

Supplementary Materials

Macrocycle as a “Container” for Dinitramide Salts

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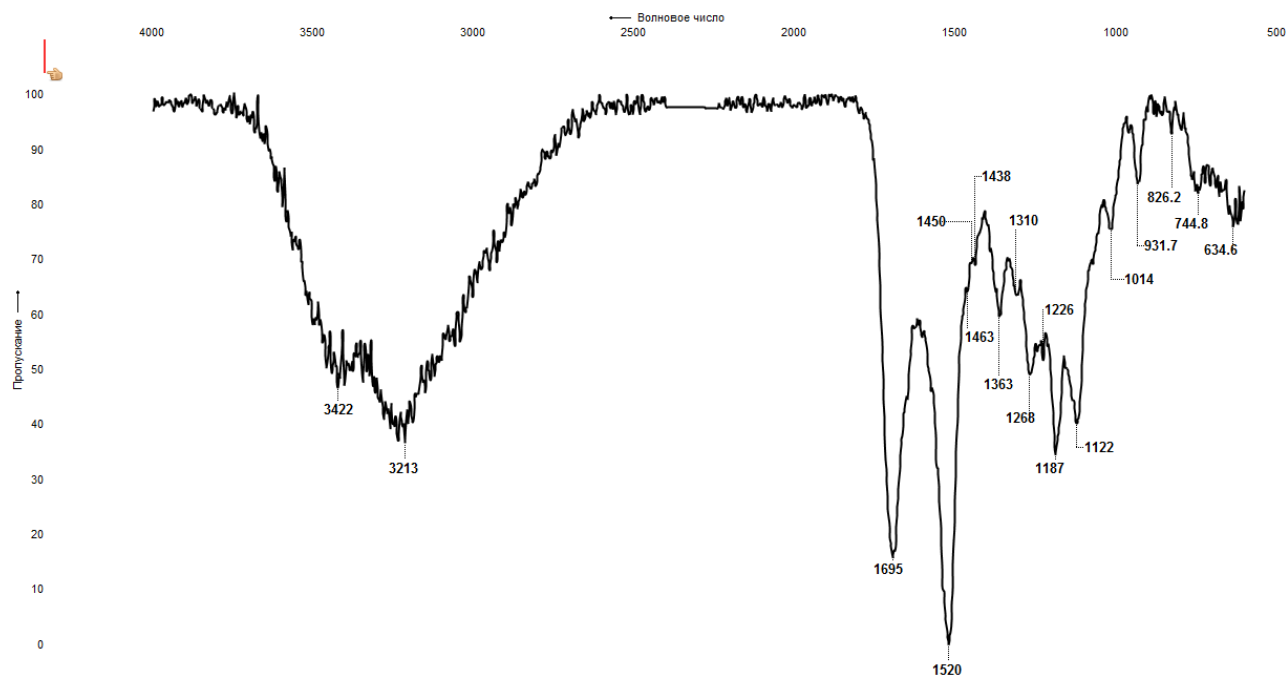


Figure S1. IR spectrum of **7**

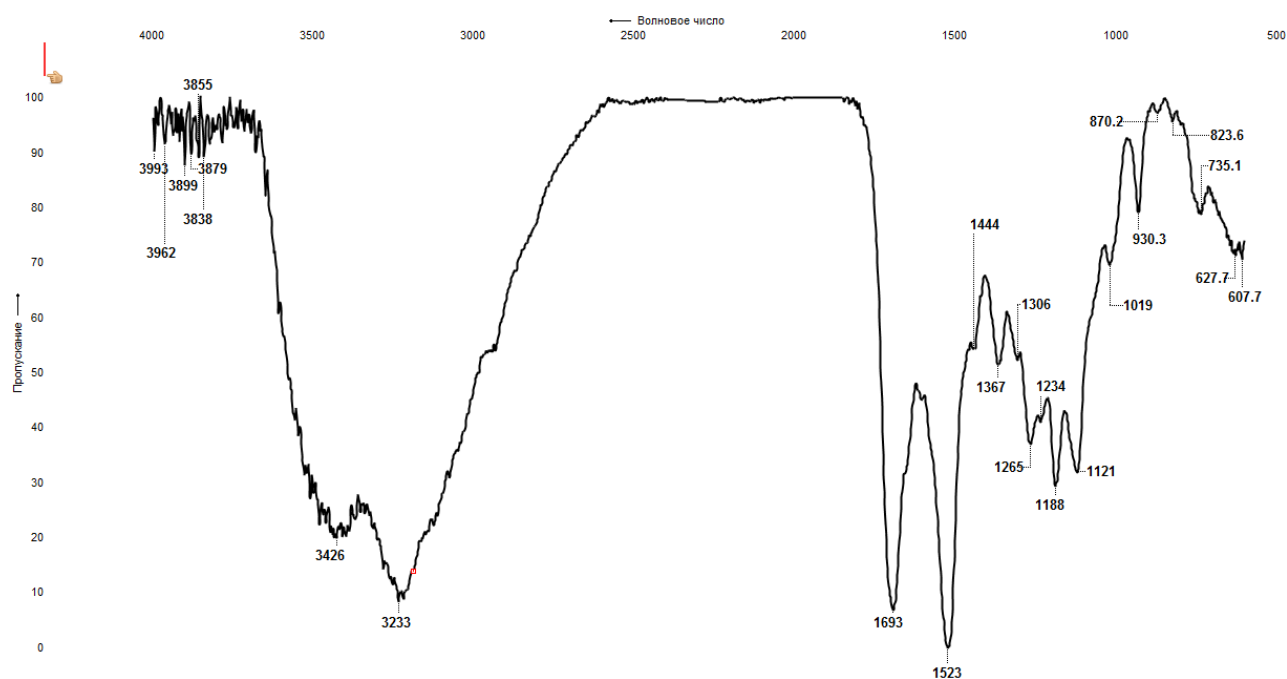


Figure S2. IR spectrum of **8**

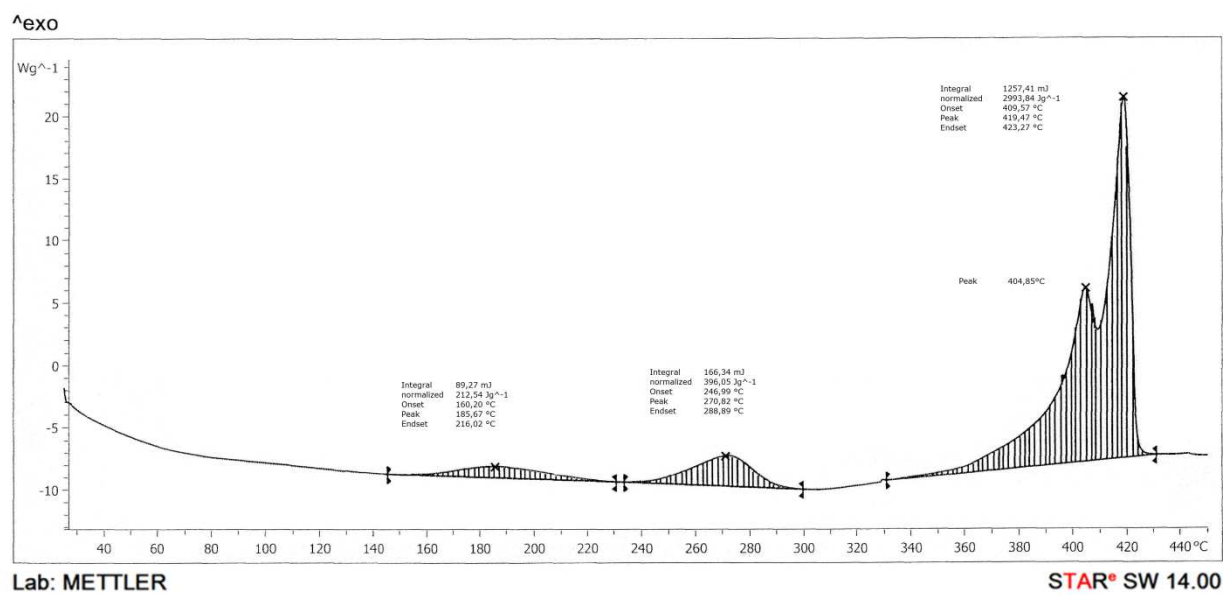


Figure S3. DSC of 7

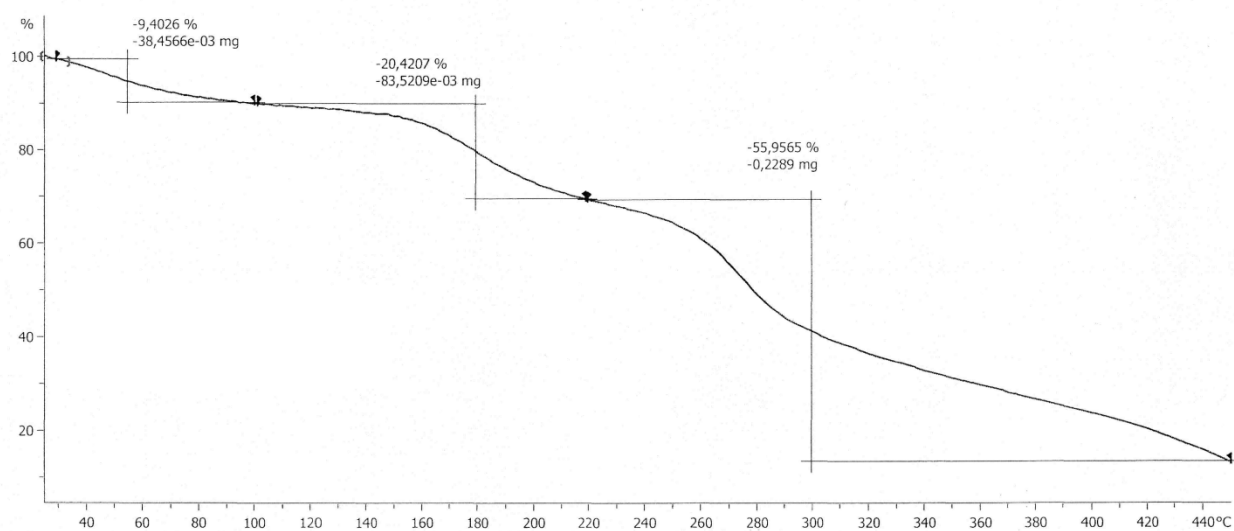


Figure S4. TGA of 7

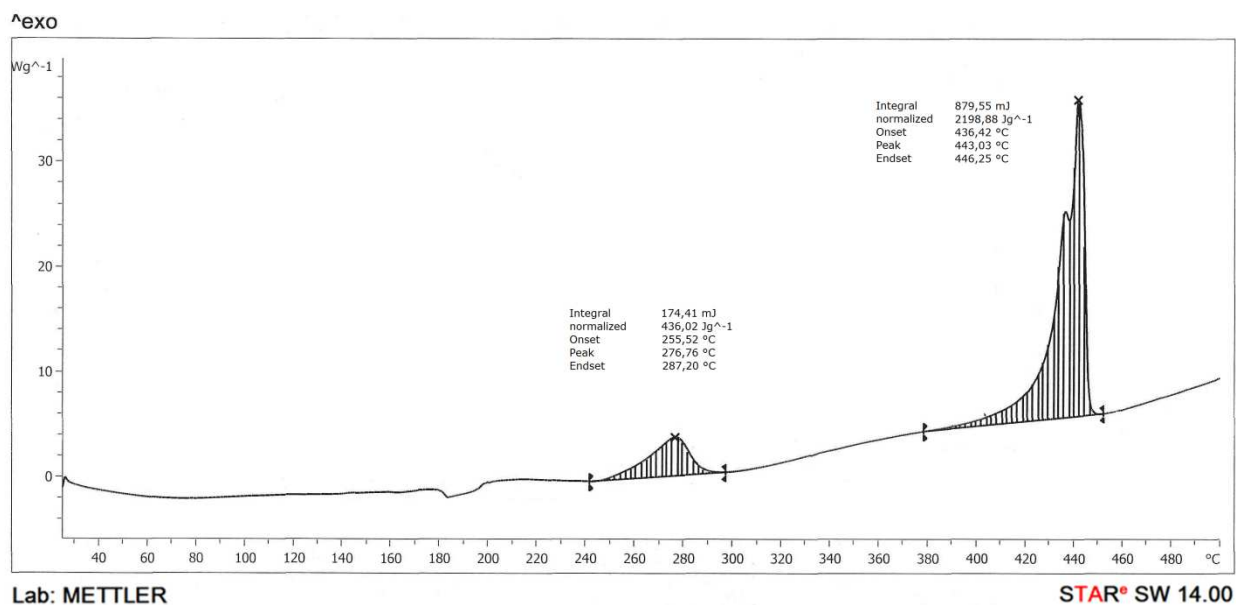
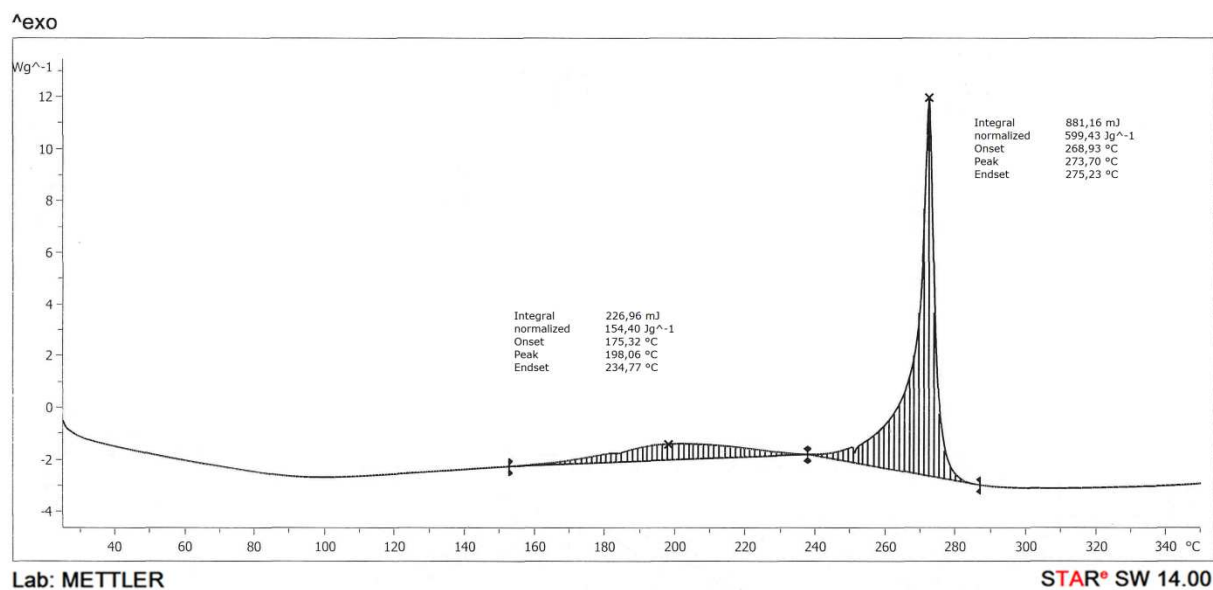


Figure S5. DSC of 8

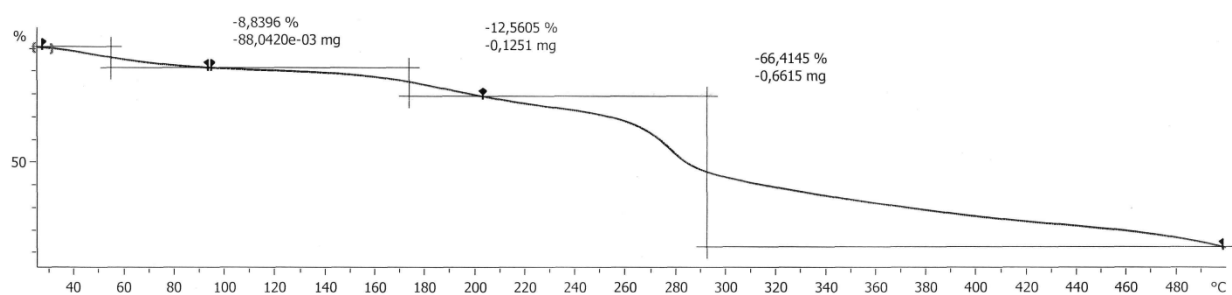
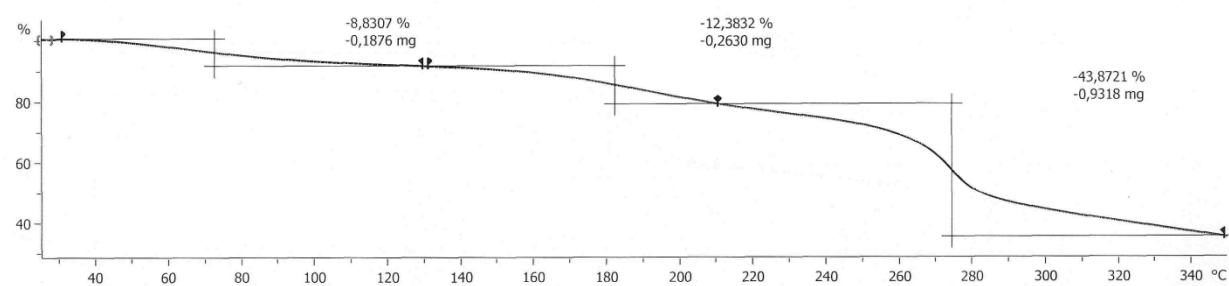


Figure S6. TGA of 8

**Testing compound 8 for burning rate of
KNO₃/Zr pyrotechnic composition**

The following formulation was employed as the model composition: 52% zirconium (PCZr-1 grade (powdered calciothermic Zr), technical specifications No. 48-4-234-84, particle size 1–15 µm) and 48% potassium nitrate (chemically pure grade, GOST R 4217-77, particle size 63–160 µm).

Compound **8** was used as the burning-rate modifier composed of (MZ)₅ Ni[N(NO₂)₂]₂ 10H₂O with added 3.71% Ni.

Table S1. Burning rate of model composition (no additives)

Sample #, sensor #	<i>l</i> , mm	time, s	<i>u</i> , mm/s	mean <i>u</i> , mm/s
1.1-2	4.28	0.11864	36,07552	33.9783
1.2-3	4.40	0.11967	36,76778	
1.3-4	4.34	0.12108	35,84407	
2.1-2	4.40	0.12851	34,23858	
2.2-3	4.22	0.12901	32,71140	
2.3-4	4.18	0.13071	31,97944	
3.1-2	4.40	0.12910	34,08211	
3.2-3	4.22	0.14007	30,12779	
3.3-4	4.24	* failure	-	

Charge density: 2.82–2.95 g/cm³.

* failure – simultaneous short circuit of sensors no.3 and no.4.

Table S2. Burning rate with 0.5% **8**

Sample #, sensor #	<i>l</i> , mm	time, s	<i>u</i> , mm/s	mean <i>u</i> , mm/s
1.1-2	4.3	0.18004	23.88358	22.6255
1.2-3	4.2	0.18543	22.65006	
1.3-4	4.38	0.22208	19.72262	
2.1-2	4.32	0.17777	24.30065	
2.2-3	4.36	0.19379	22.49858	
2.3-4	4.22	0.20021	21.07787	
3.1-2	4.36	0.19331	22.55445	
3.2-3	4.32	0.17367	24.87476	
3.3-4	4.22	0.19124	22.06651	

Charge density: 2.76–2.84 g/cm³.

Table S3. Burning rate with 1.0% **8**

Sample #, sensor #	<i>l</i> , mm	time, s	<i>u</i> , mm/s	mean <i>u</i> , mm/s
1.1-2	4.3	0.19871	21.63958	21.4868
1.2-3	4.3	0.20220	21.26607	
1.3-4	4.3	0.19406	22.15810	
2.1-2	4.32	0.21564	20.03339	
2.2-3	4.24	0.17506	24.22027	
2.3-4	4.28	0.22028	19.42982	

3.1-2	4,22	0.19612	21.51744
3.2-3	4,22	0.20582	20.50335
3.3-4	4,24	0,18750	22,61333

Charge density: 2.81–2.91 g/cm³.

Table S4. Burning rate with 1.5% 8

Sample #, sensor #	<i>l</i> , mm	time, s	<i>u</i> , mm/s	mean <i>u</i> , mm/s
1.1-2	4.22	0.20375	20.71166	20.0348
1.2-3	4.3	0.18301	23.49598	
1.3-4	4.34	0.18423	23.55751	
2.1-2	4.54	0.23788	19.08525	
2.2-3	4.26	0.25301	16.83728	
2.3-4	4.18	0.22551	16.52109	
3.1-2	4.34	*failure		
3.2-3	4.64	*failure		
3.3-4	4.4	*failure		

Charge density: 2.81–2.87 g/cm³.

* failure – simultaneous triggering of sensors nos.1, 2 and 4.

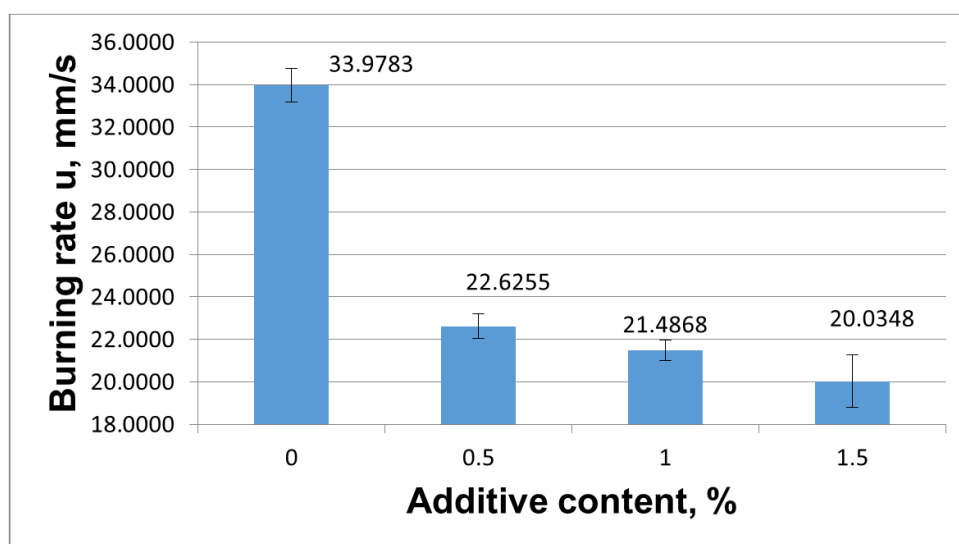


Figure S7. Effect of modifier 8 on the variation in the burning rate of KNO₃/Zr

**Testing compound 8 for burning rate of
KClO₄/Al pyrotechnic composition**

The following formulation was employed as the model composition: 70% potassium perchlorate (chemically pure grade, technical specifications No. 6-09-3801-76, particle size 63–160 μm) and 30% aluminum (ASD-4 grade, technical specifications No. 48-5-226-87, particle size 4–10 μm).

Compound **8** was used as the burning-rate modifier composed of (MZ)₅ Ni[N(NO₂)₂]₂ 10H₂O with added 3.71% Ni.

Table S5. Burning rate of model composition (no additives)

Sample #, sensor #	<i>l</i> , mm	time, s	<i>u</i> , mm/s	mean <i>u</i> , mm/s
1.1-2	5.22	1.31879	3.958174	3.857847
1.2-3	5.3	1.12713	4.702208	
1.3-4	5.32	*failure		
2.1-2	5.36	1.42547	3.760163	
2.2-3	5.4	1.75731	3.072878	
2.3-4	5.34	1.45117	3.679789	
3.1-2	5.34	1.42106	3.757758	
3.2-3	5.28	1.49087	3.541556	
3.3-4	5.44	1.23911	4.390248	

Charge density: 2.27–2.35 g/cm³.

* failure – no short circuit of sensor no.4.

Table S6. Burning rate with 0.5% **8**

Sample #, sensor #	<i>l</i> , mm	time, s	<i>u</i> , mm/s	mean <i>u</i> , mm/s
1.1-2	5.34	1.5716	3.3978	2.9385
1.2-3	5.4	1.6919	3.1917	
1.3-4	5.52	0.7069	7.8093	
2.1-2	10.88	4.2119		
2.2-3	5.36	*failure		
2.3-4	5.3	0.5734	9.2439	
3.1-2	5.42	1.8986	2.8547	
3.2-3	5.38	1.8833	2.8567	
3.3-4	5.3	1.9293	2.7471	

Charge density: 2.28–2.33 g/cm³.

** failure – simultaneous short circuit of sensors nos. 2 and 3

Table S7. Burning rate with 1.0% **8**

Sample #, sensor #	<i>l</i> , mm	time, s	<i>u</i> , mm/s	mean <i>u</i> , mm/s
1.1-2	5.38	4.1184	1.3063	2.3835
1.2-3	5.42	2.4752	2.1897	
1.3-4	5.40	1.7472	3.0907	

2.1-2	5.36	5.3675	0.9986
2.2-3	5.38	1.9157	2.8084
2.3-4	5.42	1.3289	4.0786
3.1-2	5.40	3.6334	1.4862
3.2-3	5.50	2.3696	2.3211
3.3-4	5.40	1.7026	3.1716

Charge density: 2.25–2.3 g/cm³.

Table S8. Burning rate with 1.5% **8**

Sample #, sensor #	<i>l</i> , mm	time, s	<i>u</i> , mm/s	mean <i>u</i> , mm/s
1.1-2	5.26	1.6196	3.2477	2.6643
1.2-3	5.42	2.2380	2.4218	
1.3-4	5.22	0.6380	8.1814	
2.1-2	5.5	1.8686	2.9434	
2.2-3	5.28	2.8244	1.8694	
2.3-4	5.34	1.4407	3.7065	
3.1-2	5.34	4.1069	1.3003	
3.2-3	5.28	2.8503	1.8524	
3.3-4	5.54	1.3945	3.9728	

Charge density: 2.28–2.32 g/cm³.

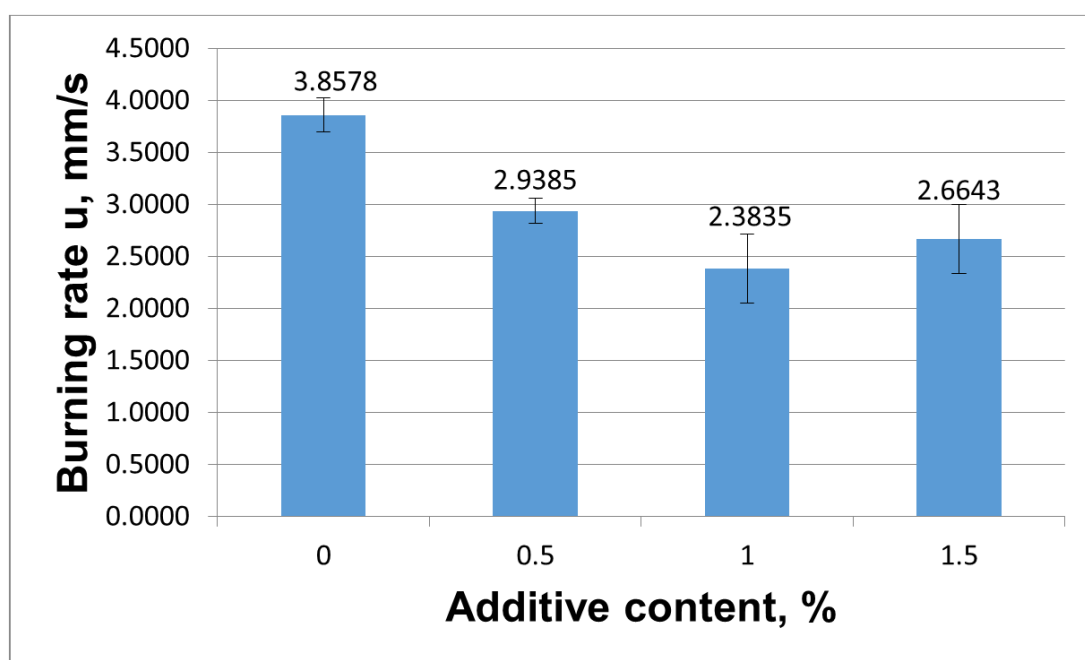


Figure S8. Effect of **8** on the burning rate of the KClO₄/Al pyrotechnic composition