Crystal structures, thermodynamics and accelerating thermal decomposition of RDX: Two new energetic coordination polymers based on Y-shaped ligand of tris(5-aminotetrazole)triazine

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Table S1.Crystal data and structure refinement details for **1** and **2***.

	1	**2**
Empirical formula	$Zn_2C_{12}H_{18}O_5N_{36}$	$PbZnC_6H_6O_2N_{18}$
CCDC	1884884	1848810
Formula weight	875.35	634.85
Crystal system	Monoclinic	Triclinic
Space group	$P2_1/c$	P-1
a/ Å	12.4524(16)	7.2877(9)
b/ Å	9.1886(10)	7.4427(8)
c/ Å	25.7031(3)	13.6865(17)
α/°	90	83.102(7)
β/°	93.345(3)	85.643(6)
γ/°	90	81.066(5)
V/ Å^3	2936.1(6)	726.8(15)
Z	4	2
$\rho_{calc.}$/g·cm^{-3}	1.980	2.901
μ/mm^{-1}	1.735	13.278
F(000)	1760.0	592.0
GOOF on F^2	1.046	0.998
R_1/wR_2 [$I>2\sigma(I)$]	0.0869/0.2461	0.0444/0.0925
R_1/wR_2 [all data]	0.1881/0.2899	0.0667/0.1011

* $R_1 = \Sigma\left\|F_0\right|-\left|F_c\right\| / \Sigma\left|F_0\right|$, $wR_2 = [\Sigma(F_o^2 - F_c^2) / \Sigma w(F_0)^2]^{1/2}$

Table S2 Bond lengths for **1** and **2**.

1	Atom	Atom	Length/ Å
	Zn1	O3	1.984(8)
	Zn1	N19	2.100(10)
	Zn1	N13	1.996(10)
	Zn2	N11#1	2.126(10)
	Zn2	N25	2.285(10)
	N11	Zn2#2	2.126(10)
	Zn1	N18	2.006(10)
	Zn1	N8	2.339(10)
	Zn2	O5	2.025(8)
	Zn2	N36	2.010(10)
	Zn2	N22	2.031(9)
[1]+X,-1+Y,+Z; [2]+X,1+Y,+Z			
2	Pb1	O1#1	2.416(9)
	Pb1	O2	2.426(8)
	Pb1	N16#2	2.779 (10)
	Zn1	N1	1.969(9)
	Zn1	N15#3	2.031(10)
	N15	Zn1#3	2.031(10)
	Pb1	O1	2.357(7)
	Pb1	N2	2.785(11)
	Zn1	O1	2.128(8)
	Zn1	N9	1.966(9)
	Pb1#1	O1	2.416(8)
	Pb1#4	N16	2.779(10)
[1]1-X,1-Y,2-Z; [2]+X,+Y,1+Z; [3]1-X,1-Y,1-Z; [4]+X,+Y,-1+Z			

Table S3 Bond angles for **1** and **2**.

1	Atom	Atom	Atom	Angle/°
	O3	Zn1	N18	117.7(4)
	O3	Zn1	N8	83.5(3)
	N18	Zn1	N19	97.1(4)
	N19	Zn1	N8	174.2(3)
	N13	Zn1	N19	101.9(4)
	O5	Zn2	N11#1	85.3(4)
	O5	Zn2	N22	124.2(4)
	N36	Zn2	O5	104.8(4)
	N36	Zn2	N25	84.3(4)
	N22	Zn2	N11#1	101.3(4)
	N12	N11	Zn2#2	122.3(8)
	N17	N18	Zn1	126.5(8)
	N20	N19	Zn1	127.4(7)
	N35	N36	Zn2	128.5(8)
	C8	N25	Zn2	124.4(8)
	N12	N13	Zn1	126.5(8)
	C7	N22	Zn2	127.2(9)
	O3	Zn1	N19	91.7(4)
	O3	Zn1	N13	110.1(4)
	N18	Zn1	N8	82.3(4)
	N13	Zn1	N18	127.6(4)
	N13	Zn1	N8	82.9(4)
	O5	Zn2	N25	87.3(3)
	N11#1	Zn2	N25	172.5(4)
	N36	Zn2	N11#1	97.6(4)
	N36	Zn2	N22	128.4(4)
	N22	Zn2	N25	82.9(4)
	N10	N11	Zn2#2	125.2(8)
	C6	N18	Zn1	125.0(8)
	N21	N19	Zn1	121.6(7)
	C4	N8	Zn1	121.8(7)
	C12	N36	Zn2	122.2(8)
	C9	N25	Zn2	121.3(8)
	N21	N22	Zn2	124.5(7)

[1]+X,-1+Y,+Z; [2]+X,1+Y,+Z

2	O1	Pb1	O1#1	74.4(3)
	O1	Pb1	O2	95.1(3)
	O1#1	Pb1	N2	131.8(3)
	O1#1	Pb1	N16#2	72.2(3)
	O2	Pb1	N16#2	148.1(3)
	N1	Zn1	O1	96.9(4)
	N9	Zn1	O1	92.5(4)
	N9	Zn1	N15#3	107.1(4)
	Pb1	O1	Pb1#1	105.6(3)
	Zn1	O1	Pb1	120.7(3)
	C1	N1	Zn1	137.9(8)
	N3	N2	Pb1	126.6(7)
	C6	N9	Zn1	139.5(9)
	C5	N15	Zn1#3	136.2(8)
	N17	N16	Pb1#4	119.6(8)
	O1#1	Pb1	O2	80.0(3)
	O1	Pb1	N2	74.0(3)
	O1	Pb1	N16#2	92.4(3)
	O2	Pb1	N2	67.7(3)
	N16#2	Pb1	N2	143.9(3)
	N1	Zn1	N15#3	102.9(4)
	N9	Zn1	N1	148.2(4)
	N15#3	Zn1	O1	92.0(4)
	Zn1	O1	Pb1#1	113.6(3)
	N2	N1	Zn1	115.3(8)
	N1	N2	Pb1	121.1(7)
	N10	N9	Zn1	114.7(7)
	N16	N15	Zn1#3	116.6(7)
	N15	N16	Pb1#4	121.3(7)

[1]1-X,1-Y,2-Z;[2]+X,+Y,1+Z;[3]1-X,1-Y,1-Z;[4]+X,+Y,-1+Z

Table S4 Hydrogen bond lengths (Å) and angles (°) for **1** and **2**.

	D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
1	O1	H1A	O2	0.85	2.38	2.793(15)	110
	O1	H1B	N29	0.85	2.13	2.938(16)	158
	O2	H2A	N9	0.85	2.47	3.155(14)	164.9
	O2	H2A	N13	0.85	2.62	3.339(14)	144
	O2	H2B	N10	0.85	2.09	2.846(14)	148
	O2	H2B	N21	0.85	2.59	3.068(12)	116
	O3	H3A	O2	0.92	1.74	2.557(13)	145
	O3	H3B	O2	0.91	2.51	3.305(13)	145
	O4	H4A	N21	0.85	2.35	3.159(14)	159
	O4	H4B	N3	0.85	2.28	2.917(14)	132
	N5	H5	N28	0.87	2.00	2.865(14)	174
	O5	H5A	N20	0.90	2.40	3.249(14)	156
	O5	H5B	N17	0.90	2.15	2.802(14)	129
	N9	H9	O1	0.87	1.99	2.853(15)	174
	N14	H14	N33	0.87	1.96	2.826(14)	173
	N23	H23	O4	0.87	1.97	2.785(14)	155
	N27	H27	N4	0.87	2.03	2.894(14)	174
	N32	H32	N15	0.87	1.92	2.769(14)	165
2	O1	H1	N18	0.85	2.05	2.870(12)	160
	O2	H2A	N11	0.89	2.51	3.307(14)	119
	O2	H2A	N12	0.89	2.52	3.266(14)	142
	O2	H2B	N17	0.89	1.97	2.686(13)	137
	N5	H5	N4	0.88	1.99	2.859(14)	169
	N13	H13	N7	0.88	2.46	3.319(13)	167
	N14	H14	N12	0.88	1.95	2.813(14)	165

Table S5 Experimental and smoothed molar heat capacities of ECPs **1** and **2** at pressure 101.3 kPa.

T/K	**1**		**2**	
	$C_{p,m}$/(J K^{-1} mol^{-1})		$C_{p,m}$/(J K^{-1} mol^{-1})	
	Exp.	smooth	Exp.	smooth
293.15	588.35	589.36	930.18	931.46
296.15	627.95	629.05	930.03	929.24
299.15	663.43	664.60	930.12	928.61
302.15	695.11	696.35	930.69	929.57
305.15	724.39	724.62	932.94	932.15
308.15	749.96	749.75	936.87	936.33
311.15	771.73	772.07	942.52	942.14
314.15	790.57	791.92	949.81	949.58
317.15	808.28	809.63	958.79	958.66
320.15	824.19	825.54	969.50	969.39
323.15	838.63	839.97	981.89	981.77
326.15	851.94	853.27	995.97	995.82
329.15	864.23	865.76	1011.75	1011.54
332.15	876.48	877.78	1029.23	1028.94
335.15	888.37	889.67	1048.40	1048.03
338.15	901.46	901.75	1069.29	1068.82
341.15	913.08	914.37	1091.87	1091.31
344.15	926.55	927.84	1116.16	1115.52
347.15	941.21	942.52	1142.16	1141.45
350.15	957.76	958.73	1169.87	1169.11
353.15	975.49	976.80	1199.28	1198.51
356.15	995.26	997.08	1230.41	1229.66
359.15	1018.41	1019.88	1263.26	1262.57
362.15	1044.52	1045.55	1297.82	1297.23
365.15	1072.78	1074.43	1334.11	1333.67
368.15	1105.07	1106.84	1372.09	1371.89

Standard uncertainties u are u(p) =1 kPa, u(T) = 0.01 K, relative uncertainty $u_r(C_{p,m})$= 1.29%.

Table S6 Thermodynamic functions of ECPs **1** and **2**, the enthalpy change, the entropy change and the gibbs free energy change by taking T = 298.15 K as the benchmark.

T/K	H_T-$H_{298.15}$/(kJ mol^{-1})		S_T-$S_{298.15}$/(J K^{-1} mol^{-1})		G_T-$G_{298.15}$/(kJ mol^{-1})	
	1	**2**	**1**	**2**	**1**	**2**
293.15	-3.1011	-4.6460	-10.488	-15.715	-2.6543E-2	-3.9148E-2
296.15	-1.2784	-1.8568	-4.3021	-6.2487	-4.3331E-3	-6.2475E-3
299.15	0.65681	0.92812	2.1993	3.1077	-1.1106E-3	-1.5485E-3
302.15	2.6927	3.7135	8.9708	12.372	-1.7827E-2	-2.4700E-2
305.15	4.8184	6.5042	15.971	21.563	-5.5151E-2	-7.5749E-2
308.15	7.0239	9.3049	23.163	30.696	-0.11378	-0.15407
311.15	9.3002	12.121	30.514	39.789	-0.19423	-0.25935
314.15	11.640	14.956	37.996	48.859	-0.29644	-0.39305
317.15	14.035	17.817	45.585	57.920	-0.42228	-0.55233
320.15	16.480	20.706	53.259	66.990	-0.57087	-0.74085
323.15	18.971	23.631	61.003	76.082	-0.74212	-0.95490
326.15	21.503	26.595	68.802	85.213	-0.93677	-1.1972
329.15	24.073	29.604	76.646	94.396	-1.1550	-1.4664
332.15	26.680	32.663	84.530	103.65	-1.3966	-1.7643
335.15	29.323	35.776	92.450	112.98	-1.6616	-2.0892
338.15	32.001	38.949	100.40	122.40	-1.9493	-2.4406
341.15	34.715	42.186	108.40	131.93	-2.2657	-2.8219
344.15	37.469	45.494	116.43	141.59	-2.6004	-3.2342
347.15	40.264	48.877	124.52	151.37	-2.9631	-3.6711
350.15	43.105	52.341	132.67	161.31	-3.3494	-4.1417
353.15	45.998	55.889	140.89	171.40	-3.7573	-4.6409
356.15	48.947	59.529	149.21	181.66	-4.1941	-5.1692
359.15	51.961	63.265	157.64	192.11	-4.6554	-5.7313
362.15	55.047	67.102	166.20	202.75	-5.1423	-6.3239
365.15	58.215	71.045	174.91	213.59	-5.6534	-6.9474
368.15	61.474	75.101	183.79	224.65	-6.1883	-7.6039

Standard uncertainties u are u(p) =1kPa, u(T) = 0.01 K.

u(H_T-$H_{298.15K}$) = u$_r$($C_{p,m}$)($C_{p,m}$ / J mol^{-1} K^{-1})[T/K-298.15 K].

u(S_T-$S_{298.15K}$)= u$_r$($C_{p,m}$)($C_{p,m}$ / J mol^{-1} K^{-1})[ln(T/298.15 K)].

Table S7.Calculated parameters used in the detonation reactions for **1** and **2**.

	ECPs (hartree)	ZnO (hartree)	Pb (hartree)	H_2O (hartree)	NH_3 (hartree)	C (hartree)	N_2 (hartree)	ΔE_{det} (hartree)	ΔE_{det} ($kcalg^{-1}$)	ΔH_{det} ($kcalg^{-1}$)
1	-2944.5869	-142.0943	-	-76.3776	-56.5045	-37.738	-109.447	2.4088	1.7268	1.992
2	-1437.0478	-142.0943	-3.9251	-76.3776	-56.5045	-37.738	-109.447	0.8251	0.8155	0.965

Table S8. Calculated parameters of detonation velocity and detonation pressure for **1** and **2**.

	ρ ($g\ cm^{-3}$)	N ($mol\ g^{-1}$)	M ($g\ mol^{-1}$)	Q ($kcal\ g^{-1}$)	D ($km\ s^{-1}$)	P (GPa)
1	1.980	0.0259	25.06	1.992	8.69	35.41
2	2.901	0.0168	25.69	0.965	7.84	34.75

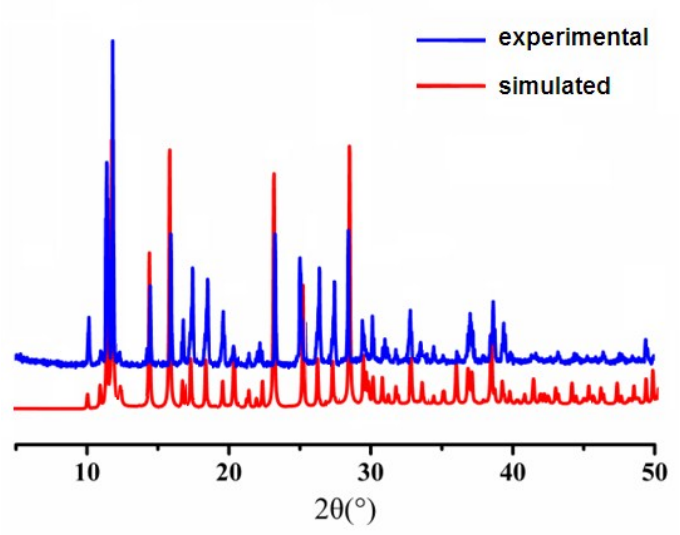

Figure S1 PXRD curve of **1**

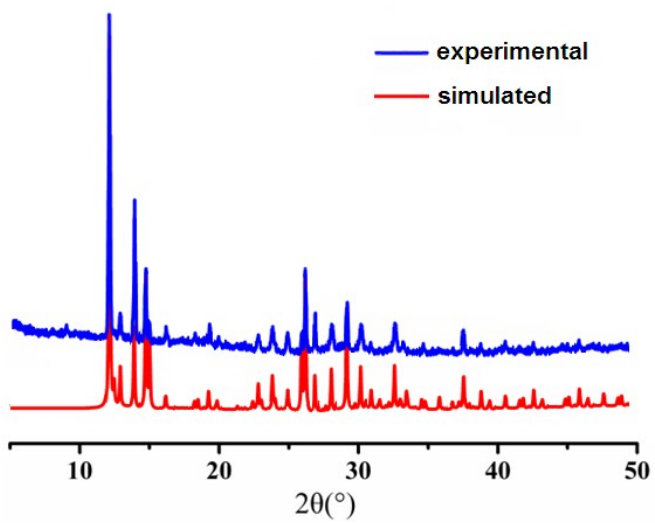

Figure S2 PXRD curve of **2**