetic Materials*, S. N. Bulusu, Ed (Kluwer Academic Publishers, Dordrecht, 1990), p. 605.

IV-105. D. Price and T. P. Liddiard, Jr., "The Small-Scale Gap Test; Calibration and Comparison with the Large Scale Gap Test," U.S. Naval Ordnance Laboratory report NOLTR 66-87 (1966).

IV-106. D. Price, "Gap Tests and How They Grow," *Minutes of the Twenty Second Explosives Safety Seminar* (Anaheim, California, 1986), Vol. I, p. 365.

IV-107. D. Price, "Effect of Particle Size on the Sensitivity of Porous HE," *J. Energ. Mater.* **6**, 283 (1988).

IV-108. T. P. Liddiard, J. W. Forbes, and D. Price, "Physical Evidence of Different Chemical Reactions in Explosives as a Function of Stress," *Proceedings, Ninth Symposium (International) on Detonation* (Portland, Oregon, 1989), Office of the Chief of Naval Research report OCNR 113219-7, Vol. II, p. 1235.

IV-109. T. L. Spivak, D. Betancourt, and J. H. O'Connor, "Insensitive High Explosives Gap Test Data," Naval Surface Warfare Center report NSWC TR 88-282 (1988).

IV-110 C. B. Storm and J. R. Travis, "Molecular Composition, Structure, and Sensitivity of Explosives," *Structure and Properties of Energetic Materials* (Boston, Massachusetts, 1992), D. H. Liebenberg, R. W. Armstrong, and J. J. Gilman, Eds (Materials Research Society, Pittsburgh, Pensylvania, 1993), p. 25.

IV-111. L. R. Dosser, S. Siwecki, T. M. Beckman, and T. C. Girmann, "Laser Ignition of Energetic Materials With a Pulsed Neodymium-Doped YAG Laser," *Proceedings, International Conference on Lasers* 1988 (Pub. 1989), p. 589.

IV-112. J. Sharma and F. J. Owens, "XPS Study of UV and Shock Decomposed Triamintrinitrobenzene," *Chem. Phys. Lett.* **61**, 280 (1979).

IV-113. F. J. Owens, "Molecular Studies of the Mechanism of Initiation of Energetic Materials," Report of Working Group Meeting on Detonation Phenomena, SRI, Menlo Park, CA (1979).

IV-114. F. J. Owens, "On the Possibility of the Role of Phonon Relaxation Processes in Shock Induced Chemical Reactions in Organic Solids," *Theoret. Chim. Acta* **55**, 319 (1980).

IV-115. F. J. Owens, "Molecular Orbital Calculation of Indices of Impact and Shock Induced Reactivity in Trinitroaromatic Molecules," *Shock Waves in Condensed Matter—1987*, Y. M. Gupta, Ed (Plenum Press, New York, 1988), p. 857.

IV-116. J. Sharma, J. C. Hoffsommer, D. J. Glover, C. S. Coffey, R. Santiago, A. Stolovy, and S. Yasuda, "Comparative Study of Molecular Fragmentation in Sub-Initiated TATB Caused by Impact, UV, Heat and Electron Beams," *Shock Waves in Condensed Matter—1983,* J. R. Asay, R. A. Graham, G. K. Straub, Eds. (Elsevier Science Publishers, 1984), p. 543.

IV-117. J. Sharma, C. S. Coffee, J. C. Hoffsommer, and D. J. Glover, "Study of Hot Spots in Impacted TATB Before and After Localized Ignition," *Am. Phys. Soc. Bull.* **29**, 750 (1984).

IV-118. J. Sharma, J. C. Hoffsommer, D. J. Glover, C. S. Coffey, J. W. Forbes, T. P. Liddiard, W. L. Elban, and F. Santiago, "Sub-Ignition Reactions at Molecular Levels in Explosives Subjected to Impact and Underwater Shock," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSWC MP 86-194, p.725.

IV-119. J. Sharma, J. W. Forbes, C. S. Coffey, and T. P. Liddiard, "The Physical and Chemical Nature of Sensitization Centers Left From Hot Spots Caused in Triaminotrinitrobenzene by Shock or Impact," *J. Phys. Chem.* **91**, 5139 (1987).

IV-120. J. Sharma, J. W. Forbes, C. S. Coffey, and T. P. Liddiard, "The Nature of Reaction Sites and Senstization Centers in TATB and TNT," *Shock Waves in Condensed Matter—1987*, S. C. Schmidt and N. C. Holmes, Eds (Elsevier Science Publishers, New York, 1988), p. 565.

IV-121. J. Sharma, B. C. Beard, J. Forbes, C. S. Coffey, and V. M. Boyle, "Physical and Chemical Nature of Hot Spots in TATB and HMX," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSWC MP 86-194, Vol. II, p.897.

IV-122. J. Sharma and B. C. Beard, "XPS Study of Hot Spots and Sensitization Centers in Energetic Materials," *Chemistry and Physics of Energetic Materials*, S. N. Bulusu, Ed (Kluwer Academic Publishers, Dordrecht, 1990), p. 587.

IV-123. J. Sharma, B. C. Beard, and M. Chaykovsky, "Correlation of Impact Sensitivity with Electronic Levels and Structure of Molecules," *J. Phys. Chem.* **95**, 1209 (1991).

IV-124. J. Sharma, "Chemistry of Energetic Materials Under Shock Caused via Electronic Exitations," *Shock Compression of Condensed Matter—1991*, S. C. Schmitt, R. D. Dick, J. W. Forbes, and D. G. Tasker, Eds (Elsevier Science Publishers, New York, 1992), p. 639.

IV-125. J. Sharma and B. C. Beard, "Spectroscopy of Reacted Surfaces," R*oy. Soc. London, Phil. Trans.* **A339**, 285 (1992).

IV-126. J. Sharma and B. C. Beard, "Electronic Excitations Preceeding Shock Initiation in Explosives," *Structure and Properties of Energetic Materials*, Boston, Massachusetts, 1992, D. H. Liebenberg, R. W. Armstrong, and J. J. Gilman, Eds (Materials Research Society, Pittsburgh, Pennsylvania, 1992) p. 189.

IV-127. D. Demske, N. Brazell, W. E. Farley, S. Miller, and R. Warnes, "Intense Electron Beam Detonation of TATB Explosives," *Proceedings, Ninth Symposium (International) on Detonation* (Portland, Oregon, 1989), Office of the Chief of Naval Research report OCNR 113291-7, Vol. II, p. 1131.

IV-128. N. R. Greiner, D. S. Phillips, J. D. Johnson, and F. Volk, "Diamonds in Detonation Soot," *Nature* **333** No. 6172, 440 (1988).

IV-129. N. C. Blais, N. R. Greiner, and W. J. Fernandez, "Detonation Chemistry Studies of Energetic Materials Using Laboratory Scale Samples," *Chemistry and Physics of Energetic Materials*, S. N. Bulusu, Ed (Kluwer Academic Publishers, Dordrecht, 1990), p. 477.

IV-130. B. W. Dodson, E. L. Venturini, and J. W. Rogers, Jr., "Subthreshold Generation of Free Radicals in Shock-Loaded Organic Solids," *Shock Waves in Condensed Matter—1987*, Y. M. Gupta, Ed (Plenum Press, New York, 1988), p. 897.

IV-131. A. M. Renlund and W. M. Trott, "Spectroscopic Studies of Initiation and Detonation Chemistry," *J. Phy. Colloq.* **C4** (1987) C4-179.

IV-132. A. M. Renlund and W. M. Trott, "Spectroscopic Studies of Shocked and Detonating Explosives," *Shock Waves in Condensed Matter—1987*, S. C. Schmidt and N. C. Holmes, Eds (Elsevier Science Publishers, New York, 1988), p.988.

IV-133. W. M. Trott and A. M. Renlund, "Single-Pulse Raman Scattering Study of Triaminotrinitrobenzene Under Shock Compression," *J. Phys. Chem.* **92**, 5921 (1988).

IV-134. W. M. Trott and A. M. Renlund, "Pulsed-Laser-Excited Raman Spectra of Shock-Compressed Triaminotrinitrobenzene," *Proceedings, Ninth Symposium (International) on Detonation* (Portland, Oregon, 1989), Office of the Chief of Naval Research report OCNR 113291-7, Vol. I, p. 153.

IV-135. M. F. Foltz, "Pressure Dependence of the Reaction Propagation Rate of TATB at High Pressure," *Propellants, Explos., Pyrotech.* **18**, 210 (1993).

IV.136. L. E. Fried and A. J. Ruggiero, "Energy Transfer Dynamics and Impact Sensitivity," *Structure and Properties of Energetic Materials* (Boston, Massachusetts, 1992), D. H. Liebenberg, R. W. Armstrong, and J. J. Gilman, Eds (Materials Research Society, Pittsburgh, Pennsylvania, 1993), p. 35.

IV-137. C. L. Mader and J. D. Kershner, "The Three-Dimensional Hydrodynamic Hot-Spot Model," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSWC MP 86-194, p. 42.

IV-138. P. K. Tang, J. N. Johnson, and C. A. Forest, "Modeling Heterogeneous High Explosive Burn With an Explicit Hot-Spot Process," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSWC MP 86-194, p. 52.

IV-139. D. E. Maiden, "A Hot Spot Model for Calculating the Threshold for Shock Initiation of Pyrotechnics and Explosives," *Proceedings, International Symposium on Pyrotechnics and Explosives,* Beijing, China, 1987 (China Academic Publishers 1987) p. 594.

IV-140. A. L. Nichols, C. M. Tarver, and S. K. Chidester, "Modeling Thermal Explosion and Hot Spot Growth in HMX and TATB," *Paper Summaries, Tenth International Detonation Symposium* (Boston, Massachusetts, 1993), Naval Surface Weapons Center report NSWCDD/MP-92/456, p. 358.

IV-141. A. B. Donaldson and D. O. Lee, "Comparative Thermal Behavior of HMX and TATB Base Explosives," Sandia National Laboratories report SC-DR-72-0729 (1972).

IV-142. A. B. Donaldson and D. O. Lee, "Test Results on the Effect of Heating a Confined High Explosive," Sandia National Laboratories report SLA-74-0345 (1974).

IV-143. D. O. Lee and A. B. Donaldson, "Qualitative Comparison of TATB and PBX 9404 Behavior When Preheated and Ignited Under Confinement," Sandia National Laboratories report SAND78-0561 (1978).

IV-144. E. A. Lundstrom, "A Hot Spot Variation of the Forest Fire Burn Model for Condensed Heterogeneous Explosives," *Twenty-Second International Annual Conference of ICT*, (Karlsruhe, Federal Republic of Germany, 1991) p. 8/1–8/16.

IV-145. A. Popolato, J. J. Ruminer, A. S. Vigil, N. K. Kernodle, and D. L. Jaeger, "Thermal Response of Explosives Subjected to External Heating," Los Alamos Scientific Laboratory report LA-7667-MS (1979).

V. AGING AND COMPATIBILITY

A. Introduction

When materials are aged for extended time periods (weeks or months) in close contact under confinement, they are frequently changed by decomposition or decomposition products through the influence of temperature pressure, radiation, or other external stimuli. Such changes can affect the properties and performance of the explosives and components; TATB is no exception. These changes are called compatibility problems when they affect the behavior and performance of a weapon part or component.

Aging tests have been carried out since the early 1970s in various configurations, from coupons to full-scale mockups. Decomposition and/or other reactions are usually expressed as amount of gases evolved. Pertinent results from tests with TATB, its mixtures, and other materials of interest are summarized below. Unconfined samples were run as controls and for comparison.

B. Aging Tests

The early aging (surveillance) tests were carried out by Loughran, Wewerka, Cady, and Rogers at LASL with TATB and X-0219, the materials being stored at 175 and 204°C in ampoules containing 200 torr of dry air for periods of one to eight weeks. The X-0219 survived the 175°C/2 wk test well, but it showed an 11% weight loss after 204°C/2 wk. Thus, X-0219 was deemed unsuitable for use in Plowshare applications. TATB showed similar weight loss after 204°C/2 wk.

Samples of TATB were irradiated in a ^{60}Co source by Loughran and Wewerka at LASL in 1973 at 0.26, 0.52, 2.1, 10, and 21 Mrad, then aged in ampoules under 200-torr air at 175°C for 2, 4, 8, and 16 weeks. Thermal decomposition started at lower temperature, and the rate was higher for the more highly irradiated material. These researchers also studied the use of free-radical inhibitors (quinone, anthraquinone, butene-1, and NO) to slow the decomposition rate of TATB. Results of tests at 177 and 204°C over 2 to 16 weeks under 200 torr air, butene-1, or NO indicated that none of these materials stabilized TATB.

Later in 1973, Loughran and Wewerka studied TATB, X-0219, and X-0272 formulations in long-term stability tests in ampoules in brass and aluminum Henkin cells. The Al Henkin cells had much lower TATB decomposition rates than did the brass cells in the 204°C tests. The surface of the brass cells turned dark blue, similar in appearance to the blue of copper amine complexes. After 204°C/8 wk the unconfined TATB had evolved gas at almost ten times the rate of the Al-confined material (Fig. V-1).

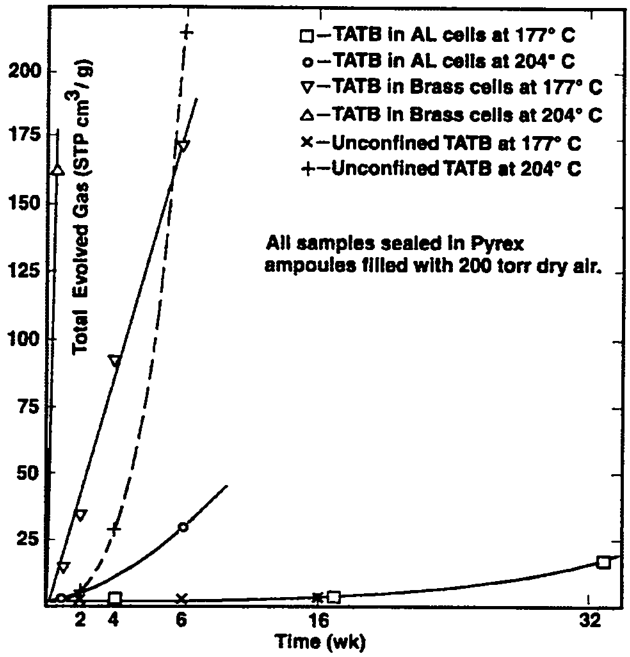

Fig. V-1. Gas evolution data for TATB after eight-weeks storage in Henkin cells at 177 and 204°C, and comparison with unconfined tests.

Maienschein, Nichols III, and Wardell at LLNL in 1993 reported on reactions of LX-17 and its combustion products with a molten metal (Nd/Fe 75/25 at %) at high temperatures.[V-1] Kinetic data taken with gas mixtures of CO and H_2O and larger-scale tests with LX-17 showed that the reactions were slow and incomplete, so there was no significant contribution to the energy release rate. The IHE was held in tantalum (Ta) vessels and instrumented with Ta thermocouples. The LX-17 preheated to between 227 to 237°C showed effective flame temperatures of 827 to 1127°C and burn rates of 0.08 to 0.11 mm/s, depending on the extent of gas confinement by molten metal. They also noted that molten metal was not oxidized, nor did it disperse when in contact with deflagrating LX-17; therefore, no significant energy release was provided above that of the deflagrating IHE. An induction time of 5 to 30 s was observed in the deflagration. The concept of effective flame temperature leads to a unique temperature for a given HE only with defined confinement conditions; for example, weak confinement, such as a layer of molten metal, is sufficient to raise the effective flame temperature by 300°C.

Results from DTA and TGA studies indicate that a detectable exothermic reaction occurs between TATB and Cu, Fe, or Zn in the 400 to 500°C temperature region at 40°C/min heating rate. Iron accelerates the decomposition rate of TATB more than does Cu or Zn, and Al and SiO_2 do not change the rate. TGA runs, at 338 and 357°C, showed that TATB evolves gaseous products at an ever-increasing rate until the TATB is completely decomposed. Neither the metals nor the initial decomposition products catalyzed decomposition of the excess TATB.

Cady at LANL found that after temperature cycling (from 4 to 77°C) for about one year, precipitated TATB had a surface area reduction from 21 m^2/g to 11 m^2/g, and that polysaccharide coating did not stabilize the TATB surface area as it had for micronized TATB. Osborn at MHSMP conducted thermal aging studies for micronized ultrafine, dry and wet TATB samples for 14 days at 90°C for the wet and 121°C for the dry samples. Results indicate a range of surface areas from 2 m^2/g to 3 m^2/g for dry- and wet-aminated TATB, and from 3 m^2/g for wet-aminated, polysaccharide-coated TATB to 5.5 m^2/g for dry-aminated, polysaccharide-coated TATB.

Pritchard at LLNL conducted a compatibility study of TATB mixtures with three binders, Estane 5702-F1, Kel-F 800, and Viton A (RX-03-AY, RX-03-AX, and RX-03-AZ, respectively) at 120°C for one, two, or four months.[V-2] Test results were analyzed by a pattern-recognition scheme. All units displayed physical changes, chemical analyses found no gross chemical changes, the primary off-gassing products from the HEs alone were H_2, N_2, and CO_2. The conclusions were that RX-03-AX and RX-03-AZ seemed to be suitable for long-term service; the decomposition of the binder in RX-03-AY cast some doubt on the long-term stability of this formulation. Additional testing was recommended.

Compatibility tests of many materials were carried out with TATB at MHSMP. For example, in 1979 Myers and Copeland carried out "coupon" tests on TATB and X-0290 in close proximity to stainless steel, aluminum, uranium alloys, and similar materials.[V-3,V-4] The coupon stacks were placed in sealed canisters and aged at elevated temperatures for 6, 12, and 18 months. The canisters were gas-sampled by CRT periodically, and the samples were tested for mechanical strength at completion of the test series. Test temperatures ranged from 50 to 100°C. The metals showed some corrosion, but suffered no effects from the chlorine impurities. Stress and strain were greater at higher test temperatures.

During the late 1970s and early 1980s, Taylor and Andrews at LANL conducted numerous materials compatibility studies and automated the data collection process for these accelerated aging tests.

In 1980, Foster of MHSMP tested glycerine and a heat-transfer fluid with TATB and RX-03-DI by DTA and CRT.[V-5] No compatibility problems were observed.

Mechanical properties of the explosives of interest were determined before and after thermal aging; results are reported in Section III. Hammon and Althouse at LLL tested bond strength and compatibility of Explostick 473 with RX-03-BB in 1976. They found no problems. Richardson of MHSMP recently studied the tensile and shear strength of glue bonds between LX-17 and Explostik 473 at 24 and 71°C.[V-6] No deterioration was found after 2 months of aging at ambient or elevated temperatures.

C. References for Section V

V-1. J. L. Maienschein, A. L. Nichols III, and J. F. Wardell, "Reactions of TATB-Based Explosive With Molten Metal," Lawrence Livermore National Laboratory report UCRL-JC-114162 Preprint (1993).

V-2. R. H. Pritchard, "Initial Compatibility Evaluation of TATB Plastic-Bonded Explosive," Lawrence Livermore Laboratory report UCRL-77897 Preprint (1976).

V-3. L. C. Myers, "PBX 9502 Coupon Test," Mason & Hanger, Silas Mason, Company, Inc., Pantex Plant report MHSMP-79-7 (1979).

V-4. R. J. Copeland, "Joint TATB/D38 Compatibility Study," Mason & Hanger, Silas Mason, Company, Inc., Pantex Plant report MHSMP-79-52 (1979).

V-5. P. A. Foster, "The Compatibility of Explosives With UCON Heat Transfer Fluid and Glycerine," Mason & Hanger, Silas Mason, Company, Inc., Pantex Plant report PXD-80-06 (1980).

V-6. B. R. Richardson, S. H. Stoner, C. M. Walkup, and M. C. Burriss, "Investigation of the Adhesive Bonding of LX-17," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-92-24 (1992) (Report UCNI, Distribution Limited).

VI. ACCIDENTS/SAFETY

A. Introduction

TATB is so insensitive to accidental ignition and initiation that it is now machined and drilled routinely without safety devices such as remote machining. However, health precautions are still necessary.

McGuire and Guarienti at LLNL summmarized the safety criteria and tests in a paper presented at the Twenty-First Explosives Safety Seminar in 1984.[VI-1] They listed the tests required to define and classify an explosive as an IHE, that is, "...explosive substances which, although mass detonating, are so insensitive that there is a negligible probability of accidental initiation or transition from burning to detonation." Corley at the Air Force Armament Laboratory (AFL) detailed IHE evaluation techniques at the same meeting.[VI-2]

The results from safety tests, such as thermal decomposition, friction, or electrical hazards are listed in Sections III and IV.

B. Drilling

Up to the time that TATB was studied for use as a production explosive, operations with HEs were carried out remotely to avoid accidents that might cause property damage and even loss of life. Urizar and Rohwer at LANL examined the drilling procedure for TATB with a view to eliminating remote handling of this insensitive HE. A test was set up to measure temperatures at the drill tip. Results of this drilling test were that the maximum temperature reached at the drill tip was 230°C. The method used by the British, an incremental drilling and withdrawing technique, would keep the drill-tip temperature even lower (Table VI-1).

TABLE VI-1. Results From Drilling Tests

Explosive/Depth	Density (g/cm^3)	Mean Maximum Temperature (°C) 3/16-in. Drill	Mean Maximum Temperature (°C) 1/16-in.Drill
X-0219/2 in. /1 in.	1.912	159	200
	1.912	72	--
X-0290/2 in. /1 in.	1.894	210	221
	1.894	167	--
TATB	1.88	114	115

C. Pressing/Machining

One pressing incident was noted at LANL. A pellet-pressing punch-and-die set failed during operation because the pressing conditions were set incorrectly. The press closed much faster than normal, causing an ultimate applied force of ~10 tons; The upper punch failed and the lower one broke; the TATB burned but did not detonate.

D. Toxicology

An extensive, in-depth toxicological study on TATB and TCB was conducted by Sasmore at SRI and published by Johnson and Cole at LLNL.[VI-3] Results from TATB dust explosions showed that TATB settled in the lungs and lymphatic system of rats, causing lung lesions, and that

TATB does not have a high explosibility index at the exposure levels of 0, 100, 1000, 2000 mg/m^3) used in these tests.

E. References for Section VI

VI-1. R. R. McGuire and R. P. Guarienti, "DOE Hazard Classification for Insensitive High Explosives (IHE)," *Minutes of the Twenty-First Explosives Safety Seminar* (Houston, Texas, 1984) Vol. I, p. 501.

VI-2. J. D. Corley, "Insensitive High Explosives Evaluation Techniques," *Minutes of the Twenty-First Explosives Safety Seminar* (Houston, Texas, 1984) Vol. I, p. 41.

VI-3. J. S. Johnson and L. A. Cole, "Ninety Day Study of Inhaled TATB and 1,3,5-Trichlorobenzene in Rats," Stanford Research Institute, Menlo Park report UCRL-15398 with Appendix (1981), and S/C 8525409.

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This compilation was begun in 1980 as a collaborative effort between B. M. Dobratz at LLNL and A. Popolato at LANL with the approval and encouragement of R. R. McGuire at LLNL and L. C. Smith at LANL. The project was put on hold in 1982 by H. L. Flaugh at LANL, because problems with TATB particle size and processing needed to be resolved. Popolato had retired, and Dobratz had become a Technical Staff Member at LANL. In 1992, J. C. Dallman asked the present author to complete this project.

I thank J. Dallman of Group DX-2 at LANL for the opportunity to write this report and for his continuing support and encouragement. I also am grateful to T. Benziger, H. Flaugh, L. Hatler, R. Rabie, J. Dick, J. Wackerle, J. Vorthman, W. Seitz, and J. Bdzil from Los Alamos, and to R. Simpson and P. Urtiew of LLNL for their helpful suggestions and candid comments.

This report can be published now, thanks to the dedication, perseverance, and skills of Wendy Burditt, Group CIC-1.

APPENDIX A. List of Organic Impurities in TATB and PBX 9502

1-Amino-3,5-dichloro-2,4,6-trinitrobenzene
1-Chloro-3,5-diamino-2,6-dinitrobenzene
1-Chloro-3,5-diamino-2,4,6-trinitrobenzene
1-Chloro-3,5-dinitro-2,4,6-triaminobenzene
1-Chloro-3,5-dinitro-2,4,6-trinitrobenzene
1,3-Diamino-5-chloro-4,6-dinitrobenzene
1,3-Diamino-5-chloro-2,4,6-trinitrobenzene
1,3-Diamino-5,6-dichloro-2,4-dinitrobenzene
3,5-Dichloro-2,4,6-trinitroaniline
1,3-Dinitro-2,4,5,6-tetrachlorobenzene
1,3-Dinitro-2,4,6-triaminobenzene
1,3-Dinitro-3,4,5-trichloroaniline
1,3-Dinitro-2,4,6-trichlorobenzene
2,4-Dinitro-3,5,6-trichloroaniline
2,6-Dinitro-3,4,5-trichloroaniline
3,5-Dinitro-2,4,6-trichloroaniline
1,3,5-Triamino-2-chloro-4,6-dinitrobenzene
1,3,5-Triamino-4-chloro-2,4-dinitrobenzene
1,3,5-Triamino-4-chloro-2,6-dinitrobenzene
1,3,5-Triamino-6-chloro-2,4-dinitrobenzene
1,3,5-Triamino-2,4-dinitrobenzene
1,3,5-Trichloro-2,4,6-trinitrobenzene
2,3,5-Trichloro-4,6-dinitroaniline
3,4,5-Trichloro-2,6-dinitroaniline
2,4,6-Trichloro-1-nitrobenzene
2,4,6-Trichloro-3,5-dinitroaniline

APPENDIX B: TEST RESULTS

TABLE B-1. Strength of TATB Mixtures at Various Temperatures and Before and After Temperature Cycling/Aging.

Formulation	Test Temp (°C)	Diametric Disk Ustre (MPa)	Diametric Disk Ustra (%)	Tensile Ustre (MPa)	Tensile Ustra (%)	Compression Ustre (MPa)	Compression Ustra (%)	Compression Tstra* (%)
TATB				5.07	0.08	13.79	2.0	
LX-17		4.32	0.37	9.11	0.38	23.42	2.24	7.44
wet aminated		4.32	0.36	10.73	0.38	23.42	2.24	7.44
+emulsion aminated		2.61	0.26	5.96	0.28	15.39	1.76	8.77
dry aminated		4.57	0.33	9.14	0.40	22.09	1.69	5.43
LX-17-0	-20	7.20	0.53	12.30	0.33			
	+55					5.29	0.5	
temperature cycled	-54					10.6	0.27	
	+21					8.7	0.29	
	+74	6.47			0.43	2.5	0.31	
PBX 9502			4.55	0.33	9.26	0.27	25-28	1.8-2.9
PBX 9502 + 0.15% Dapon M						8.48		
TATB/HMX/Estane 2/95/3	-54					50.0		
	-18					31.83		
	+24					14.53		
	+74					6.66		
71/25/4		2.84	0.33					
66/30/4		2.73	0.28					
63/27/10	-54		10.07					
	+25		9.38					
	110		0.28			8.29		
61/35/4		2.66	0.26					
46/50/4		2.50	0.19					
45/45/10	-54		12.80					
	+25		9.38					
	110		1.12			9.90		
TATB/HMX/Kel-F 63/27/10	100		1.23					
TATB/TNT/Al 40/40/20			5.10			34.66		
RX-03-BB				8.32	0.31	17.65	1.8	6.60
				9.65	0.34	20.68	2.2	
temperature cycled	+60			7.68	0.22	17.17	1.83	
	+80			7.60	0.31	16.96	2.0	
	100			7.60	0.35	15.99	2.1	
RX-03-DI				11	0.26	34.47	2.2	
RX-03-DN							17.93	2.6
RX-03-DU				6.41	0.28			

TABLE B-1. Continued

Formulation	Test Temp (°C)	Diametric Disk Ustre (MPa)	Diametric Disk Ustra (%)	Tensile Ustre (MPa)	Tensile Ustra (%)	Compression Ustre (MPa)	Compression Ustra (%)	Compression Tstra* (%)
RX-03-DY		5.11	0.10					
RX-03-EY		1.34	0.51	2.01	0.26	8.25	2.11	
RX-26-AF		2.97	0.22					
RX-03-BB				8.32	0.31	17.65	1.8	6.60
				9.65	0.34	20.68	2.2	
temperature cycled	+60			7.68	0.22	17.17	1.83	
	+80			7.60	0.31	16.96	2.0	
	100			7.60	0.35	15.99	2.1	
RX-03-DI				11	0.26	34.47	2.2	
RX-03-DN							17.93	2.6
RX-03-DU				6.41	0.28			
RX-03-DY		5.11	0.10					
RX-03-EY		1.34	0.51	2.01	0.26	8.25	2.11	
RX-26-AF		2.97	0.22					
RX-26-AF	-54			9.97	0.17	46.59	1.14	
	+21	4.36	0.24	11.28	1.54			
	+74	0.40	0.21	5.13	1.40			
X-0219	-18					34.60		
	+24					21.66		
	+49					12.4		
	+74					8.55		
X-0253 ambient						16.05		
X-0272	-18			4.77		off-scale		
	+24			5.06		off-scale		
	+49			2.41		16.07		
	+74			0.73		7.64		
X-0407	-54			7.6		43.06		
ambient				5.9		25.78		
	+72			3		12.19		
X-0433		5.65	0.30	9.92	0.17	31.96	3.05	
X-0450		2.76	0.35	4.00	0.23	16.40	2.01	

*Ustre = ultimate stress, Ustra = ultimate strain, Tstra = terminal strain

Table B-2. Temperature and Time to Explosion Data for TATB Formulations.

		Time		
Explosive	Temperature (°C)	(s)	(h)	Test
LX-17-1	235	67,464	18.79	ODTX
pressed	242	41,904	11.64	ODTX
	252	22,248	6.18	ODTX
	261	10,944	3.04	ODTX
bulk granule	255	58,320	16.2	ODTX
	265	30,312	8.42	ODTX
	276	15,624	4.34	ODTX
bulk machining waste	245	78,336	21.76	ODTX
	256	39,096	10.86	ODTX
	266	21,996	6.11	ODTX
PBX 9502	214	86,400	24.0	ODTX
ambient	245	25,416	7.06	ODTX
	251.5	20,304	5.64	ODTX
	263.3	8,995	2.50	ODTX
aged 6 mo/100°C	247.4	20,520	5.7	ODTX
	252.6	15,480	4.3	ODTX
	263.6	6,912	1.92	ODTX
aged 12 mo/100°C	239.8	27,432	7.62	ODTX
	245	21,672	6.02	ODTX
	256.3	8,424	2.34	ODTX
	259.5	6,955	1.93	ODTX
	250	138,600	38.5	LSTX
	254	198,000	55.0	LSTX
	215	64,800	18.0	ARC
heating rate 20°C/min	340	1,100	0.31	LSTX
RX-26-AF	171	49,968	13.88	ODTX
ambient	174.4	31,680	8.8	ODTX
	181	19,656	5.46	ODTX
	185	13,104	3.64	ODTX
	192	7,560	2.1	ODTX
aged 6 mo/100°C	169.4	49,176	13.66	ODTX
	177.6	24,480	6.8	ODTX
	182.3	17,064	4.74	ODTX
	188.9	7,632	2.12	ODTX
	201.5	3,384	0.94	ODTX
aged 12 mo/100°C	172.6	44,388	12.33	ODTX
	175.7	32,040	8.9	ODTX
	180.8	19,152	5.32	ODTX
	185.3	11,520	3.2	ODTX
	190	7,776	2.16	ODTX
X-0407 average	215.82	7,854.4	2.18	ARC
X-0450	177.6	31,860	8.85	ODTX
	187	14,400	4.0	ODTX
	195	6,997	1.94	ODTX
X-0541 average	207.15	3,962.3	1.10	ARC
X-0547 average	224.94	6,549.6	1.82	ARC

Table B-3. Results From CRTs Carried Out at LLNL

Explosive	Temperature (°C)	Time (h)	Total Gases (cm^3 [STP]/g)
PBX 9502	120	48	0.0 - 0.5
RX-26-AF	100	48	0.054 ± 0.008
with Rocketdyne TATB	100	96	0.065 ± 0.003
	100	144	0.075 ± 0.003
	120	24	0.089 ± 0.009
	120	48	0.128 ± 0.005
	120	96	0.202 ± 0.010
	120	144	0.267 ± 0.010
	140	24	0.297 ± 0.015
	140	48	0.473 ± 0.012
	140	96	0.857 ± 0.044
	140	144	1.205 ± 0.052
	160	24	1.712 ± 0.132
	160	48	1.284 ± 0.43
with Hercules TATB	100	48	0.009 ± 0.002
	120	24	0.022 ± 0.003
	120	48	0.034 ± 0.001
	120	96	0.068 ± 0.008
	120	144	0.116 ± 0.013
	140	48	0.155 ± 0.010
	160	48	0.791 ± 0.087
RX-26-AW	100	48	0.007 ± 0.000
	120	24	0.0136± 0.0021
	120	48	0.016 ± 0.003
	120	96	0.026 ± 0.001
	120	144	0.039 ± 0.003
	140	48	0.096 ± 0.006
	160	48	0.672 ± 0.059
RX-26-AY	100	48	0.0086± 0.0009
	120	24	0.0118± 0.0005
	120	48	0.017 ± 0.002
	120	96	0.025 ± 0.002
	120	144	0.046 ± 0.011
	140	48	0.086 ± 0.003
	160	48	0.712 ± 0.035
TATB/HMX 50/50	100	48	0.008 ± 0.000
	120	24	0.025 ± 0.003
	120	48	0.036 ± 0.005
	120	96	0.028 ± 0.001
	120	144	0.071 ± 0.004
	140	48	0.107 ± 0.025
	160	48	0.793 ± 0.101

Table B-4. Corner-Turning Test Data From MHSMP

Formulation	Density (g/cm^3)	Density %TMD	BET (m^2/g)	Temperature (°C)	Particle Type	Corner-Turning Distance (mm)
LX-17-1	1.908			+21		31.22
PBX 9502	1.886			+21		16.06
	1.886			-54		26.50
	1.875			+21		11.30
	1.875			-54		17.79
	1.869			+21		10.01
	1.869			-54		14.63
PBX 9503			2.86	+21		3.33/4.47
			1.45	+1		5.67/6.74
			0.87	+21		failed
RX-03-DI		97.84		+21		4.2
		98.15		+21		28.2
		98.46		+21		37.6
TATB/HMX/Kel-F 90/5/5	1.9403			+21	production	16.5 ± 1.0
				-54	production	25.3 ± 0.2
				+21	micronized	13.6 ± 2.1
				-54	micronized	failed
80/15/5	1.9369			+21	50/50	4.1 ± 1.0
				-16	production	6.2 ± 0.9
				-54	micronized	6.9 ± 0.6
			2.86	-54	micronized	failed
			1.45	-54	micronized	failed
			1.45	+21		failed
			0.87	-54	micronized	failed/7.8
			0.87	+21	micronized	failed
					micronized	10.2/11.3
	1.8975	98.01		-54		9.5
				+21		6.8
75.5/19.5/5	1.8956	98.00		-54		7.0
				+21		5.1
75/25/5	1.9336			+21	coarse	4.9 ± 0.5
				-54	coarse	4.9 ± 0.2
				+21	fine	1.6 ± 0.6
				-54	fine	3.0 ± 1.2
70/25/5	1.8940	98.03		-54		4.8
X-0433	1.896	97.88		+21		4.13
	1.8			+21	micronized	1
	1.8			-54	micronized	2.1
		97.90		-54		14.64
	1.800	92.89		+21		1.21
		92.91		-54		2.27

Table B-5. Corner-Turning Data For PBX 9502

Density of Test Piece	Booster Diameter	Corner-Turning Distance (mm)		Corner-Turning Radius (mm)		Volume of Radius
(g/cm^3)	(mm)	(experiment)	(model)	(experiment)	(model)	(mm^3)
Temperature -55°C						
1.870	12.0	17.94±1.26	14.30	17.46	14.80	5,800
1.870	15.0	15.80±0.93	12.88	18.12	15.96	6,500
1.883	12.0	25.17±1.66	22.04	21.19	18.90	18,300
1.886	15.0	21.74±4.48	20.64	18.12	21.22	19,300
1.900	15.0	failed, no light beyond the fifth slit				
Temperature 25°C						
1.874	9.0	15.27±0.49	12.05	13.20	10.59	3,100
1.869	13.0	10.35±0.22	7.41	14.15	12.12	1,900
1.883	9.0	18.62±0.68	16.49	16.92	12.38	5,200
1.887	13.0	13.02±0.64	11.19	14.15	13.12	3,300
1.902	9.0	failed, no light beyond third slit				
1.901	13.0	27.24±0.52	23.61	21.36	21.22	22,900
Temperature 75°C						
1.875	7.0	12.54±0.59	13.90	16.62	8.92	2,500
1.877	8.5	11.35±0.46	10.17	13.10	9.46	2,000
1.885	7.0	16.57±0.98	13.51	12.82	10.57	3,400
1.883	8.5	11.22±0.56	8.48	13.10	9.26	1,600
1.901	7.0	32.72±1.30	35.44	20.50	13.25	14,500
1.902	8.5	30.24±1.93	30.90	20.68	15.69	17,600

Table B-6. LLNL Cylinder-Test Data

Formulation	Density (g/cm^3)	Density (%TMD)	$R-R_0$ (mm)	Velocity (km/s) Wall	Velocity (km/s) Detonation
LX-17	1.900	97.90	5	1.2600	7.597
			19	1.4539	
LX-17-1	1.917	98.60	5	1.7850	7.656
			19	1.9561	
PBX 9502	1.880	97.01	5	1.7446	7.650
			19	1.9384	
RX-03-AT	1.893	97.96	5	1.7500	7.580
			19	1.9397	
RX-03-AU	1.885	97.10	19	1.4590	7.729
RX-03-DJ	1.852	97.70	19	1.4520	7.586
RX-03-DM	1.868	97.60	19	1.4590	7.662
RX-03-DY	1.846	96.80	5	1.6656	7.573
			19	1.9150	
RX-03-EI	1.885	97.80	5	1.6912	7.621
			19	1.9201	
RX-03-EJ	2.032	98.45	5	1.4909	7.440
			19	1.7505	
RX-03-EK	1.966	98.20	5	1.7732	7.537
			19	1.8065	
RX-03-EL	2.087	98.42	5	1.4378	7.349
			19	1.7234	
RX-03-EN	1.891	97.70	5	1.7093	7.591
			19	1.9309	
RX-03-EO	2.003	98.69	5	1.6173	7.070
			19	1.9466	
RX-03-ER	1.970	99.13	5	1.7043	7.369
			19	1.8156	
RX-03-EX	1.800	98.20	5	1.7162	7.501
			19	2.0345	
RX-03-EY	1.808	--	5	1.6354	7.541
			19	1.9723	

Table B-6. Continued

Formulation	Density (g/cm^3)	Density (%TMD)	R-R$_0$ (mm)	Velocity (km/s) Wall	Velocity (km/s) Detonation
RX-03-FG	1.833	98.77	5	1.6829	7.718
			19	1.9189	
RX-26-AF	1.838	98.30	5	1.8984	8.239
			19	2.1670	
RX-26-AV	1.747	89.90	19	1.3410	6.562
RX-26-AY	1.888	98.74	5	1.8578	8.247
			19	2.1806	
RX-26-BI	1.896	99.60	5	1.9640	8.217
			19	2.1872	
RX-26-BM	1.973	97.20	5	1.6216	7.407
			19	1.8342	
RX-26-BN	1.936	98.22	5	1.6956	7.852
			19	1.9670	
RX-26-BO	1.934	97.30	5	1.4979	7.108
			19	1.6774	
RX-26-BS	--	--	5	1.2711	7.099
RX-26-BV	1.907	--	no detonation		
RX-26-BW	1.880	--	5	1.2158	7.040
			19	1.4270	
RX-26-BX	1.901	--	no detonation		
RX-26-BY	1.900	--	5	1.2433	7.313
			19	1.5175	
RX-26-CA	1.772	97.85	5	1.9616	8.297
			19	2.1995	
RX-34-AE	1.880	96.76	5	1.9132	6.751
			19	2.1576	
RX-36-AI	1.817	95.38	5	1.5135	8.411
			19	1.7476	
TATB	1.800	92.88	5	1.2828	7.478
			19	1.4674	
	1.860		5	1.49	7.76

TABLE B-7. Results of LANL Drop-Weight Impact Tests With Type 12 Tooling

Explosive Composition (wt %)	Drop Height (cm)	Comments	Designation
DATB	>320		
DATB/Estane 5703/$BaCO_3$ 37/9.5/53.5	>320		X-0262
DATB/Estane/Oxamide 55.5/14.3/30.2	>320		X-0263
DATB/Sylgard 182	>320		X-0384-20
DATB/Talc/Estane 42.8/46.2/11.0	>320		
DATB/TiO_2/Estane 37.4/53/9.6	>320		
DATB/Viton 95/5	>320		X-0299
DATB recyled/DATB raw/Viton A 63.33/31.67/5	>320		
DATB/Viton A/$BaCO_3$ 35.1/14.1/50.8	>320		X-0264
TATB	>320	Cordova	
	>320	Hercules	
	>320	Livermore	
	>320	Pantex	
	>320	Rocketdyne	
	>320	Teledyne McCormick-Selph	
	>320	UTC	
	>320	Superfine	
	>320	γ-irradiated 160 h	
	>320	Bromine-treated	
	>320	Ultrafine, saccharide coated	
	>320	UV-irradiated	
TATB/acrylate binder 70/30	>320		
TATB/AN 1/9 molar ratio	211		
1/3 molar ratio	285		
TATB/AN/ADNT 1.24/1.24/1 molar ratio	111		
1.3/4/3 molar ratio	110		
TATB/Dapon M 90/10	>320	Cured PBX	
TATB/EAK 20/80	116		
TATB/Elwax/B^2 wax 94/3/3	>320		
90/5/5	>320		
TATB/Epoxy HG 18 95/5	>320		
TATB/Estane 95/5	>320		
90/10	>320		
TATB/Estane 5714-F1 95/5	>320		X-0238
TATB/Fairy Dust 90/10	>320	1:2 wt ratio	
TATB/HMX 85/15	>320		
75/25	>320		
TATB/HMX/Estane 70/25/5	>320		
5/92/3	47.9		
2/95/3	39.9		
TATB/HMX/Estane 5703 F-1 46.64/49.28/4.10	180		RX-26-AF
51/46/3	148		
43/55/2	106		
29/70/1	55.6		
TATB/HMX/Estane 5703 F-1/Dye 70/25/5/0.4	>320		X-0396
TATB/HMX/Estane/Dye 60.6/34.9/4.1/0.4	252	fine HMX	X-0450
51/46/3/0.3	130		X-0371
TATB/HMX/Kel-F 95/0.1/5	>320		PBX 9502
TATB/HMX/Kel-F/purple dye 79.8/15/5/0.2	>320		X-0351, PBX 9503
TATB/HMX/Kel-F 75/20/5	3 Es* in 25 drops at 320		X-0321
70/20/10	>320		
60/35/5	>320		X-0320
50/45/5	67.0		X-0319

TABLE B-7. Continued

Explosive Composition (wt %)	Drop Height (cm)	Comments	Designation
TATB/HMX/Kel-F 800 92.5/5/2.5	>320		X-0353
90.25/4.75/5	>320		X-0341
87.5/10/2.5	>320		X-0354
85.5/9.5/5	>320		X-0342
85/12.5/2.5	>320		X-0358
82.5/15/2.5	>320		X-0355
80.75/14.25/5	>320		X-0343
80/15/5	166		PBX 9503, X-0351
77.5/20/2.5	>320		X-0356
71.25/23.75/5	210		X-0344
70/25/5	>320		
47.5/45/7.5	80.4		X-0319
45/45/10	187		
TATB/HMX/Kel-F 800/Purple dye 80/15/5/0.5	>320		X-0351
TATB/HMX/Kel-F 800/Vivid-blue pigment 50/45/5/0.27	90.2		X-0319
/Dye 90.25/4.75/5/0.4	>320		X-0341
80.75/14.25/5/0.4	>320		X-0343
80/15/5/0.2	>320		
50/45/5/0.4	120		X-0319
TATB/HMX/Kel-F 800/Red-orange pigment 49.02/44.12/4.90/1.96	101		X-0319
/Vivid-blue pigment 45/45/10/0.27	95.5	at 150°C	PBX 9503
/Hi Viz pigment 50/45/5/0.3	111		X-0219
/Dye 79.83/14.96/5/0.2	78.8		X-0319
45/45/10/0.4	>320		PBX 9503
	135		X-0219
37.8/57/5/0.2	58.0		
19.8/70/10/0.2	74.3		
18.8/76/5/0.2	47.9		
3/91.8/5/0.2	39.9		
TATB/HMX/Kel-F 820-800 63/27/10	>320		
40/50/10	69.6		
20/70/10	53.7		
TATB/HMX/Kraton 1650 47.1/49.7/3.2	67		RX-26-AX
TATB/HMX/Kraton G-6500 70/25/5	320		
47.1/49/7/3.2	67		RX-26-AW, -AX
TATB/HMX/Kraton G-6500/Hyvac oil 70/25/2.24/2.76	>320		
51.4/46.3/1.03/1.27	172		
43/55/0.9/1.10	98.3		
29/70/0.45/0.55	56.4		
/Irganox 1010 24.32/72.97/1.3/1.4/0.03	52.7		X-0298
TATB/HMX/W/PS/DOP 6.74/6.60/85.36/0.8/0.5	>320		
TATB/$KClO_4$/Astrel-360	97.5	Proprietary	
TATB/$KClO_4$/Dapon M/$PbCrO_4$	58.0	Proprietary	
TATB/Kel-F/Cumar R-16 95/5/0.15	>320		
TATB/Kel-F 800 99.5/0.5	>320		X-0331
99/1	>320		X-0332
98/2	>320		X-0333
97.5/2.5	>320		X-0297
92.5/7.5	>320		X-0291, LX-17
90/10	>320		X-0219
95/5	>320		X-0290, PBX 9502

TABLE B-7. Continued

Explosive Composition (wt %)	Drop Height (cm)	Comments	Designation
TATB/Kel-F 800 99.5/0.5 (continued)			
95/5	>320	Thermal study from RT to 74°C	X-0290
90/10	>320		X-0219
TATB/Kel-F 800/Al 77/5/18	>320		
TATB/Kel-F 800/Dioctyl Sebacate 95/4.8/0.2	>320	wet aminated	X-0458
TATB/Kel-F 800/Oil 90/5/5	>320		
/Purple dye 80/15/5/0.5	>320		
TATB/Kel-F 3700	>320		X-0219
TATB/Kel-F 5500 95/5	>320		X-0290
TATB/Kel-F 800/Dapon-M 95/5/0.15	>320		
/Fluorolube MO-10 90/8/2	>320		
/Fluorolube LG-160 90/8/2	>320		
90/9/1	>320		
90/9.5/05	>320		
TATB/Kel-F 800/Kraton G-6500 95/5/0.2	>320		
/Lecithin 95/5/0.2	>320		
/Phenolic microballoons	>320		X-0394
/Polyethylene fibers/Selane 186-A 95/4/5/0.15	>320		X-0339
/Versamid 125 95/5/0.2	>320		
/Wax-10-200 90/8/2	>320		
TATB/Kraton 98/2	>320		X-0296
TATB/Kraton G-6500/Hivac oil 97.6/1.68/0.72	>320		X-0345
TATB/PBX 9502/Kel-F 800 66.35/30/3.5	>320	machine scrap	PBX 9502
TATB/PBX 9502/Kel-F 800 47.5/50/2.5	>320	machine scrap	PBX 9502
TATB/PETN 70/30	80.4		
TATB/PETN/Kel-F 800 75/20/5	162		
70/25/5	144		X-0407
65/30/5	58.6		
TATB/PETN/Kel-F 800/Blue dye 69.8/25.0/5.0/0.2	33.6-51.3	micronized TATB	X-0407
TATB/Phenoxy 96.9/3.1	>320		X-0329
TATB/PNF elastomer 90/10	>320		
TATB/Polysar 306 95/5	>320		X-0497
TATB/PS/Poly(phenylene oxide) 97.2/2.52/0.28	>320		X-0330
TATB/PS/DOP 94/4.5/1.5	>320		
TATB/PYX 50/50	>320		
TATB/RDX 85/15	>320		
80/20	>320		
75/25	>320		
TATB/RDX/acrylate 70/30 (90/10)	>320		
TATB/RDX/acrylate 70/30 (70/30)	2 Es* in 12 drops at 320		
TATB/Ta/Kel-F 800 65.2/31.0/3.8	>320		
TATB/TNT 99.9/0.1	>320		
60/40	1 E* in 9 tests at 320		
50/50	2 Es* in 9 tests at 320		
40/60	288		
30/70	269		
20/80	177		
10/90	150		
TATB/TNT/Al 40/40/20	6 Es* in 17 tests at 320		
/Kel-F 800 94.9/0.1/5	>320		

TABLE B-7. Continued

Explosive Composition (wt %)	Drop Height (cm)	Comments	Designation
TATB/Vibrathane 5003 98/2	>320		X-0219
95/5	>320		X-0219
TATB/Vistalon 404 95/5	>320		X-0498
TATB/Vistanex Tufflo 6026/D32 Microballoons 86/12/2	>320		
TATB/W/PS/DOP 13.46/85.24/0.8/0.5	>320		
TCTNB	1 E* in 25 drops at 320		

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*E=Event

TABLE B-8. Results of LLNL Drop-Weight Impact Tests

Explosive Composition (wt %)	Drop Height (cm)	Comments	Designation
DATB/HMX/Viton 20/70/10	64	5 kg, ρ = 1.83-1.86	LX-03-0
TATB/BTF 50.6/49.4	44		RX-36-AB
TATB/BTF/NH_4ClO_4 36.42/2.50/61.08	21	TMD 1.944	RX-34-AD
31.99/10.0/58.01	22	TMD 1.941	RX-34-AG
TATB/Estane 5702 F-1 97/3	>177	TMD 1.946, MHSMP	RX-03-AJ
TATB/Estane 5702 F-1 94/6	>177	TMD 1.866	RX-03-AE
TATB/HMX 46.6/53.4	63		RX-36-AF
TATB/HMX/BTF 15.2/69.9/14.4	54		RX-36-AC
TATB/HMX/BTF 58.6/22.4/46.0	68		RX-36-AD
TATB/HMX/BTF/Viton 14.44/66.40/14.16/5.0	53	TMD 1.9053	RX-36-AI
TATB/HMX/Kraton 48/48/4	>112		RX-03-DA
TATB/HMX/Kraton/Vistanex 48/48/2/2	>177		RX-03-DD
TATB/Kel-F 800 97.5/2.5	>177		RX-03-BC
95/5	>177	14% <20 micron	RX-03-AR
	>177	TMD 1.940, ρ = 1.70	RX-03-AU
92.5/7.5	>177	TMD 1.944, ρ = 1.89-1.94	RX-03-BB
91/9	>177	TMD 1.946, superfine, slurry	RX-03-AH
90/10	>177	TMD 1.946, ρ = 1.92, MHSMP	RX-03-AB, X-0219
TATB/Kel-F 800/Al 74/6/20	161	TMD 2.067	RX-03-EJ
83.25/6.75/10	161	TMD 2.008	RX-03-EK
64.75/5.25/30	161	TMD 2.129	RX-03-EL
55/4.5/40	161	TMD 2.196	RX-03-EM
TATB/Kel-F 800/AP/Al 74.0/6.0/12.4/7.6	145	TMD 1.981	RX-03-ER
TATB/Kraton/Tufflo Oil 95.13/3.24/1.63	>177	TMD 1.833	
TATB/Phenoxy PKHJ 96.3/3.7 RX-03-DI	>177	TMD 1.893 ρ = 1.848	
TATB/TNT 95/5	>177		RX-03-DH
TATB/Viton A 95.5/4.5	>177	14% <20 micron	RX-03-AT
A 91/9	>177	TMD 1.927, MHSMP	RX-03-AF

Table B-9. Gap-Test Results For TATB and TATB Formulations

Explosive Name or Composition	Density (g/cm^3)	Voids (%)	50% Point (mm)	Test	Reference	Comments
		in Dural				
TATB	1.7		0 to 0.025	S	LANL	50µ**
	1.7		0.042	S	LANL	20µ
	1.7		0.025 to 0.051	S	LANL	5µ
	1.881	2.9	22.78	L	LANL	
TATB/HMX/Estane 2/95/3	1.841	54.07		L	LANL	
TATB/HMX/Kel-F 800 90.25/4/75/5	1.907	1.7	26.24	L		
85.5/9.5/5	1.905	1.7	37.16	L		
80.75/14.24/5	1.898	2.0	43.23	L		
75.25/23.75/5	1.893	2.1	43.51	L		
TATB/$KClO_4$ 95/5	1.905	2.9	22.6	L	LANL	
90/10	1.924	3.0	22.28	L	LANL	regular
90/10	1.923	3.1	19.81	L	LANL	blm***
TATB/Kel-F 800 95/5	1.895	2.4	22.33	L		
X-0219	1.920		14.73	L*	LANL	
	1.880	2.5	46.91	L	LANL	
X-0319	1.897	1.5	47.19	L	LANL	
	1.883	2.2	48.74	L	LANL	
	1.850	3.9	52.86	L	LANL	
X-0320	1.881	2.4	46.74	L	LANL	
X-0321	1.881	2.7	42.85	L	LANL	
X-0341	1.884	2.89	29.40	L	LANL	RT
X-0343	1.879	2.94	42.88	L	LANL	RT
X-0351	0.88		no reaction	L	LANL	
X-0407	1.860	2.225		L	LANL	
		in brass				
PBX 9502	1.895	2.4	6.8	M	LANL	+80°C
	1.895	2.4	3.38	M	LANL	RT
	1.845	5.0	9.2	M	LANL	
	1.894	2.47	2.57	L	LANL	-75°C
RX-03-BB	1.906		2.0	M	MHSMP	
	1.900		1.73	M	MHSMP	RT
	1.887		2.36	M	MHSMP	2 mo/100°C
	1.888		2.22	M	MHSMP	8 mo/100°C
	1.893		1.91	M	MHSMP	4 mo/80°C
	1.894		2.41	M	MHSMP	8 mo/100°C
	1.899		2.16	M	MHSMP	8 mo/60°C
	1.858		±4.7	M	MHSMP	cycl30d -50 +92°C
	1.851		4.95	M	MHSMP	cycl150d -50+92°C
	1.848		5.46	M	MHSMP	cycl250d-50 +92°C
RX-03-DI	1.847		1.95	M	MHSMP	
TATB	1.883		5.17	M		
	1.865	3.8	0.127	S	LANL	prod
	1.750	9.7	0.36	S	LANL	1.5% Cl superfine
	1.700		0.38	S	LANL	13µ
	1.700		0.36	S	LANL	0.2% Cl
	1.700		0.38	S	LANL	~20µ, 0.15% Cl
	1.700		0.05	S	LANL	fine
	1.600	17.4	0.36	S	LANL	1.5% Cl superfine

Table B-9. Continued

Explosive Name or Composition	Density (g/cm^3)	Voids (%)	50% Point (mm)	Test	Reference	Comments
TATB (continued)	1.200	38.1	0.20	S	LANL	1.5% Cl superfine
	1.000	48.4	0.13	S	LANL	superfine
	0.777	60.0	0.13	S	LANL	superfine
TATB/HMX/Estane5/92/3	1.839	1.6	2.057	S	LANL	
2/95/3	1.803	3.5	3.632	S	LANL	
TATB/PYX 50/50	1.760	4.9	1.2	S	LANL	
X-0219	0.777	60.0	0.13	S	LANL	superfine
	1.000	48.4	0.13	S	LANL	superfine
	1.200	38.1	0.20	S	LANL	superfine
	1.502	22.5	0.38	S	LANL	superfine
	1.702	12.2	0.36	S	LANL	superfine
	1.801	7.1	0.41	S	LANL	superfine
X-0290	1.894	2.5	4.57	1-in.	LANL	
	1.895	2.4	4.17	1-in.	LANL	
	1.895		2.34	1-in.	LANL	-78°C
	1.895		3.78	1-in.	LANL	+25°C
	1.895		5.54	1-in.	LANL	+80°C
X-0297	1.880	3.1	5.79	1-in.	LANL	
X-0407	1.859		1.6	S	LANL	
		in aluminum				
TATB/TNT/Al 40/40/20	1.90	0.7	31.3	L	LANL	
	1.870	2.3	34.39	L	LANL	
X-0329	1.856	2.3	17.6	L	LANL	

* L - LSGT (41.275 mm), M - PXGT (24.5 mm),
S - SSGT (12.7 mm)

** µ - particle size

*** blm - ball milled

APPENDIX C. BIBLIOGRAPHY

General

B. M. Dobratz and P. C. Crawford, "LLNL Explosives Handbook, Properties of Chemical Explosives and Explosive Simulants," Lawrence Livermore National Laboratory report UCRL-52997 Change 2 (1985).

B. T. Federoff, O. E. Sheffield, and S. M. Kaye, "Encyclopedia of Explosives and Related Items," U.S. Army Research and Development Command report PATR 2700, Vols. 1-10 (1960-1983).

C. Gaudin, R. Ousset, and R. Teissier, "Insensitive High Explosives," *International Annual Conference of ICT* (Karlsruhe, Federal Republic of Germany, 1982), p. 391.

T. R. Gibbs, and A. Popolato, "*LASL Explosive Property Data,*" (University of California Press, Berkeley, 1980).

D. Haishan, "Properties and Technology of High Explosives," *Chengdu Baozha Yu Chongji* (Explosions and Shock Waves) No. 3, (1982), 86.

L. C. Smith, "Explosives Research and Development, Recommendations and Comments On Unsolved Problems," Los Alamos Scientific Laboratory report LA-8124-MS (1979).

T. Urbanski, "Heat Resistant Explosives," in *Chemistry and Technology of Explosives*, Vol. 4, (Pergamon Press, New York, 1984), Ch. 7.

T. Urbanski and S. K. Vasudeva, "Heat Resistant Explosives," *J. Sci. Ind. Res.* **37**, 250 (1978).

Synthesis: Laboratory Scale

Z. L. Estes, "Chlorine Free Synthesis of TATB," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-77-24 (1977).

Z. L. Estes, "Trichloronitrosobenzene - A Raw Material for TATB Synthesis," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-77-25 (1977).

M. K. Hadhoud, S. A. Shokry, A. K. El Morsi, and S. Ragab, "Study of Kinetics and Analysis of the Amination of Pentanitroaniline to Produce TATB," *Seventeenth International Annual Conference of ICT* (Karlsruhe, Federal Republic of Germany, 1986), paper 54/1 to 18.

M. E. Hill, "Large Scale Laboratory Preparation of 1,3,5-Trinitro-2,4,6-Tribromobenzene," U.S. Naval Ordnance Laboratory report NAVORD 3709 (1953).

S. A. Shokry, S. K. Shawki, and A. K. El Morsi, "TATB Plastic-Bonded Compositions," *Twenty-First International Annual Conference of ICT* (Karlsruhe, Federal Republic of Germany, 1990) paper 100/160.

R. J. Spear and W. S. Wilson, "Recent Approaches to the Synthesis of High Explosive and Energetic Materials: A Review," *J. Energ. Mater.* **2**, 61 (1984).

Y. Wei, "Preparation of 1,3,5-Triamino-2,4,6-Trinitrobenzene," *Yingyong Huakue* **7**, 70 (1990).

Synthesis: Large-/Pilot Plant-Scale

S. Calsson and H. Schmid, "High-Energy Explosives and Their Manufacturer," Nobelkrut AB, SE Pat. Appl. 90/3,724 (1990), EUR Appl. EP 487, 472 (1992).

I. J. Dagley, R. P. Parker, L. Montelli, and C. N. Loneys, "Mixed High Explosives for Insensitive Booster Compositions," Materials Research Laboratory, Australia report MRL-TR-92-22 (1993).

D. Double and R. P. Bright, "Chemically Bonded Ceramic Armor With Embedded Explosive Charges," Cemcom Corp., U.S. Pat. Appl. 72,501 (1987). EUR Pat. Appl. EP 299, 253 (1989).

A. A. Duncan, "Inter- and Intra-Laboratory Sieve Analysis of TATB," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-77-43 (1977).

A. A., Duncan, "TATB Interlaboratory Sieving Study," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-83-09 (1983).

Z. L. Estes and J. G. Locke, "Pilot Plant Synthesis of TCTNB From Trichloronitrosobenzene," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-78-27 (1978).

G. L. Flowers, "Characterization of Binders Used in High Explosives and the Effect of Binder Strength on Impact Sensitivity of Explosives," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-85-42 (1985) (report UCNI).

H. Kerviel and P. Charrue, "Explosive Powders and Their Manufacture," Commissariat a l'Energie Atomique, FR Pat. Appl. 91/441 (1991), EUR Pat. Appl EP 495, 714 (1992).

B. Li, "Plastic-Bonded Explosive Based on Bis(β,β,β-Trinitroethyl-N-Nitro)Ethylenediamine," *Baozha Yu Chongji* **8**, 261 (1988).

J. G. Locke and R. W. Ashcraft, "Sparger Aminated TATB Progress Report," Mason & Hanger, Silas, Mason, Company, Inc., Pantex Plant report MHSMP-89-34 (1989) (report UCNI).

J. G. Locke, "Amination of Trichlorotrinitrobenzene Using a Ring Sparger," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-80-45 (1980).

J. G. Locke, "Continuous Amination of TCTNB to TATB," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-90-06 (1990) (report UCNI).

J. G. Locke, "Low Chlorine TATB Produced by Emulsion Amination," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-80-14 (1980).

J. G. Locke and W. T. Quinlan, "Thermal Purification of TATB Containing Chloronitrobenzenes," Mason & Hanger Silas Mason Company, Inc., Pantex Plant report MHSMP-82-3 (1982).

J. G. Locke, "Sparger Aminated TATB Fraction Factorial Experiment," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-83-37 (1983) (report UCNI).

J. G. Locke, "Synthesis of Fine Particle TATB by a Wet-Amination Process," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-89-34 (1989) (report UCNI).

J. G. Locke and R. W. Ashcraft, "Sparger Aminated TATB Progress Report," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-82-37 (1982).

J. G. Locke and Z. L. Estes, "Emulsion Amination of TCTNB," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-78-26 (1978).

Preparation: TATB Formulations

R. W. Ashcraft, "A Mathematical Model for Oven Drying of LX-17," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-85-18 (1985) (report UCNI).

J. A. Crutchmer, "Mechanical Pressing Study of Several Explosives," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-89-17 (1989) (report UCNI).

J. D. Harrell, "A Study for Pressing LX-17 Explosive," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-82-45 (1982).

R. D. Harold, "PBX Binders, "Allied Signal Aerospace Company," Kansas City Division report KCP-613-4224 (1989).

H. D. Johnson, A. G. Osborn, and T. L. Stallings, "TATB PBX Formulations," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-76-5 (1976).

P. D. Lunney and R. W. Ashcraft, "Moisture Sorption in Pressed LX-17-0: Thermodynamic Equilibrium and Transport Properties," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-84-25 (1984) (report UCNI).

G. W. Neff, "Holston-Pantex LX-17 Formulation Comparison," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-81-38 (1981).

A. G. Osborn, "LX-17-1 Processing Variables Experiment," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-87-08 (1987).

T. W. Stull and J. Sandoval, "Moisture Retardation of Micronized TATB Pellets Through Parylene Coating," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-80-43 (1980).

Analyses

R. W. Ashcraft, "Numerical Method for Titration End Point Determination," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-75-40 (1975).

A. J. Bailey, M. Bellerby, and S. A. Kinloch, "The Identification of Bonding Agents for TATB/HTPB Polymer Bonded Explosives," *Phil. Trans. Soc. London* **A339**, 321 (1992).

C. C. Blair, "Analysis of Chloride in TATB by X-Ray Fluorescence. Progress report October to December 1975," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-76-5 (1976).

N. E. Chisum, "Applications of Negative Ion Analyses on the Elan 250 ICP-SM," *At. Spectrosc.* **12**, 155 (1991).

G. L. Clink, "^{13}C FT-NMR Analysis of the Isolated By-Products of TATB," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-80-37 (1980).

G. L. Clink, "Carbon-13 NMR Identification of the Amination Products of the 1,3,5-Trichlorotrinitrobenzene TATB Substrate," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-83-30 (1983) (report UCNI).

G. L. Clink, "Fluorine-19 NMR Analysis of the Kel-F 800 Polymer System: The Quantitative Determination of the Perfluorodecanoate Emulsifier Content," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-83-41 (1983) (report UCNI).

G. L. Clink, "Fluorine-19 NMR Evidence for the Molecular Stability of Kel-F 800 in the Presence of TATB and Its Congeners," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-84-29 (1984) (report UCNI).

G. L. Clink, "An NMR Procedure for the Analysis of the Ammonium Content of TATB," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-75-54 (1974).

N. J. Dosanjh and D. A. J. Wase, "Oxygen Uptake Studies on Various Sludges Adapted to Waste Containing Chloro-, Nitro-, and Amino-Substituted Xenobiotics," *Water Res.* **21**, 205 (1987).

B. D. Faubion and C. C. Blair, "Chloride Analysis of TATB," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-75-20 (1975).

C. S. MacDougall, "Assay of TCTNB for T4CDNB and TCDNB," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-76-17 (1976).

C. S. MacDougall, "Liquid Chromatographic-Spectrophotometric Assay for TATB in TATB," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-77-18 (January–March 1977).

J. M. Poyet, M. Vignaud, and H. Prigent, "Use of Exclusion Chromatography for the Control of Inert and Explosive Compositions," Spectra 2000, **122**, 47 (1987).

J. Sandoval, "Titrimetric Determination of Water in TATB Using Karl Fischer Reagent," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-80-59 (1980).

C. L. Schaffer, "Compositional Analysis of PBX 9503 - A TATB/Kel-F Formulation," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-81-55 (1981).

C. L. Schaffer, "Compositional Analysis of RX-28-AF - A TATB/HMX/Estane PBX," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-80-61 (1980).

C. L. Schaffer, "Determination of Inorganic Chlorides in TATB/Kel-F 800 Explosives," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-83-40 (1983). (report UCNI).

C. L. Schaffer, "Kel-F Analysis in LX-17," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-84-53 (1984) (report UCNI).

C. L. Schaffer, "Quantitative Analysis of TATB Impurities by Thin Layer Chromatography," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-83-06 (1983).

C. L. Schaffer, "Recrystallization of TATB for Analytical Standard," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-80-03 (1980).

C. L. Schaffer, and W. T. Quinlin, "HPLC Assay Methods for TATB," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-85-62 (1985) (report UCNI).

C.-S. Tan, C. W. Wong, and B.-S. Chen, "Separation of Toluene-Trichlorobenzene Mixture With CO_2 At Elevated Pressures," *Separation Sci. Tech.* **26**, 1245 (1991).

A. C. Teter, "The Analysis of TATB/Phenoxy Formulations by HSLC," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-79-39 (1979).

A. C. Teter, "Synthesis and Isolation of Byproduct Impurities in TATB," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-84-16 (1984). (report UCNI).

R. D. Worley, "Fluorescence X-Ray Analysis for Chlorine in TATB," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-79-57 (1979).

Properties: Chemical and Physical

H. H. Billon and M. A. Parry, "The Viscosity of TATB Types A and B Suspensions in Molten TNT: General Characteristics," Materials Research Laboratory, Australia report MRL-TR-91-24 (1991).

J. L. Bredas, C. Dehu, F. Meyers, and J. Zyss, "Theoretical Insight Into the Quadratic Nonlinear Optical Response of Organics: Derivatives of Pyrene and Triaminotrinitrobenzene," *Proceedings, Nonlinear Optical Properties of Organic Materials IV*, K. D. Sweer, Ed, (SPIE-International Society for Optical Engineering, San Diego, California, 1991) p. 98.

J. L. Bredas, F. Meyers, B. M. Pierce, and J. Zyss, "On the Second-Order Polarizability of Conjugated π-Electron Molecules With Octupolar Symmetry: the Case of Triaminotrinitrobenzene," *J. Amer. Chem. Soc.* **114**, 4928 (1992).

J. L. Bredas and F. Meyers, "Conjugated Organic Molecules with Octupolar Symmetry: Novel Compounds With Large Quadratic Nonlinear Optical Properties," Special Publication - Royal Society of Chemistry 1993, p. 129.

B. L. Deopura and V. D. Gupta, Vibrational Spectra of 1,3,5-Triamino-2,4,6-Trinitrobenzene, *J. Chem. Phys.* **54**, 4013 (1971).

V. D. Gupta and B. L. Deopura, Low Frequency Neutron Spectrum of 1,3,5-Triamino-2,4,6-Trinitrobenzene, *Mol. Phys.* **19**, 589 (1970).

P. C. Hariharan, W. S. Koski, J. J. Kaufman, and R. S. Miller, AB Initio MODPOT/VRDDO/MERGE Calculations on Energetic Compounds. III. Nitroexplosives: Polyaminopolynitrobenzenes (Including DATB, TATB, and TETRYL), *Int. J. Quant. Chem.* **23**, 1493 (1983).

M. Joffre, Yaron, R. J. Silbey and J. Zyss, "Second-Order Optical Nonlinearity in Octupolar Aromatic Systems," *J. Chem. Phys.* **97**, 5607 (1992).

J. M. Leclercq, E. Lavenir, J. Leclercq, J. Boileau, S. Odiot, and M. Blain, "Molecular Structure of Aromatic Nitro Derivatives. IV. The Singlet Electronic States of 1,3,5-Triamino-2,4,6-Trinitrobenzene (TATB) in D_{3h} Symmetry," *Propellants, Explos., Pyrotech.* **9**, 201 (1984).

M. H. Miles, D. Gustavson, and K. L. DeVries, "Stress-Induced Radical Generation in TATB," *J. Mater. Sci.* **18**, 3243 (1983).

M. H. Miles and K. L. DeVries, "Molecular Decomposition of Polymeric Binders and Energetic Materials," *Ind. Eng. Chem. Prod. Res. Dev.* **23**, 304 (1984).

L. C. Myers and C. C. Blair, "An Investigation of the Crystallinity of Kel-F, Viton, and Estane," Mason & Hanger, Silas Mason, Inc., Pantex Plant report MHSMP-76-17 (1976).

L. C. Myers and H. D. Johnson, "An Investigation of Binder Crystallinity on the Mechanical Properties of a Plastic-Bonded Explosive," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-877-5 (1976).

H. S. Nalwa, T. Watanabe, and S. Miyata, "A Comparative Study of H-Nitroaniline, 1,5-Dinitrobenzene and 1,3,5-Triamino-2,4,6-Trinitrobenzene and their Molecular Engineering for Second Order Nonlinear Optics," *Opt. Mater.* **2**, 73 (1993).

A. M. O'Connell, A. I. Rae, and E. N. Maslen, "A Discussion of the Distribution of Bonded Electron Density," *Acta Crystallogr.* **21**, 208 (1966).

M. D. Pace, "A Review of Paramagnetic Resonance Products in Condensed Phase Energetic Materials," *Proceedings, Ninth Symposium (International) on Detonation* (Portland, Oregon, 1989), Office of the Chief of Naval Research report OCNR 113291-7, Vol. II, p. 987 (1989).

R. P. Parker, "Establishment of A Super Small-Scale Cookoff Bomb (SSCB) Test Facility at MRL," Material Research Laboratory, Australia report MRL-TR-89-9 (1989).

W. E. Patterson, "Hydrostatic Density Determination of High Explosive Parts," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-92-19 (1992) (report UCNI).

G. Vergoten, G. Fleury, M. Blain, and S. Odiot, "Molecular Structure of Aromatic Nitro Derivatives. 5. Vibrational Spectra and Normal Coordinate Analysis of 1,3,5-Triamino-2,4,6-Trinitrobenzene," *J. Raman Spectrosc.* **16**, 143 (1985).

J. J Wolff, S. F. Nelson, P. A. Petillo, and D. R. Powell, "Structures of Tris(Donor)-Tris(Acceptor)-Substituted Benzenes. I. Steric, Polar, and Hydrogen-Bonding Effects in Triaminotrinitrobenzene," *Chem. Ber.* **124**, 1719 (1991).

Properties: Mechanical

J. E. Field, S. J. P. Palmer, P. H. Pope, R. Sundararajan, and G. M. Swallowe, "Mechanical Properties of PBX's and Their Behaviour During Drop Weight Impact," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSW MP 86-194, p. 635.

J. E. Field, M. A. Parry, S. J. P. Palmer, and J. M. Huntley, "Deformation and Explosive Properties of HMX Powders and Polymer Bonded Explosives," *Proceedings, Ninth Symposium (International) on Detonation* (Portland, Oregon, 1989), Office of the Chief of Naval Research report OCNR 113291-7, Vol. II; p. 886.

H. D. Johnson, "Mechanical Properties of [a] TATB/Kel-F 800 Formulation," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-76-7 (1976).

H. D. Johnson, "Thermal Growth and Mechanical Properties of RX-03-BB," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-76-17 (1976).

L. C. Myers and H. D. Johnson, "An Evaluation of a Mechanical Property Test for Small Samples of Plastic Bonded Explosives," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-76-30 (1976).

L. C. Myers and H. D. Johnson, "An Investigation of the Effect of Binder Crystallinity On the Mechanical Properties of a Plastic Bonded Explosive," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-77-05 (1977).

A. G. Osborn, "Evaluation of Low Growth TATB PBX Using Water-Aminated TATB," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant, report MHSMP-85-08 (1985) (report UCNI).

A. G. Osborn, R. W. Ashcraft, and T. L. Stallings, "The Effect of Pressing Conditions on RX-03-EY Physical Properties," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-89-26 (1989).

A. G. Osborn, J. A. Crutchmer, N. O. Rhoton, and C. L. Brasher, "Evaluation of Ultrafine TATB Processing Variables," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-85-27 (1985) (report UCNI).

E. Patzak, "Shear, Tensile, and Compressive Stress Behavior of Plastic-Bonded Explosives," *Proceedings, International Annual Conference of ICT* (Karlsruhe, Federal Republic of Germany, 1982), p. 447.

B. R. Richardson, S. H. Stoner, C. M. Walkup, and M. C. Burris, "Investigation of the Adhesive Bonding of LX-17-1," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-92-24 (1992) (report UCNI).

D. G. Sullivan, J. R. Anthony, and R. W. Ashcraft, "High Explosive Lathe Machining Modeling Program," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-91-16 (1991) (report UCNI).

Properties: Thermal

T. B. Brill, P. J. Brush, K. J. James, J. E. Shepherd, and K. J. Pfeiffer, "T-Jump/FT-IR Spectroscopy: A New Entry into the Rapid, Isothermal Pyrolysis Chemistry of Solids and Liquids," *Appl. Spectrosc.* **46**, 900 (1992).

T. B. Brill and K. J. James, "Thermal Decomposition of Energetic Material. 61. Perfidy in the Amino-2,4,6-Trinitrobenzene Series of Explosives," *J. Phys. Chem.* **97**, 8752 (1993).

T. B. Brill and K. J. James, "Kinetics and Mechanisms of Thermal Decomposition of Nitroaromatic Explosives," *Chem. Rev.* 2667 (1993)

T. B. Brill and J. E. Shepherd, "Interpretation of Time-To-Explosion Tests," *Paper Summaries, Tenth International Detonation Symposium* (Boston, Massachusetts, 1993), Naval Surface Weapons Center report NSWCDD/MP-92/456 p.307.

J. M. Brosse, C. Kassel, C. Michaud, and S. Poulard, "Laboratory Scale Sensitivity Testing of Insensitive High Explosives," *Proceedings, Seventh Symposium (International) on Detonation* (Annapolis, Maryland, 1981), Naval Surface Weapons Center report NSWC MP 82-334, p. 965.

J. Cao, "Critical Shock Initiation Problem of PBX 9404 and TATB in Diverging Geometry," *Baozha Yu Chongji* **6**, 350 (1986).

C. Castille, E. Germain, and R. Belmas, "Physical Origin of Hot Spots in Pressed TATB Explosive Compositions," *Propellants, Explos., Pyrotech.* **17**, 249 (1992).

C. Castille, D. Banville, P. Raynier, and T. Belmas, "Experimental Study and Numerical Modeling of Thermal Ignition and Combustion of High Heterogeneous Explosives," Paper Summaries, *Ninth Symposium (International) on Detonation* (Portland, Oregon, 1989), p.1070.

J. F. Cau, "On the Use of Electromagnetic Velocity Gauges in Explosives," *Proceedings, Tenth International Detonation Symposium* (Boston, Massachusetts, 1993), Naval Surface Weapons Center report NSWCDD/MP-92/456, p. 470.

F. Chaissé, J. M. Servas, J. Aveillé, J. Baconin, N. Carion, and P. Bongrain, "A Theoretical Analysis of The Shape of a Steady Axisymmetrical Reactive Shock Front in Cylindrical Charges of High Explosive. A Curvature--Diameter Relationship," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSWC MP 86-194, p. 159.

H. Cherin, "Influence of Microstructure on Explosive Compositions Sensitivity," *Paper Summaries, Tenth International Detonation Symposium* (Boston, Massachusetts, 1993), Naval Surface Weapons Center report NSWCDD/MP-92/456, p. 150.

J. M. Chevalier, N. Carion, J. C. Protat, and J. C. Redasse, "Propagation Phenomena on the Detonation Wave Front," *Paper Summaries, Tenth International Detonation Symposium* (Boston, Massachusetts, 1993), Naval Surface Weapons Center report NSWCDD/MP/92/456, p. 71 and *Phys, Rev. Lett.* **71**, 712 (1993).

R. Chirat and J. Baute, "An Extensive Application of WCA Equation of State for Explosives," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSWCDD/MP 86-194, p. 751.

R. Chirat and G. Pittion-Rossillon, "A Theoretical Equation of State for Detonation Products: Application to Twelve CHNO Explosives," *Combust. and Flame* **45**, 147 (1982).

J. A. Crutchmer "Skid Sensitivity of Large-Scale Sensitive Pole Billets," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-82-34 (1982).

P. Deneuville, C. Gaudin, Y. de Longueville, and J. Mala, "Comparison of TATB and DINGU Explosive Properties," *Proceedings, Seventh Symposium (International) on Detonation* (Annapolis, Maryland, 1981), Naval Surface Weapons Center report NSWC MP 82-334, p. 540.

G. Eden and R. A. Belcher, "The Effects of Inert Walls on the Velocity of Detonation in EDC35, an Insensitive High Explosive," *Proceedings, Ninth Symposium (International) on Detonation* (Portland, Oregon, 1989), Office of the Chief of Naval Research report OCNR 113291-7, p.831.

G. Eden, R. A. Belcher, M. I. Andrew, and W. R. Marlow, "Frozen Hot Spots" in Shocked EDC35, An Insensitive High Explosive," *Proceedings, Ninth Symposium (International) on Detonation* (Portland, Oregon, 1989), Office of the Chief of Naval Research report OCNR 113291-7, Vol. II, p.1253.

K. K. Feng, W. K. Chung, and B. C.-Y. Lu, "Calculation of Detonation Products By Means of The Cs Hard-Sphere Equation of State," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSWC MP 86-194, p. 805.

V. M Gerasimov, V. A. Gubachev, V. A. Vakin, I. E. Plaksin, and V. I. Shutov, "Initial Phase of Formation of Detonation Wave In Solid Explosive Substances During Multiple Initiations," *Khim. Fiz.* **12**, 734 (1993).

A. P. Glazkova and Yu. A. Kazarova, "Self-Inhibition During TATB Combustion," *Fiz. Gozeniya* **28**, (6) 37 (1992) (trans. Combust, Expl, Shock Waves **28**, 605), and *Proceedings, Twenty-Third International Annual Conference of ITC* (Karlsruhe, Federal Republic of Germany, 1992) p. 67/1 to 67/9.

D. Grief, S. H. Ward, and G. D. Coley, "Run to Detonation in TATB," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSWC MP 86-194, p.380.

Y. He and D. Jing, "The Shape of Detonation Front and the Detonation Velocity," S. C. Schmidt, J. W. Shaner, G. A. Samara, and M. Ross, Eds (High Pressure Science and Technology, American Institute of Physics, New York, 1994), Part 2, p. 1365.

M. Held, "Corner-Turning Distance and Detonation Radius," *Propellants, Explos., Pyrotech.* **14**, 153 (1989).

M. Hertzberg, K. L. Cashdollar, I. A. Zlochower, and G. M. Green, "Explosives Dust Cloud Combustion," *Proceedings Twenty-Fourth Symposium (International) on Combustion* (The Combustion Institute, Pittsburgh, Pennsylvania, 1992), p. 1837.

F. Hosoya, K. Shiino, and K. Itabashi, "Electric Spark Sensitivity of Heat-Resistant Polynitroaromatic Compounds," *Propellants, Explos., Pyrotech* **16**, 119 (1991).

F. Hosoya, Y. Wada, K. Shuno, T. Wainai, K. Stabaski, M. Tamura, and T. Yoshida, "Synthesis of Heat-Resistant Nitro-compounds and their Estimation of Explosibility IV. The Under-Water Small Scal Gap Test and the Electric-Spark Test of Poynitro-Compounds," *Kogio Kayaku* **53**, 14 (1992).

Y. K. Huang and A. L. Arbuckle, "A Semi-Analytical Approach to Shock Initiation in Heterogeneous Explosives," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weaons Center report NSWC MP 86-194, p. 943.

C. D. Hutchinson, "The Initiation of TATB-Based Insensitive High Explosives in Diverging Geometry," *Twenty-First International Annual Conference of ITC* (Karlsruhe, Federal Republic of Germany, 1988), 38/1 to 38/10.

C. D. Hutchinson, "Experimental Studies Condemning the Response of Intermediate Explosives to Thermal Stimuli," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSWC MP 86-194, p. 1105.

C. D. Hutchinson, G. C. W. Foan, H. R. Lawn, and A. G. Jones, "Initiation and Detonation Properties of the Insensitive High Explosive TATB/Kel-F 800 95/5," *Proceedings, Ninth Symposium (International) on Detonation* (Portland, Oregon, 1989), Office of the Chief of Naval Research report OCNR 11329-7, Vol. II, p. 123.

G. H. Johansson and P. A. Persson, "Density and Pressure in the Chapman-Jouguet Plane as Functions of Initial Density of Explosives," *Nature* **212**, 1230 (1966).

B. D. Lambourn and D. C. Swift, "Application of Whitham's Shock Dynamics Theory to the Propagation of Divergent Detonation Waves," *Paper Summaries, Tenth International Detonation Symposium* (Boston, Massachusetts, 1993), Naval Surface Weapons Center report NSWCDD/MP-92/456, p. 784.

H. H. Licht, "Performance of Castable IHE Formulations," Institute Franco-Allemanddes Recherches report ISL-CO-217/88 (1988).

J. Liu, J. Jia, X. Ji, X. Jiang, and D. Ding, "A Study of SDDT Behavior of Several Insensitive Explosives," *Proceedings, Seventeenth International Pyrotechnic Seminar* (1991) Vol. 2, p. 780.

L. C. Myers, "X-0290 Coupon Test," Mason & Hanger, Silas Mason, Company, Inc., Pantex Plant report MHSMP-77-11 (1977).

M. Nicollet, R. Beluas, J. P. Plotard, B. Udiment, and M. Leroy, "Initiation of a Mixed TATB/HMX Composition by Single and Double Shocks, Propellants," *Explos., Pyrotech.* **18**, 128 (1993).

V. I. Pepekin and Yu. A. Lebedev, "Criterion for Evaluating the Detonation Parameters in Explosives," *Dokl. Akad. Nauk, SSSR*, **234**, (6) 1391 (1977) (trans. p. 630).

M. Pinègre, J Aveillé, M. Leroy, J. C. Protat, R. Chéret, and N. Camarcat, "Expansion Isentropes of TATB Compositions Released Into Argon," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSWC MP 86-194, p.815.

D. Pirotais, J. P. Plotard, and J. C. Braconnier, "Numerical Simulation of Jet Penetration of HMX and TATB Explosives," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSWC MP 86-194, p. 337.

S. A. Shackelford, "Mechanistic Relatioships of the Decomposition Process to Combustion and Explosion Events From Kinetic Deuterium Isotope Effect Investigations," *Chemistry and Physics of Energetic Materials*, S. N. Bulusu Ed., (Kluwer Academic Publishers, Dordrecht, 1990) p. 433.

H. Shi and D. Jing, "Global Calibration of Constitutive Relationships in Explosive Reaction Zone," *Proceedings, Ninth Symposium (International) on Detonation* (Portland, Oregon, 1989), Office of the Chief of Naval Research report OCNR 113291-7, p. 252.

E. V. Shorokhov and B. V. Litvinov, "Shock Compressibility of the TATB-Based Explosive Composition in the Pressure Range from 0.1 to 40 GPa," *Proceedings, Thirteenth AIRAPT International Conference on High Pressure Science and Technology* (1991) (Pub. 1992), p. 866, and *Khim. Fiz.* **12**, 722 (1993).

T. L. Stallings, "The Effect of HMX Particle Size on the Firing Performance of X-0433," Mason & Hanger, Silas Mason Company, Inc., Pantex Plant report MHSMP-90-09 (1990) (report UCNI).

A. Stolovy, A. I. Nameson, J. B. Aviles, Jr., E. C. Jones, and J. M. Kidd, "Exothermal Reactions in TATB Initiated by an Electron Beam," *J. Chem Phys.* **78**, p. 229

A. Stolovy, A. I. Namenson, J. B. Aviles, Jr., E. C. Jones, Jr., and J. M. Kidd, "Thermal Initiation of High Explosives by Electron Heating," *J. Energ. Mater.* **5**, 181 (1987).

J. Vanpoperynghe, J. Sorel, J. Aveille, and J. C. Adenis, "Shock Initiation of TATB and HMX Explosive Compositions," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSWC MP 86-194, p. 892.

J. Vanpoperynghe, J. Sorel, and H. C. Pujols, "Experiments and Numerical Simulation of High Explosive Delayed and Lowed Detonation," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSWC MP 86-194, p. 135.

F. Volk, "Detonation Products of Cast High Explosives," *Proceedings, Thirteenth International Pyrotechnic Seminar* (1988) p. 835.

F. E. Walker, "Correlation Between Reaction Dynamics Experiments and the Detonation of Explosives," *Propellants, Explos., Pyrotech.* 15, 190 (1990).

Y. Wei and P. Zheng, "The Divergence and Transmission of Detonation Wave. I. The TATB/HMX Boosters," *Proceedings, Seventeenth International Pyrotechnic Seminar* (1991) Vol. 2, p. 864.

W. Xiong, "A Method for Evaluating the Detonation Performance and the Metal Accelerating Ability of Explosives," *Proceedings, International Symposium on Pyrotechnics and Explosives* (Beijing, China, 1987), D. Jing Ed. (China Academic Publishers, 1987), p. 707.

G. Yuxian, P. Guoshu, S. Jialiang, X. Laibin, W. Aigin, and Z. Quangin, "The Detonation Reaction of Heterogeneous Composite Explosive," *Proceedings, Eighth Symposium (International) on Detonation* (Albuquerque, New Mexico, 1985), Naval Surface Weapons Center report NSWC MP 96-194, p. 1011.

Y. Zhang, L. Mi, M. Wang, and J. Zhang, "Research of Metal Jet to Penetrate and Initiate the Explosive," *Baozha Yu Chongji* **10**, 345 (1990).

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