

Supporting Information

Alkaline Metal and Alkaline Earth Metal Salts of Di(1H-tetrazol-5-yl)Methanone (DTO): Energetic Catalysts for Ammonium Perchlorate Decomposition

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Table S1 X-ray crystallographic data for compounds 1, 2, 3, 4

	1	2	3	4
Formula	C ₃ H ₆ N ₈ Na ₂ O ₄	C ₆ H ₂₀ N ₁₆ Na ₄ O ₁₂	C ₃ H ₂ K ₂ N ₈ O ₂	C ₃ K _{0.5} N ₈ ORb _{1.5}
M (g mol ⁻¹)	264.14	600.34	260.33	311.86
Cryst. Syst.	triclinic	orthorhombic	monoclinic	triclinic
Space group	<i>P</i> -1	<i>Pnma</i>	<i>P2</i> ₁	<i>P</i> -1
a (Å)	6.5949(13)	6.8000(14)	7.1376(14)	4.4887(9)
b (Å)	8.7129(17)	7.5000(15)	17.029(3)	7.5710(15)
c (Å)	9.1609(18)	24.200(5)	7.6232(15)	12.714(3)
α (°)	102.33(3)	90	90	97.31(3)
β (°)	90.26(3)	90.	111.38(3)	92.74(3)
γ (°)	105.15(3)	90	90	106.32(3)
V (Å ³)	495.34(19)	1234.2(4)	862.8(3)	409.70(16)
Z	2	2	4	2
ρ (g cm ⁻³)	1.771	1.615	2.004	2.528
T (K)	153.15	153.15	153.15	153.15
F (000)	268.0	616.0	520.0	294.0
μ (mm ⁻¹)	0.225	0.202	1.093	9.226
Reflns. collected	3918	2553	5224	3076
Indep. Reflns.	2206	1138	2768	1429
Params.	154	109	271	129
R _{int} .	0.0348	0.0285	0.0270	0.0329
S	1.105	1.264	1.053	1.099
R1 (I>2σ(I)) ^a	0.0407	0.0940	0.0255	0.0329
R1 (all data)	0.0437	0.0844	0.0260	0.0359
wR2 (I>2σ(I)) ^a	0.1046	0.1869	0.0620	0.0726
wR2 (all data)	0.1110	0.1878	0.0623	0.0742
Largest diff. peak /hole (e Å ⁻³)	0.33/-0.35	0.39/-0.66	0.22/-0.28	0.56/-0.57
CCDC	2078900	2078909	2078919	2078913

^aR1 = $\Sigma||F_o| - |F_c||/\Sigma|F_o|$. wR2 = $[\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$; w = $1/[\sigma^2(F_o^2) + (xP)^2 + yP]$.

Table S2 X-ray crystallographic data for compounds 5, 6, 7

	5	6	7
Formula	C ₃ H ₁₀ MgN ₈ O ₆	C ₃ H ₁₀ CaN ₈ O ₆	C ₃ H ₁₀ N ₈ O ₆ Sr
M (g mol ⁻¹)	278.50	294.27	341.81
Cryst. Syst.	orthorhombic	orthorhombic	orthorhombic
Space group	<i>Pbcn</i>	<i>P2₁2₁2₁</i>	<i>P2₁2₁2₁</i>
a (Å)	11.890(2)	6.5466(13)	6.6230(13)
b (Å)	16.700(3)	12.561(3)	12.839(3)
c (Å)	11.228(2)	13.047(3)	13.282(3)
α (°)	90	90	90
β (°)	90	90	90
γ (°)	90	90	90
V (Å ³)	2229.4(8)	1072.9(4)	1129.3(4)
Z	8	4	4
ρ (g cm ⁻³)	1.659	1.822	2.010
T (K)	153.15	153.15	153.15
F (000)	1152.0	332.0	680.0
μ (mm ⁻¹)	0.200	0.627	4.814
Reflns. collected	5924	4309	4560
Indep. Reflns.	2515	2250	2529
Params.	164	163	163
R _{int.}	0.0439	0.0289	0.0364
S	1.116	1.049	1.073
R1 (I>2σ(I)) ^a	0.0589	0.0354	0.0312
R1 (all data)	0.0687	0.0362	0.0320
wR2 (I>2σ(I)) ^a	0.1288	0.0823	0.0726
wR2 (all data)	0.1363	0.0831	0.0732
Largest diff. peak /hole (e Å ⁻³)	0.36/-0.35	0.26/-0.26	0.34/-0.96
CCDC	2078915	2078916	2078917

^aR1 = $\Sigma||F_o| - |F_c||/\Sigma|F_o|$. wR2 = $[\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$; w = $1/[\sigma^2(F_o^2) + (xP)^2 + yP]$.

Table S3. The first exothermic decomposition peak temperatures tested at different heating rates of compounds **1** to **7**.

compound	The first exothermic decomposition peak temperatures (°C)			
	5°C·min ⁻¹	10°C·min ⁻¹	15°C·min ⁻¹	20°C·min ⁻¹
1	252.3	254.2	256.1	257.5
2	258.8	260.2	261.4	262.8
3	223.5	225.2	227.3	229.0
4	242.3	244.1	246.2	248.0
5	220.1	221.9	223.5	225.0
6	200.6	202.3	203.8	205.2
7	201.7	203.8	208.4	210.6

Figure S1. DSC curve of **1**.

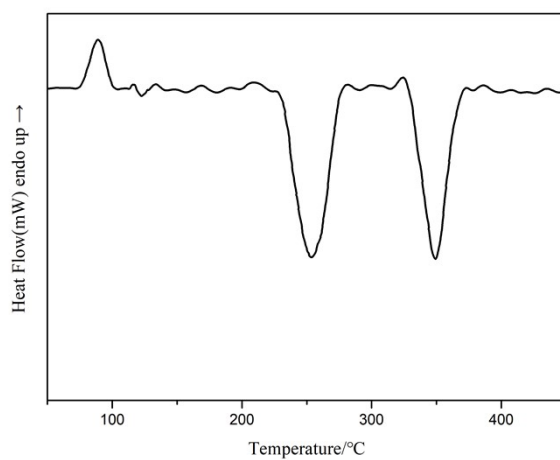


Figure S2. DSC curve of **2**.

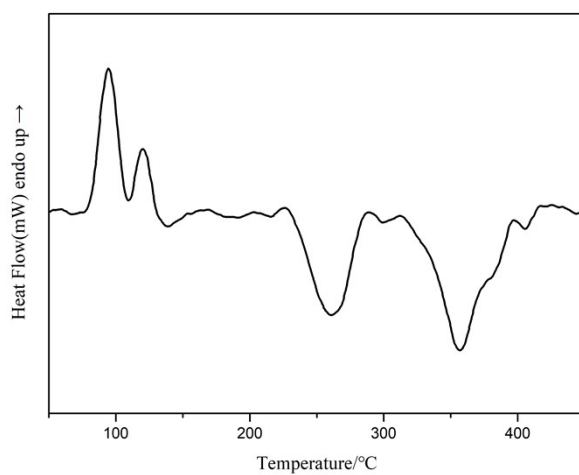


Figure S3. DSC curve of **3**.

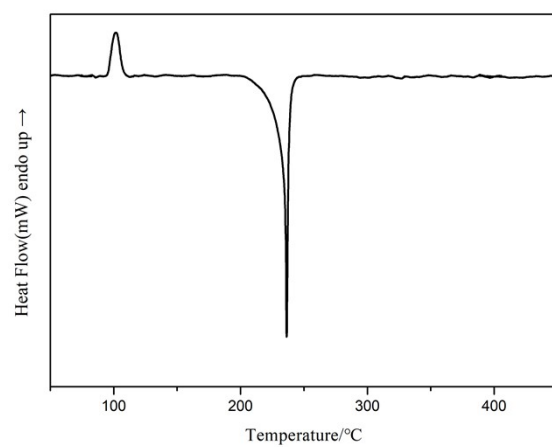


Figure S4. DSC curve of **4**.

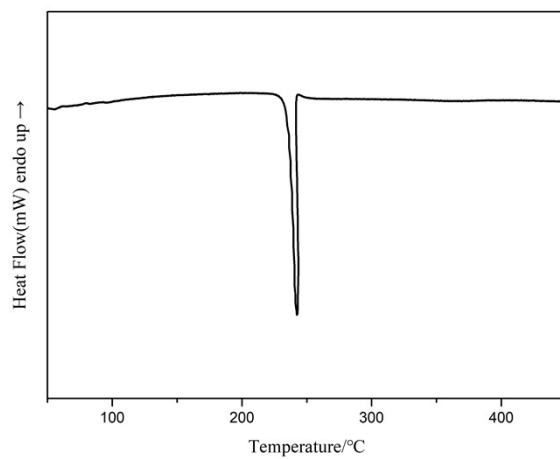


Figure S5. DSC curve of **5**.

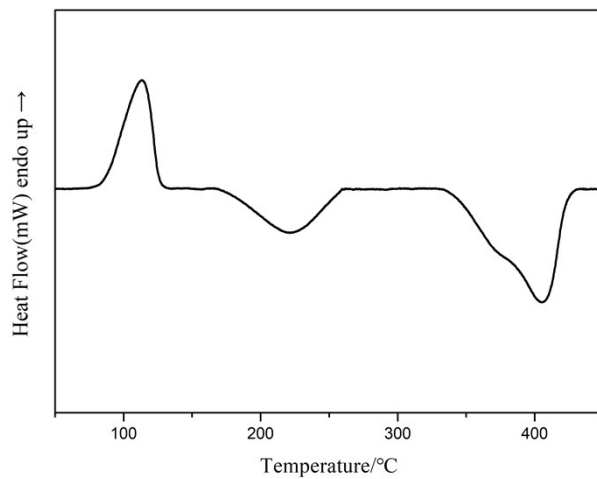


Figure S6. DSC curve of **6**.

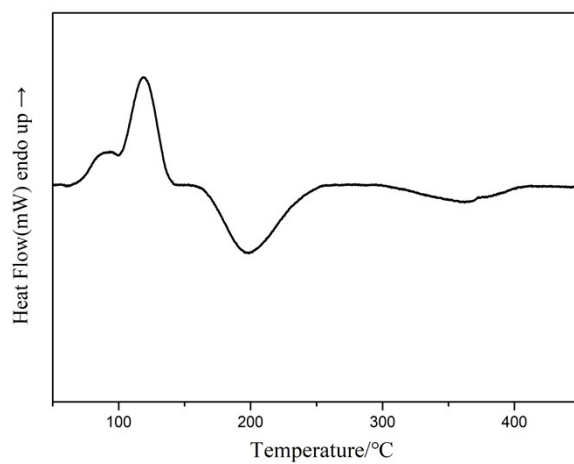


Figure S7. DSC curve of **7**.

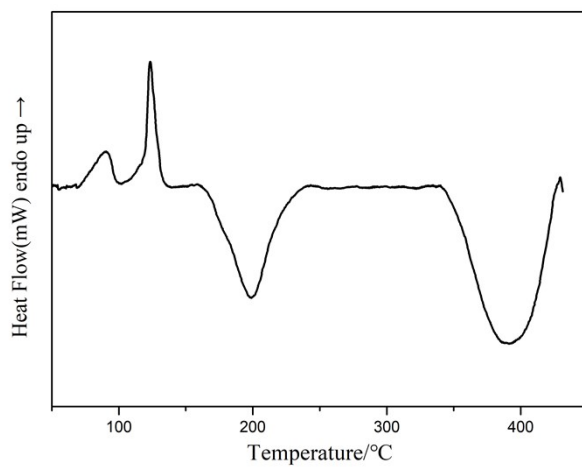


Figure S8. TG-DTG curve of **1**.

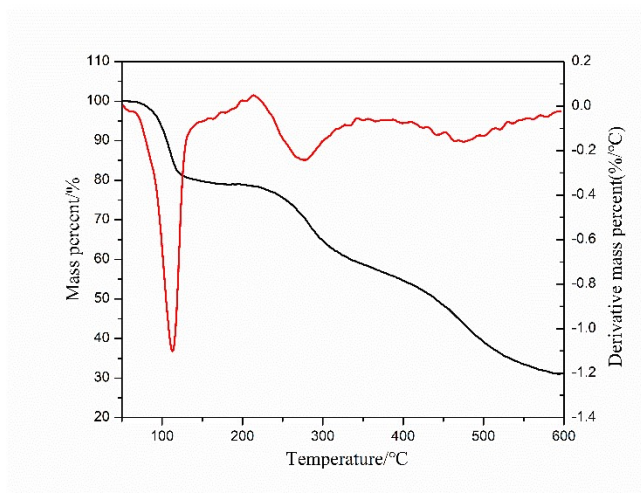


Figure S9. TG-DTG curve of **2**.

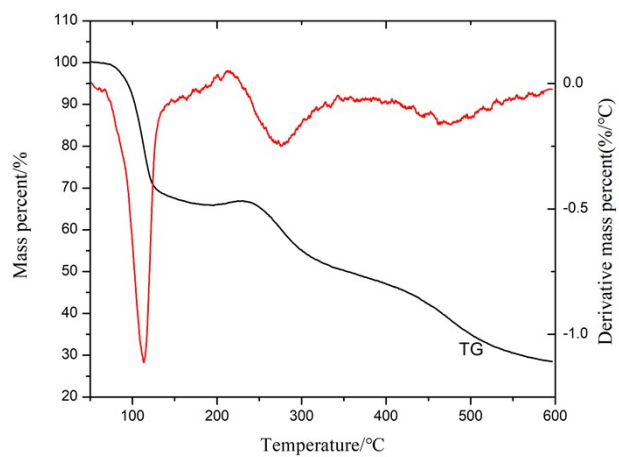


Figure S10. TG-DTG curve of **5**.

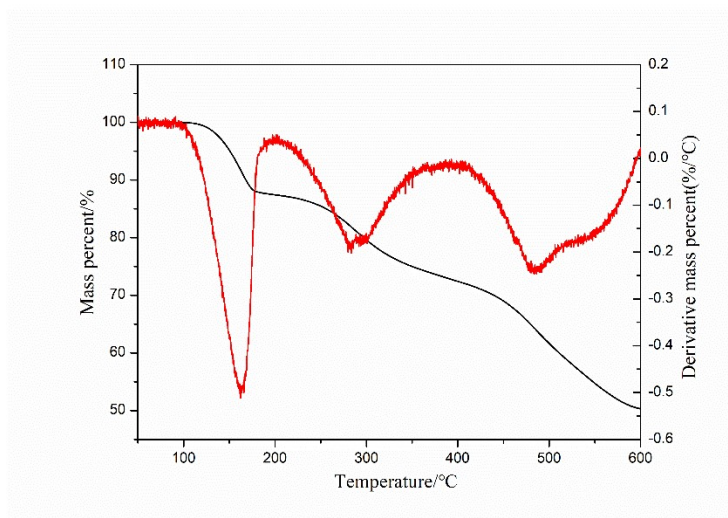


Figure S11. TG-DTG curve of **6**.

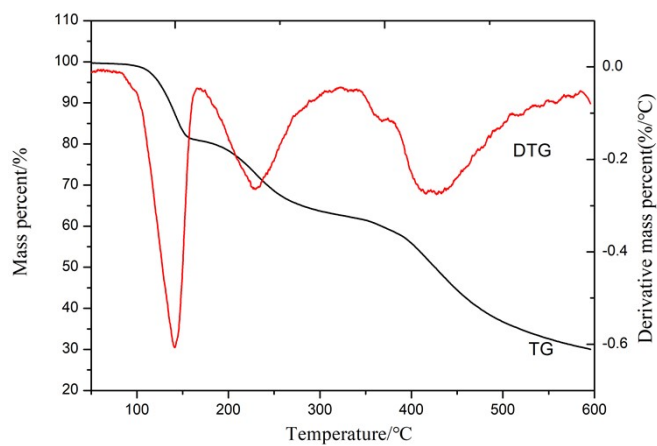


Figure S12. TG-DTG curve of **7**.

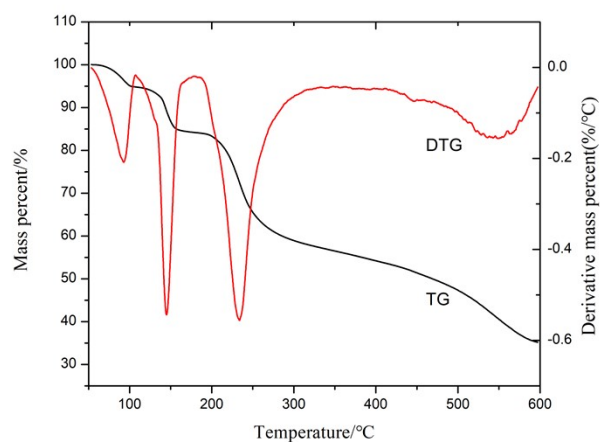


Figure S13. DSC curves of mixed **1+AP**, **3+AP**, **4+AP** and **7+AP**.

