

Supporting Information

A π -stacking highly stable insensitive energetic inner salt and its insensitive energetic salts

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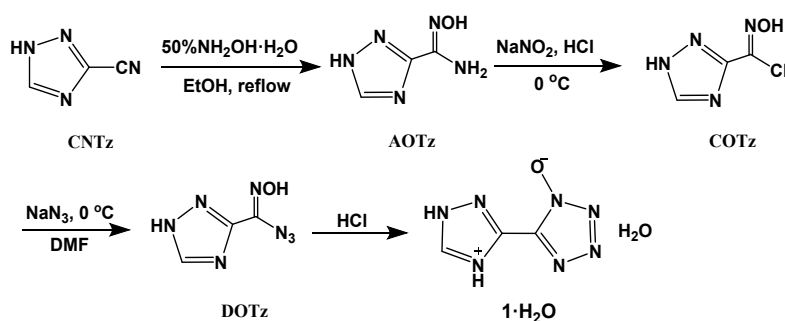
Experimental Section

Safety Precautions! Carefully! Although we experienced no difficulties in the synthesis and characterization of these materials, small-scale syntheses are strongly encouraged. All of the compounds should be handled with extreme care, and eye protection and gloves must be worn at all times.

General Methods. Chemical reagents and solvents were purchased from Aladdin (Shanghai, China) and used as supplied without further purification. ^1H NMR and ^{13}C NMR spectra were obtained using a JEOL GSX 600 MHz nuclear magnetic resonance (NMR) spectrometer in a DMSO solution by using tetramethylsilane as an internal standard. Fourier transform infrared (FT-IR) spectra were recorded on a Nicolet-5700 FTIR spectrometer by using pressed KBr pellets to evaluate the chemical bonding of the samples from 4000 cm^{-1} to 400 cm^{-1} . Elemental analyses (C, H, and N) were conducted using a Vario EL CUBE device. DSC was performed by a Q200 DSC instrument (TA Instruments, United States) at a heating rate of $10\text{ }^\circ\text{C min}^{-1}$ in flowing high-purity nitrogen. TGA was performed with an STA 449 F5 TGA instrument (Netzsch Instruments, Germany) at a heating rate of $10\text{ }^\circ\text{C min}^{-1}$ in flowing high-purity nitrogen.

Synthesis of 5-(1*H*-1,2,4-triazol-4-ium-3-yl)-1*H*-tetrazol-1-olate monohydrate ($\text{TzTO}\cdot\text{H}_2\text{O}$, $1\cdot\text{H}_2\text{O}$):

5-(1*H*-1,2,4-triazol-4-ium-3-yl)-1*H*-tetrazol-1-olate monohydrate was synthesized through four reaction steps, as shown in Scheme S1.



Scheme S1 Synthesis pathway of $1\cdot\text{H}_2\text{O}$

1*H*-1,2,4-triazole-3-hydroxamamide (AOTz): 1*H*-1,2,4-triazole-3-carbonitrile (4.70 g, 50 mmol) was suspended in 30 mL ethanol, added 0.75 mL of 50 wt% aqueous hydroxylamine into the suspension, which reacted with reflux at $90\text{ }^\circ\text{C}$ for 2 h. The mixture was cooled to room temperature, and filtered, and dried to yield 6.22 g (98%) of the white powder crystal. $T_d(\text{DSC}, 10\text{ }^\circ\text{C}\cdot\text{min}^{-1})$: $197\text{ }^\circ\text{C}$. ^1H NMR (DMSO- d_6 , 600 MHz) δ/ppm : 14.28 (1H, NOH), 9.98 (1H, NH), 8.04 (1H, CH), 5.84 (2H, NH_2). ^{13}C NMR (DMSO- d_6 , 150 MHz) δ/ppm : 150.09, 148.06, 143.38. IR (KBr) ν/cm^{-1} : 3434, 1657, 1426, 1339, 1282, 1098, 984, 873, 804, 535. Elemental analysis (%) calcd for $\text{C}_3\text{H}_5\text{N}_5\text{O}$ (127.11): C 28.35, H 3.97, N 55.10; found: C 28.32, H 4.01, N 55.09.

1*H*-1,2,4-triazole-3-carbohydroximoylchloride (COTz): 1*H*-1,2,4-triazole-3-hydroxamamide (2.54 g, 20 mmol) was suspended in 15 mL water and 27.5 mL concentrated hydrochloric acid. At $0\text{ }^\circ\text{C}$, a saturated

solution of NaNO₂ (1.42 g, 20 mmol) was slowly added dropwise to the suspension. After the dropwise addition, the reaction was carried out at low temperature for 2.5 h, filtered and dried to yield 2.45 g (94%) of white product. *T_m*(DSC, 10 °C·min⁻¹): 130 °C. *T_d*(DSC, 10 °C·min⁻¹): 206 °C. ¹H NMR (DMSO-*d*₆, 600 MHz) δ/ppm: 12.67 (1H, NOH), 8.98 (1H, NH), 8.61 (1H, CH). ¹³C NMR (DMSO-*d*₆, 150 MHz) δ/ppm: 155.23, 146.27, 128.73. IR (KBr) ν/cm⁻¹: 3452, 1675, 1541, 1475, 1278, 1178, 1033, 979, 937. Elemental analysis (%) calcd for C₃H₃ClN₄O (146.53): C 24.59, H 2.06, N 38.24; found: C 24.63, H 2.04, N 38.21.

1H-1,2,4-triazole-3-carbohydroximoylazine (DOTz): *1H-1,2,4-triazole-3-carbohydroximoylchloride* (0.876 g, 6 mmol) was suspended in DMF. At 0 °C, 0.5 g sodium azide (0.77 mmol) was added in batches. The suspension was stirred for 30 min and 50 mL of water was added. The mixture was placed in the refrigerator at -18 °C for 2 h, and a white solid was precipitated, filtered, and dried to yield 0.872 g (95%). *T_{melt}*(DSC, 10 °C·min⁻¹): 113 °C. *T_d*(DSC, 10 °C·min⁻¹): 145 °C. ¹H NMR (DMSO-*d*₆, 600 MHz) δ/ppm: 15.27 (1H, NOH), 11.90 (1H, NH), 8.97 (1H, CH). ¹³C NMR (DMSO-*d*₆, 150 MHz) δ/ppm: 163.06, 146.73, 138.45. IR (KBr) ν/cm⁻¹: 3458, 1675, 1541, 1475, 1278, 1178, 1033, 979, 937, 800, 617, 489, 466. Elemental analysis (%) calcd for C₃H₃N₇O (153.11): C 23.53, H 1.98, N 64.04; found: C 23.55, H 2.01, N 64.02.

5-(1H-1,2,4-triazol-4-ium-3-yl)-1H-tetrazol-1-olate monohydrate (TzTO·H₂O): *1H-1,2,4-triazole-3-carbohydroximoylazine* (3.06 g, 20 mmol) was suspended in 50 mL of concentrated hydrochloric acid, and the reaction was stirred at room temperature for 12 h and 150 mL of water was added. White product was filtered, and dried to yield 3.283 g (96%). *T_{melt}*(DSC, 10 °C·min⁻¹): 114 °C. *T_d*(DSC, 10 °C·min⁻¹): 261 °C. ¹H NMR (DMSO-*d*₆, 600 MHz) δ/ppm: 8.92 (2H, 2NH), 6.75 (1H, CH). ¹³C NMR (DMSO-*d*₆, 150 MHz) δ/ppm: 148.30, 146.32, 141.80. IR (KBr) ν/cm⁻¹: 3433, 1650, 1384, 1092, 987, 862, 532. Elemental analysis (%) calcd for C₃H₅N₇O₂ (171.14): C 21.06, H 2.95, N 57.30; found: C 21.03, H 2.98, N 57.33.

General procedure for the synthesis of the energetic salts 2–4.

5-(1H-1,2,4-triazol-4-ium-3-yl)-1H-tetrazol-1-olate monohydrate (0.171 g, 1 mmol) was dissolved in a few milliliters of distilled water. A solution of aqueous ammonia (1 mmol), hydroxylamine (1 mmol), and hydrazine monohydrate (1 mmol), was added. The reaction mixture was stirred for 0.5 h and the solvent was evaporated under reduced pressure. The solid obtained was purified by washing with ether.

Ammonium 5-(1H-1,2,4-triazol-4-ium-3-yl)-1H-tetrazol-1-olate (2). White solid (96% yield). DSC (10 °C min⁻¹): 282 °C (dec). ¹H NMR (DMSO-*d*₆, 600 MHz) δ/ppm: 8.20 (6H, 2NH, NH₄⁺). IR (KBr) ν/cm⁻¹: 3399, 2379, 1648, 1401, 1097, 987, 860, 534. Elemental analysis (%) calcd for C₃H₆N₈O (170.16): C 21.18, H 3.55, N 65.86; found: C 21.13, H 3.58, N 65.87. BAM drop hammer: ≥ 40 J; friction tester: ≥ 360 N.

Hydroxylammonium 5-(1H-1,2,4-triazol-4-ium-3-yl)-1H-tetrazol-1-olate (3). White solid (94% yield). DSC (10 °C min⁻¹): 238 °C (dec). ¹H NMR (DMSO-*d*₆, 600 MHz) δ/ppm: 11.08 (1H, NOH), 8.33 (5H,

2NH, NH₃⁺). ¹³C NMR (DMSO-*d*₆, 150 MHz) δ /ppm: 149.15, 146.41, 136.62. IR (KBr) ν /cm⁻¹: 3398, 1647, 1426, 1098, 987, 861, 534. Elemental analysis (%) calcd for C₃H₆N₈O₂ (186.16): C 19.36, H 3.25, N 60.20; found: C 19.38, H 3.21, N 60.22. BAM drop hammer: ≥ 40 J; friction tester: ≥ 360 N.

Hydrazinium 5-(1*H*-1,2,4-triazol-4-ium-3-yl)-1*H*-tetrazol-1-olate (4). White solid (95% yield). DSC (10 °C min⁻¹): 264 °C (dec). ¹H NMR (DMSO-*d*₆, 600 MHz) δ /ppm: 8.54 (7H, 2NH, NH₂, NH₃⁺). ¹³C NMR (DMSO-*d*₆, 150 MHz) δ /ppm: 147.67, 147.11, 139.99. IR (KBr) ν /cm⁻¹: 3399, 1646, 1092, 986, 862, 535. Elemental analysis (%) calcd for C₃H₇N₉O (185.18): C 19.46, H 3.81, N 58.63; found: C 19.48, H 3.85, N 58.69. BAM drop hammer: ≥ 40 J; friction tester: ≥ 360 N.

Nuclear magnetic resonance.

The structure of energetic compounds **1-4** was characterized by NMR. The deuterium reagent is DMSO. We have shown by solubility tests that energetic salts **2-4** are slightly soluble in the tested solvents. Therefore, ¹³C NMR of energetic salt **2** has not been obtained. ¹H NMR and ¹³C NMR of energetic compounds **1-4** are shown in Figs. S1-S7.

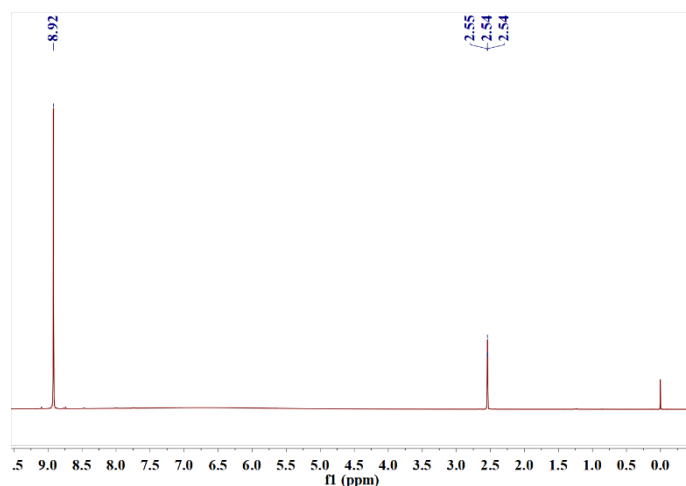


Fig. S1 ¹H NMR spectra of **1**·H₂O

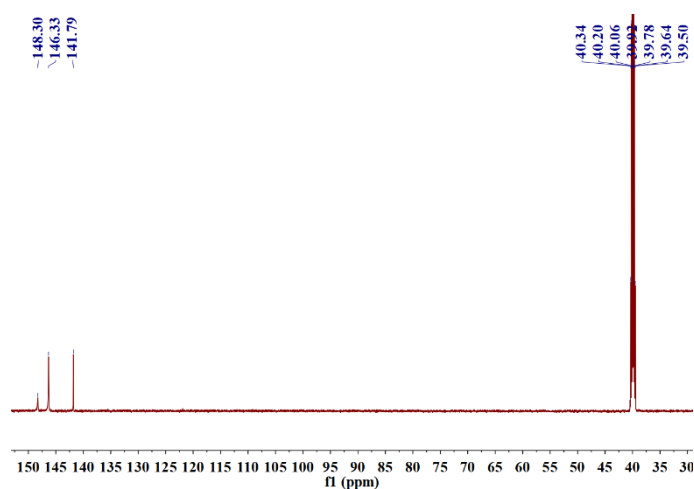


Fig. S2 ¹³C NMR spectra of **1**·H₂O

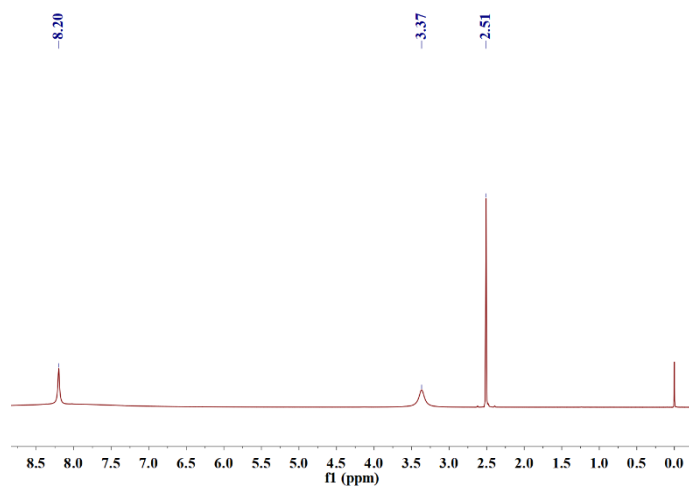


Fig. S3 ¹H NMR spectra of **2**

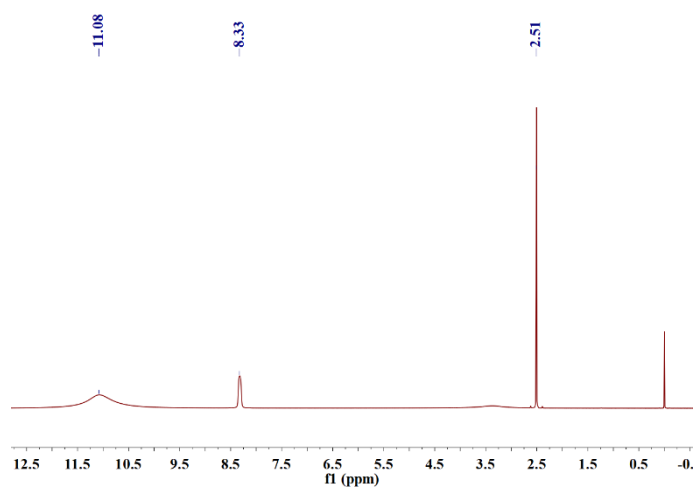


Fig. S4 ¹H NMR spectra of **3**

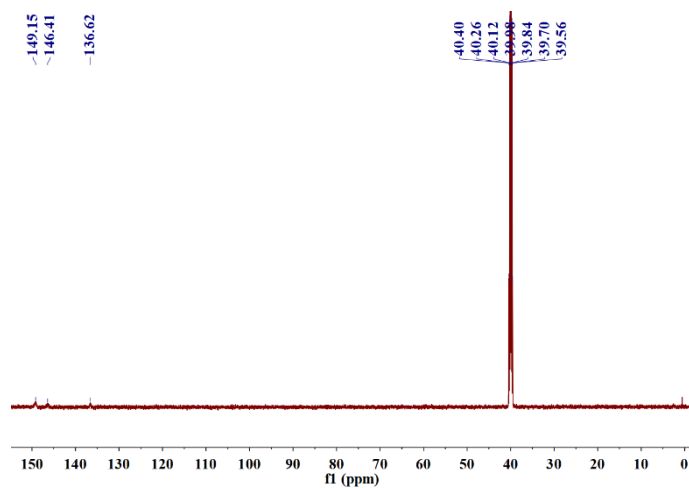


Fig. S5 ¹³C NMR spectra of **3**

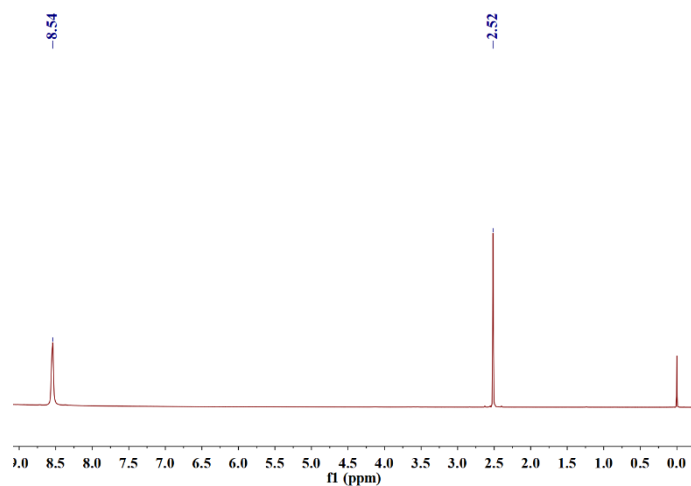


Fig. S6 ^1H NMR spectra of **4**

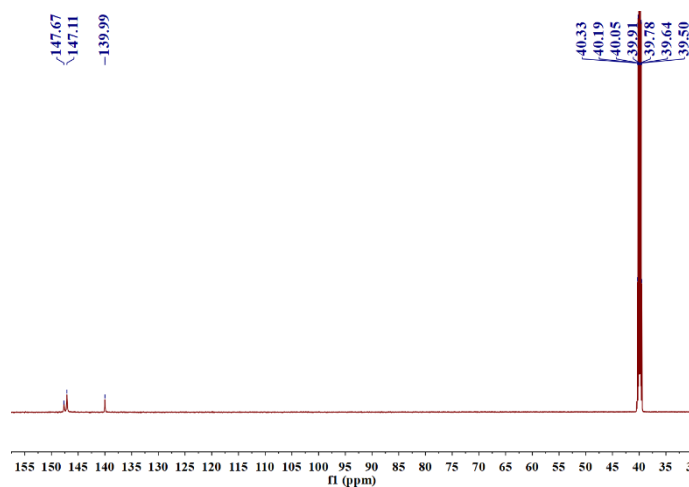


Fig. S7 ^{13}C NMR spectra of **4**

X-ray Crystallography.

The single crystals of **1-4** were cultured via a slow solvent evaporation method. Data were collected using a three-circle Bruker platform diffractometer equipped with a SMART APEX II CCD detector. All calculations were performed using the Crystal Structure crystallographic software package except for refinement, which was performed using SHELXL2.^[1] Hydrogen atoms were added theoretically and refined with riding model position parameters and fixed isotropic thermal parameters.

Table S1. Crystal data and structure refinement parameters of **1-4**

Compounds	1·H₂O	2	3	4
Empirical formula	C ₃ H ₅ N ₇ O ₂	C ₃ H ₆ N ₈ O	C ₃ H ₆ N ₈ O ₂	C ₃ H ₇ N ₉ O
Formula weight	171.14	170.16	186.16	185.18
CCDC number	2171804	2189511	2189512	2189513
Crystal size/mm ³	0.20×0.20×0.20	0.20×0.20×0.20	0.20×0.20×0.20	0.20×0.20×0.20
Crystal system	Orthorhombic	Monoclinic	Monoclinic	Monoclinic
Space group	<i>Pna</i> 2 ₁	<i>Cc</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> [Å]	8.2815(3)	3.6672(3)	12.7140(16)	12.9556(15)
<i>b</i> [Å]	16.56970(10)	24.648(2)	8.0602(10)	8.7565(10)
<i>c</i> [Å]	4.7742(3)	7.3252(7)	7.0415(8)	6.4841(8)
<i>α</i> [Å]	90	90	90	90
<i>β</i> [Å]	90	98.280(3)	95.899(3)	104.077(3)
<i>γ</i> [Å]	90	90	90	90
<i>V</i> [Å ³]	655.13(5)	655.21(10)	717.77(15)	713.50(15)
<i>Z</i>	4	4	4	4
<i>T</i> [K]	296(2)	296(2)	296(2)	296(2)
<i>ρ</i> [g cm ⁻³]	1.735	1.725	1.723	1.724
<i>μ</i> [mm ⁻¹]	0.146	0.139	0.145	0.139
<i>F</i> (000)	352	352	384	384
	-9 ≤ <i>h</i> ≤ 9	-4 ≤ <i>h</i> ≤ 3	-15 ≤ <i>h</i> ≤ 15	-15 ≤ <i>h</i> ≤ 15
Index range	-17 ≤ <i>k</i> ≤ 19	-30 ≤ <i>k</i> ≤ 25	-9 ≤ <i>k</i> ≤ 9	-10 ≤ <i>h</i> ≤ 10
	-5 ≤ <i>l</i> ≤ 5	-9 ≤ <i>l</i> ≤ 9	-8 ≤ <i>l</i> ≤ 8	-7 ≤ <i>h</i> ≤ 7
Reflections collected	2739	3026	12358	13615
<i>R</i> _{int}	0.0941	0.0350	0.0384	0.0643
Data/Restraints/Parameters	1009/1/109	1192/21/121	1262/0/119	1269/2/125
GOF on <i>F</i> ²	1.052	1.063	1.111	1.178
<i>R</i> ₁ [<i>I</i> > 2σ (<i>I</i>)]	0.0624	0.0386	0.0376	0.0572
<i>wR</i> ₂ [<i>I</i> > 2σ (<i>I</i>)]	0.1222	0.0821	0.0848	0.1306
<i>R</i> ₁ (all data)	0.1267	0.0489	0.0506	0.0794
<i>wR</i> ₂ (all data)	0.1519	0.0881	0.0913	0.1412
Largest diff. peak and hole [e Å ⁻³]	0.324/-0.403	0.171/-0.173	0.164/-0.207	0.315/-0.284

Table S2. Selected bond lengths [\AA] of **1-4**

Atoms 1-2	d (1-2) [\AA]	Atoms 1-2	d (1-2) [\AA]
1		2	
C1-N4	1.313(10)	C1-N1	1.335(4)
C1-N1	1.337(11)	C1-N4	1.338(4)
C1-C2	1.450(11)	C1-C2	1.453(4)
C2-N5	1.319(9)	C2-N6	1.314(4)
C2-N6	1.359(11)	C2-N5	1.360(4)
C3-N7	1.318(11)	C3-N7	1.305(4)
C3-N6	1.329(9)	C3-N5	1.322(4)
C3-H3	0.9300	N1-O1	1.309(3)
N1-O1	1.317(8)	N1-N2	1.348(4)
N1-N2	1.347(9)	N2-N3	1.307(4)
N6-H6	0.8600	N8-H8A	0.92(2)
N7-H7	0.8600	N8-H8B	0.87(2)
3		4	
C1-N4	1.332(2)	C1-N4	1.328(4)
C1-N1	1.333(2)	C1-N1	1.342(4)
C1-C2	1.450(2)	C1-C2	1.452(4)
C2-N6	1.320(2)	C2-N6	1.353(4)
C2-N5	1.357(2)	C3-N7	1.312(4)
N6-N7	1.349(2)	C3-N6	1.330(4)
N1-O1	1.3256(17)	N1-O1	1.323(3)
N1-N2	1.343(2)	N1-N2	1.341(3)
N8-O2	1.4058(18)	N2-N3	1.316(4)
H2-O2	0.8200	N8-H8A	0.889(18)
N8-H8A	0.8900	N8-H8B	0.896(19)
N8-H8B	0.8900	N9-H9A	0.8900

Table S3. Selected bond angles [°] of **1-4**

Atoms 1-2-3	\angle (1-2-3) [°]	Atoms 1-2-3	\angle (1-2-3) [°]
1		2	
N4-C1-N1	108.2(7)	N4-C1-N1	108.5(3)
N4-C1-C2	126.3(8)	C2-C1-N1	126.7(3)
N1-C1-C2	125.5(8)	N4-C1-C2	124.8(3)
N5-C2-N6	112.0(7)	N5-C2-N6	115.0(3)
N5-C2-C1	124.4(8)	N6-C2-C1	120.5(3)
N6-C2-C1	123.6(7)	N5-C2-C1	124.5(3)
O1-N1-C1	129.6(7)	O1-N1-C1	130.4(3)
O1-N1-N2	121.9(7)	O1-N1-N2	121.4(3)
C1-N1-N2	108.5(7)	C1-N1-N2	108.2(3)
N1-N2-N3	105.9(7)	N1-N2-N3	106.5(3)
N2-N3-N4	110.4(7)	N2-N3-N4	111.0(3)
C2-N6-C3	118.24(14)	C2-N6-N6	110.9(3)
C2-N6-H6	127.2	C3-N7-H7	124.5
3		4	
N4-C1-N1	107.99(15)	N4-C1-N1	107.7(2)
N4-C1-C2	124.39(15)	N4-C1-C2	124.8(3)
N1-C1-C2	127.61(16)	N1-C1-C2	127.5(3)
N5-C2-N6	114.59(16)	N5-C2-N6	114.8(3)
N6-C2-C1	119.28(16)	N5-C2-C1	119.8(3)
N5-C2-C1	126.13(15)	N6-C2-C1	125.4(3)
O1-N1-C1	129.58(14)	O1-N1-C1	122.0(2)
O1-N1-N2	121.39(13)	O1-N1-N2	128.9(2)
C1-N1-N2	109.03(14)	C1-N1-N2	109.1(2)
N1-N2-N3	106.17(14)	N1-N2-N3	106.1(2)
N2-N3-N4	110.66(15)	N2-N3-N4	110.3(2)
C1-N4-N3	106.15(14)	C2-N5-N7	102.2(3)
N7-C3-H3	124.8	C3-N7-N5	110.5(3)

Table S4. Selected torsion angles [°] of 1-4

Atoms(1-2-3-4)	α (1-2-3-4) [°]	Atoms(1-2-3-4)	α (1-2-3-4) [°]
1		2	
N4-C1-C2-N5	179.1(9)	N1-C1-C2-N6	171.9(3)
N1-C1-C2-N5	-0.4(12)	N4-C1-C2-N6	-6.7(5)
N4-C1-C2-N6	0.4(12)	N1-C1-C2-N5	-8.0(5)
N1-C1-C2-N6	-179.1(9)	N4-C1-C2-N5	173.3(3)
N4-C1-N1-O1	-179.7(7)	N4-C1-N1-O1	-179.0(3)
C2-C1-N1-O1	0.0(13)	C2-C1-N1-O1	2.2(5)
N4-C1-N1-N2	-0.4(9)	N4-C1-N1-N2	0.1(3)
C2-C1-N1-N2	179.2(7)	C2-C1-N1-N2	-178.8(3)
O1-N1-N2-N3	179.2(6)	O1-N1-N2-N3	179.3(3)
C1-N1-N2-N3	0.0(9)	C1-N1-N2-N3	0.2(3)
N1-N2-N3-N4	0.5(9)	N1-N2-N3-N4	-0.3(4)
N1-C1-N4-N3	0.7(9)	N1-C1-N4-N3	-0.3(3)
3		4	
N4-C1-C2-N6	-1.4(3)	N4-C1-C2-N5	-4.4(5)
N1-C1-C2-N6	-179.79(17)	N1-C1-C2-N5	175.8(3)
N4-C1-C2-N5	177.55(18)	N4-C1-C2-N6	174.5(3)
N1-C1-C2-N5	-0.8(3)	N1-C1-C2-N6	-5.3(5)
N4-C1-N1-O1	179.84(15)	N4-C1-N1-O1	-179.5(3)
C2-C1-N1-O1	-1.6(3)	C2-C1-N1-O1	0.3(5)
N4-C1-N1-N2	-0.26(19)	N4-C1-N1-N2	-0.2(3)
C2-C1-N1-N2	178.33(16)	C2-C1-N1-N2	179.5(3)
O1-N1-N2-N3	-179.83(14)	O1-N1-N2-N3	179.6(2)
C1-N1-N2-N3	0.26(19)	C1-N1-N2-N3	0.3(3)
N1-N2-N3-N4	-0.16(19)	N1-N2-N3-N4	-0.2(3)
N1-C1-N4-N3	0.15(19)	N1-C1-N4-N3	0.1(3)

Table S5. Selected hydrogen bond angles [°] of **1-4**

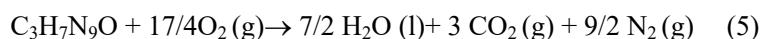
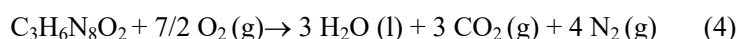
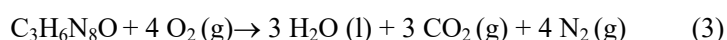
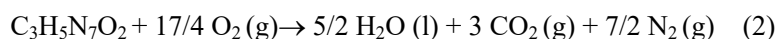
Atoms(D-H···A)	d(A···D) [Å]	Atoms(D-H···A)	d(A···D) [Å]
1		2	
N7-H7···O2	2.574	N8-H8A···O1	2.873
O2-H2A···O1	2.871	N8-H8B···N5	2.915
O2-H2A···N4	2.822	N8-H8B···O1	3.032
O2-H2B···N7	3.060	N8-H8C···N2	3.120
N6-H6···O1	2.578	N8-H8D···O1	2.942
N6-H6···N4	2.980	N7-H7···N4	2.104
3		4	
N8-H8A···N3	2.987	N8-H8A···O1	3.078
N8-H8A···N5	2.934	N8-H8B···O1	3.078
N8-H8B···O1	2.786	N9-H9A···O1	2.823
N8-H8B···N3	2.987	N9-H9B···N8	2.922
N8-H8B···O2	1.408	N9-H9C···O1	2.890
O2-H2···O1	2.630	N9-H9C···N6	3.031
O2-H2···N8	1.408	N7-H7···N4	2.843

Heats of formation

The constant-volume combustion energies of four compounds were measured by a precise oxygen bomb calorimeter. The experimental constant volume combustion energies ($\Delta_c U$) of compounds can be converted to the standard molar combustion enthalpy ($\Delta_c H_m^\theta$) based on equation (1).^[2] Their combustion reaction equation is listed as equation (2-5):

$$\Delta_c H_m^\theta = \Delta_c U + \Delta nRT \quad (1)$$

where $\Delta n = n_g(\text{products}) - n_g(\text{reactants})$, (n_g is the total molar amount of gases in the products or reactants, $R = 8.314 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$, $T = 298.15 \text{ K}$).



Based on the calculated enthalpies of combustion and known enthalpies of formation of the combustion products determined experimentally,^[3] $\Delta_f H_m^\theta(\text{H}_2\text{O}, \text{l}) = -285.83 \text{ kJ}\cdot\text{mol}^{-1}$, $\Delta_f H_m^\theta(\text{CO}_2, \text{g}) = -393.51 \text{ kJ}\cdot\text{mol}^{-1}$. The $\Delta_c U$ of **1-4** was $-1919.71 \text{ kJ}\cdot\text{mol}^{-1}$ and $-2368.58 \text{ kJ}\cdot\text{mol}^{-1}$, $-2279.48 \text{ kJ}\cdot\text{mol}^{-1}$ and $-2524.07 \text{ kJ}\cdot\text{mol}^{-1}$, respectively, measured by a precise oxygen bomb calorimeter. The $\Delta_c H_m^\theta$ of **1-4** was calculated as $-1903.61 \text{ kJ}\cdot\text{mol}^{-1}$ and $-2351.24 \text{ kJ}\cdot\text{mol}^{-1}$, $-2262.14 \text{ kJ}\cdot\text{mol}^{-1}$ and $-2505.49 \text{ kJ}\cdot\text{mol}^{-1}$, respectively.

Reference

[1] Bruker. APEX2 v2010.3-0. Bruker AXS Inc. Madison, Wisconsin, USA. **2010**.

[2] Zhang, J. H.; Jin, B.; Li, X.Y.; Hao, W. J.; Huang, T.; Lei, B.; Guo, Z. C.; Shen, J.; Peng, R. F. Study of H_2AzTO -based energetic metal-organic frameworks for catalyzing the thermal decomposition of ammonium perchlorate. *Chem. Eng. J.* **2021**, *404*, 126287–126293.