

Supporting Information

Fast explosive performance prediction via small dose energetic materials based on time-resolved image combined with machine learning

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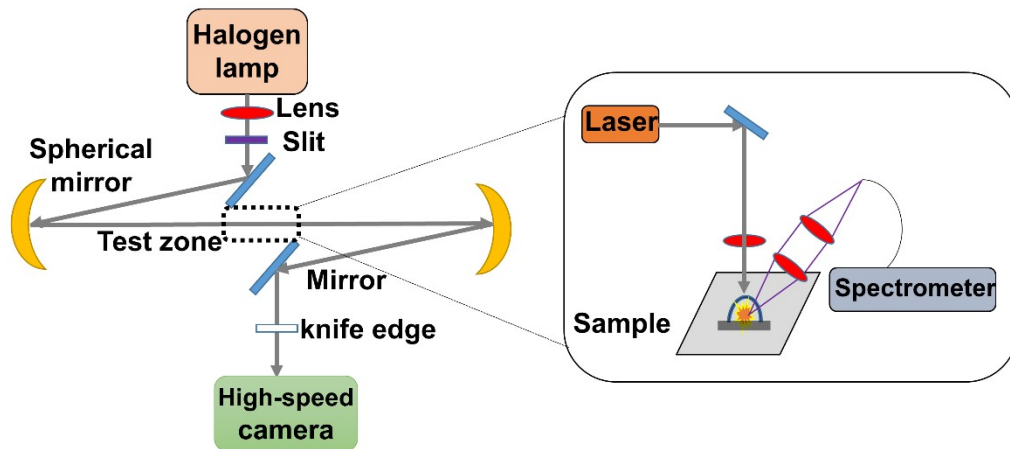
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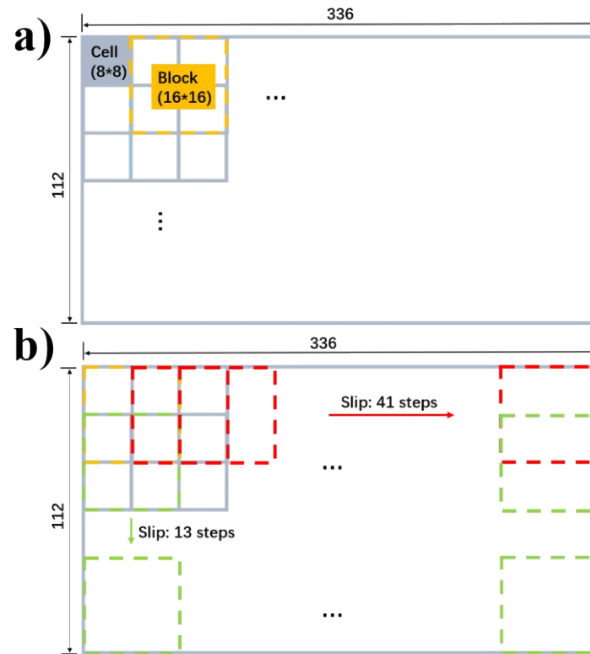
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Supplementary Figure 1. Configuration for high-speed schlieren imaging and spectrum system.



Supplementary Figure 2. Schematic diagram of image HOG feature extraction.

Supplementary Table 1. EMs information and calculated detonation parameters list.

Abbreviation /Formula	Sample number	Chemical name	Crystal Density $\rho(\text{g}/\text{cm}^3)$	DV (m/s)	HoD (-kJ/kg)	VoD (dm^3/k)	DP (GPa)	DT (k)
CL-20	D1	Hexanitrohexaazaisowurtzitane	2.038 ^a	9604	6234	732	46	4103
HMX	D2	Cyclotetramethylene tetranitramine	1.905 ^a	9193	5700	763	38	3646
RDX	D3	Cyclotrimethylene trinitramine	1.800 ^a	8818	5768	816	35	3749
TNT	D4	Trinitrotoluene	1.654 ^a	6824	4427	633	19	3222
FOX-7	D5	1,1-Diamino-2,2-dinitroethylene	1.756 ^a	8266	4588	791	28	3209
TATB	D6	Triaminotrinitrobenzene	1.940 ^a	8201	3858	670	28	2756
LLM-105	D7	2,6-Diamino-3,5-dinitropyrazine- 1-oxide	1.913 ^a	8498	4396	701	31	3137
DNAN	D8	2,4-Dinitroanisole	1.556 ^a	6174	3649	617	18	2835
NTO	D9	3-nitro-1,2,4-triazol-5-one	1.931 ^a	8479	3755	720	30	2854
1H-T	D10	Tetrazole	1.520 ^a	7656	3486	841	20	2595
5-AT	D11	Aminotetrazol	1.500 ^a	7525	2582	890	18	2069
DAT	D12	1,5-diaminodiazole	1.590 ^a	8386	2856	917	23	2120
1-MAT	D13	1-methyl-5-aminotetrazole	1.750 ^a	8632	1637	846	24	1408
H2BT	D14	Bistetrazole	1.740 ^a	8315	3715	779	25	2860
H2BTA	D15	N,N-bis-(1(2)H-tetrazol-5-yl) amine	1.860 ^a	9076	3321	806	30	2487
H2BTM	D16	Ditetrazolomethane	1.680 ^a	7794	2890	769	21	2235
H2BTE	D17	Ditetrazelethane	1.490 ^a	6720	2338	772	14	1877
C ₄ H ₇ N ₉ O ₃	D18	Ammonium N-(5-(5-amino- 1,2,4-oxadiazol-3-yl)-3H-1,2,4- triazol-3-yl) nitramidate	1.769 ^b	8324	3907	815	26	2767
C ₅ H ₁₀ N ₁₂ O ₃	D19	Aminoguanidinium N-(5-(5- amino-1,2,4-oxadiazol-3-yl)-3H- 1,2,4-triazol-3-yl)nitramidate	1.703 ^b	8136	3471	835	24	2503
C ₅ H ₈ N ₁₄ O ₃	D20	1,5-diamino-tetrazolium N-(5-(5- amino-1,2,4-oxadiazol-3-yl)-3H- 1,2,4-triazol-3-yl) nitramidate	1.763 ^b	8471	4192	812	27	2977
C ₄ H ₉ N ₁₁ O ₅	D21	Diammonium N-(5-(5- (nitramino)-1,2,4-oxadiazol-3- yl)-3H-1,2,4-triazol-3-yl) nitramidate	1.765 ^b	8433	4050	845	27	2867

C ₄ H ₁₁ N ₁₃ O ₅	D22	Dihydrazinium N-(5-(5-(nitramino)-1,2,4-oxadiazol-3-yl)-3H-1,2,4-triazol-3-yl) nitramidate	1.783 ^b	9018	4798	878	32	3146
C ₄ H ₉ N ₁₁ O ₇	D23	Dihydroxylammonium N-(5-(5-(nitramino)-1,2,4-oxadiazol-3-yl)-3H-1,2,4-triazol-3-yl) nitramidate	1.866 ^b	9135	5199	812	35	3414
C ₆ H ₁₉ N ₂₁ O ₅	D24	Di(triaminoguanidinium) N-(5-(5-(nitramino)-1,2,4-oxadiazol-3-yl)-3H-1,2,4-triazol-3-yl) nitramidate	1.676 ^b	8835	4471	905	28	2887
C ₆ H ₁₁ N ₂₁ O ₅	D25	Di(1,5-diamino-tetrazolium) N-(5-(5-(nitramino)-1,2,4-oxadiazol-3-yl)-3H-1,2,4-triazol-3-yl) nitramidate	1.786 ^b	8822	4677	833	30	3262
C ₄ H ₄ N ₈ O ₃	D26	N-(5-(5-amino-1,2,4-oxadiazol-3-yl)-3H-1,2,4-triazol-3-yl) nitramide	1.878 ^b	8484	4202	736	29	3055
C ₄ H ₃ N ₉ O ₅	D27	N-(5-(5-(nitramino)-1,2,4-oxadiazol-3-yl)-3H-1,2,4-triazol-3-yl) nitramide	1.924 ^b	9087	5317	727	36	3795

^a Density derived from CCDC. ^b Density measured by BUILD-2200 densitometer.

Supplementary Table 2. Model assessment parameters.

Targets	Model Index	R ²	MRETr	ARETr	RMSETr	MRETe	ARETe	RMSETe
Detonation Velocity	(1)	0.9851	1.45%	1.07%	88.32 m/s	3.00%	1.68%	159.97 m/s
	(2)	0.9851	1.45%	1.08%	89.27 m/s	4.79%	1.77%	194.49 m/s
	(3)	0.9866	1.46%	1.04%	86.98 m/s	3.09%	1.65%	158.21 m/s
	(4)	0.9880	1.46%	1.06%	88.06 m/s	3.02%	1.23%	138.35 m/s
	(5)	0.9861	1.45%	1.10%	90.23 m/s	3.48%	1.41%	150.32 m/s
Heat of Detonation	(1)	0.9885	7.66%	3.60%	-132.96 kJ/kg	6.68%	4.09%	-177.84 kJ/kg
	(2)	0.9907	7.67%	3.24%	-125.50 kJ/kg	6.62%	4.25%	-185.97 kJ/kg
	(3)	0.9882	7.65%	3.29%	-125.96 kJ/kg	6.85%	4.79%	-200.30 kJ/kg
	(4)	0.9871	7.66%	3.65%	-134.04 kJ/kg	7.01%	4.49%	-203.36 kJ/kg
	(5)	0.9899	7.66%	3.48%	-129.73 kJ/kg	7.80%	4.15%	-194.01 kJ/kg
Volume of Detonation	(1)	0.9891	1.43%	1.16%	9.06 dm ³ /k	3.90%	1.19%	13.30 dm ³ /k
	(2)	0.9878	1.41%	1.14%	8.86 dm ³ /k	3.20%	1.47%	14.41 dm ³ /k
	(3)	0.9814	1.40%	1.13%	8.73 dm ³ /k	5.61%	1.58%	18.15 dm ³ /k
	(4)	0.9894	1.42%	1.15%	8.99 dm ³ /k	3.58%	1.29%	12.83 dm ³ /k
	(5)	0.9936	1.39%	1.12%	8.66 dm ³ /k	1.73%	0.78%	8.40 dm ³ /k
Detonation Pressure	(1)	0.9898	6.82%	3.63%	0.92 GPa	6.75%	2.63%	0.87 GPa
	(2)	0.9920	6.81%	3.63%	0.93 GPa	5.53%	2.18%	0.78 GPa
	(3)	0.9919	6.30%	3.56%	0.91 GPa	4.73%	1.68%	0.66 GPa
	(4)	0.9917	6.67%	3.26%	0.85 GPa	4.36%	2.72%	0.87 GPa
	(5)	0.9911	6.45%	3.55%	0.91 GPa	5.37%	2.41%	0.82 GPa
Detonation Temperature	(1)	0.9846	5.14%	2.71%	72.43 K	7.70%	4.17%	142.26 K
	(2)	0.9912	4.56%	2.64%	71.01 K	4.65%	2.74%	90.62 K
	(3)	0.9865	5.02%	2.68%	71.81 K	5.81%	3.60%	123.85 K
	(4)	0.9884	4.96%	2.70%	72.43 K	6.08%	3.47%	109.29 K
	(5)	0.9847	4.77%	2.63%	70.93 K	7.20%	4.00%	136.07 K