Supporting information

Constructing energetic hydroxytetrazole with high thermal stability by connecting aminotriazole onto 1-hydroxytetrazole

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Content

1 Experimental Sections

Cautions! Strong acids, bases and other hazardous chemicals are used in the chemical

reaction process involved in this article. Wearing protective equipment during the entire experiment is strongly recommended.

General methods: Single-crystal X-ray diffraction measurements were conducted on a Bruker Smart Apex II diffractometer using Mo-Kα radiation (λ = 0.71073 Å) with a graphite monochromator at 296 K. NMR spectra were recorded on Bruker AVANCE III 500MHz at 25 ºC. The onset decomposition temperature (DSC) was measured using NETZSCH DSC204 F1 Phoenix differential scanning calorimeter at a heating rate of 5 °C min^{-1} under a dry nitrogen atmosphere. Infrared spectra (IR) were obtained on a ThermoFisher NICOLETIS10 instrument at 25 °C. Elemental analyses of C/H/N were investigated on a ThermoFisher FLASHSMART Elemental Analyzer (by multiple (5 times, 2~50 mg / times) measurements). Impact and friction sensitivities were tested by a BAM fallhammer and friction tester. Densities were determined at room temperature by employing a Micromeritics AccuPyc 1340 gas pycnometer.

1.1 Synthesis of 5-(5-amino-4H-1,2,4-triazol-3-yl)-1H-tetrazol-1-ol (ATTO)

Compound **1**[25] (3.16 g, 20 mmol) was added to 100 mL methanol solution of sodium methoxide (3.24 g, 60 mmol) in batches, stirred violently at 0 ℃ for 30min, and then heated to room temperature. Afterwards, aminoguanidine sulfate (14.8 g) was added to the mixture in batches, and then slowly heated to 60 ° C and reacted continuously for 24 hours at this temperature. After the reaction is completed, filter the mixture in hot solution and rinse the filter cake with 20 ml of methanol. Then adjust the pH of the collected methanol to weakly acidic (pH = 4) with a 20% hydrochloric acid, and filter the mixture to obtain a yellow solid product after evaporating half of the solution.

Yield 2.32 g (69.0%). ^{13}C NMR (125 MHz, DMSO-d_6): 157.88, 146.07, 141.76; ^{1}H NMR (500 MHz, DMSO-d_6): 9.47, 7.76, 6.47; IR (KBr): 3348.29, 3271.44, 3146.41, 2249.85, 1808.50, 1679.66, 1619.27, 1547.95, 1454.04, 1425.44, 1355.82, 1266.30, 1226.27, 1172.17, 1135.08, 1086.57, 1033.32, 1018.02, 975.70, 934.39, 822.21, 756.10, 734.43, 716.31, 691.63 cm^{-1}; Element analysis ($C_3N_8OH_4$), calculated (%): C 21.43, H 2.40, N 66.65; measured (%): C 21.98, H 2.11, N 66.00.

1.2 Synthesis of 5-(5-amino-1,3,4-oxadiazol-2-yl)-1H-tetrazol-1-ol (AOTO)

Compound **2**[25] (2.88 g, 20 mmol) was dispersed in a 40 mL ethanol solution, and 20 ml of water dissolved in sodium bicarbonate (4.20 g, 50 mmol) was added to the aforementioned solution in batches under stirring at room temperature. When the above mixture is stirred at room temperature for 30 min, cyanogen bromide (2.54 g, 24 mmol) is added to it. After the mixture is stirred for 24 h, 20% hydrochloric acid is added to it until the PH is 3. Then continue stirring the mixture for 1 hour, filter, and rinse the filter cake with ice water to obtain a white solid product.

Yield 2.41 g (71.3%). ^{13}C NMR (125 MHz, DMSO-d_6): 165.04, 146.40, 136.43, ^{1}H NMR (500 MHz, DMSO-d_6): 7.74; IR (KBr): 3470.21, 3409.06, 3137.82, 2697.32, 1732.83, 1659.79, 1633.65, 1506.99, 1313.01, 1245.59, 1181.80, 1155.28, 1093.72, 1020.46, 999.85, 831.88, 783.67, 746.55, 674.21, 652.79 cm^{-1}; Element analysis ($C_3N_7O_2H_3$), calculated (%): C 21.31, H 1.79, N 57.98; measured (%): C 20.46, H 2.20, N 58.87.

1.3 Synthesis of the salts (3, 4, 5 and 6) and co-crystal (ATTO-N_2H_4) of ATTO and AOTO

ATTO (0.168 g, 1 mmol) or **AOTO** (0.169 g, 1 mmol) were added to ammonia water (40 mL, 28%), hydroxylamine solution (40 mL, 50%), and hydrazine hydrate (40 mL, 85%) at room temperature, respectively. The reaction solution was stirred at room temperature for 2 h, filtered, and the corresponding crystalline products were obtained after slowly evaporating the filtrate.

For **3**, yield 0.164 g (88.6 %). ^{13}C NMR (125 MHz, DMSO-d_6): 159.82, 146.83, 137.32, ^{1}H NMR (500 MHz, DMSO-d_6): 7.44, 5.97; IR (KBr): 3562.39, 3428.05, 3309.49, 3063.05, 2851.09, 2168.36, 1634.51, 1587.78, 1502.48, 1410.46, 1362.60, 1238.68, 1205.11, 1103.10, 1050.04, 1016.25, 986.52, 751.23, 707.36, 688.93, 647.04, 579.35 cm^{-1}; Element analysis ($C_3N_9OH_7$), calculated (%): C 19.46, H 3.81, N 68.09; measured (%): C 18.88, H 4.20, N 68.87.

For **4**, yield 0.182 g (90.1 %). ^{13}C NMR (125 MHz, DMSO-d_6): 159.01, 146.91, 138.03, ^{1}H NMR (500 MHz, DMSO-d_6): 6.18; IR (KBr): 3341.78, 3174.22, 3003.27, 2687.07, 2459.98, 1666.55, 1618.55, 1592.16, 1507.71, 1444.27, 1344.61, 1241.31,

1206.08, 1126.50, 1084.91, 1058.02, 1002.94, 989.32, 868.99, 745.41, 718.41, 684.79, 660.51, 578.57 cm^{-1}; Element analysis ($C_3N_9O_2H_7$), calculated (%): C 17.91, H 3.51, N 62.67; measured (%): C 16.99, H 3.98, N 63.43.

For **5**, yield 0.169 g (91.2 %). ^{13}C NMR (125 MHz, DMSO-d_6): 164.24, 148.91, 133.06, ^{1}H NMR (500 MHz, DMSO-d_6): 7.35; IR (KBr): 3133.34, 2827.95, 1667.66, 1592.81, 1485.37, 1434.44, 1398.59, 1302.39, 1237.32, 1160.44, 1113.79, 1078.13, 1033.52, 1007.98, 970.14, 827.48, 741.78, 726.32, 673.87; Element analysis ($C_3N_8O_2H_6$), calculated (%): C 19.36, H 3.25, N 60.20; measured (%): C 20.08, H 2.72, N 61.03.

For **6**, yield 0.186 g (92.7 %). ^{13}C NMR (125 MHz, DMSO-d_6): 164.22, 149.04, 132.94, ^{1}H NMR (500 MHz, DMSO-d_6): 7.32, 7.10; IR (KBr): 3288.14, 3126.25, 2649.81, 1674.37, 1599.56, 1486.68, 1417.13, 1303.37, 1241.57, 1163.38, 1145.98, 1113.02, 1081.99, 1028.51, 1009.92, 972.02, 752.57, 740.01, 674.91, 586.55; Element analysis ($C_3N_9O_2H_7$), calculated (%): C 17.91, H 3.51, N 62.67; measured (%): C 17.00, H 4.42, N 61.83.

For **ATTO-N_2H_4**, yield 0.181 g (90.6 %). ^{1}H NMR (500 MHz, DMSO-d_6): 5.59; IR (KBr): 3397.44, 3159.34, 2812.04, 2604.71, 1655.52, 1618.08, 1536.27, 1499.73, 1415.68, 1304.84, 1229.77, 11210.19, 1152.51, 1126.02, 1037.05, 986.07, 959.24, 767.49, 744.33, 724.91, 692.01, 665.28, 589.78; Element analysis ($C_3N_9O_2H_3$), calculated (%): C 18.00, H 4.03, N 69.98; measured (%): C 17.11, H 4.42, N 70.83.

2 Crystallographic data

Table S1 Crystallography data sheet for compounds **AOTO·H_2O**, **ATTO·N_2H_4** and **3**.

Comp.	**AOTO·H_2O**	**ATTO·N_2H_4**	**3**
Formula	$C_3H_3N_7O_2·H_2O$	$C_3H_4N_8O·N_2H_4$	$C_3H_3N_8O·H_2O·NH_4$
Temperature	296(2) K	296(2) K	296(2) K
System	Monoclinic	Orthorhombic	Monoclinic

Space group	$P2_1/n$	Cmca	$P2_1/c$
Dimensions	a = 7.2861(5) Å b = 5.9922(4) Å c = 8.2491(6) Å α= 90° β= 97.669(2) ° γ = 90°	a = 6.5314(4)Å b = 25.0039(17) Å c = 9.2895(6) Å α= 90 ° β= 90 ° γ = 90°	a = 9.2271(12) Å b = 14.2917(17) Å c = 6.4999(8) Å α= 90° β= 101.078(4) ° γ = 90°
Volume/ $Å^3$	356.93(4)	1517.07(17)	841.18(18)
Z	2	8	4
Density / $g·cm^{-3}$	1.741	1.753	1.604
F(000)	192	832	424
Theta range / °	2.821 to 27.480	2.732 to 24.983	2.663 to 27.559
Index ranges	-9≤h≤9, -7≤k≤7, -9≤l≤10	0≤h≤7, 0≤k≤29, 0≤l≤11	-11≤h≤9, -18≤k≤16, -8≤l≤8
Reflections collected	3318	724	8363
Independent reflections	892 [R(int) = 0.0238]	724 [R(int) = 0.0288]	1940 [R(int) = 0.0331]
Data/restraints/ parameters	892 / 3 / 89	724 / 0 / 85	1940 / 0 / 155
Goodness-of-fit on F^2	1.083	1.060	1.056
Final R indices [I>2sigma(I)]	R1 = 0.0410, wR2 = 0.1006	R1 = 0.0743, wR2 = 0.1669	R1 = 0.0535, wR2 = 0.1430
R indices (all data)	R1 = 0.0507, wR2 = 0.1067	R1 = 0.0810, wR2 = 0.1720	R1 = 00.0738, wR2 = 0.1554
CCDC Num.	2277160	2267698	2265664

Table S2 Crystallography data sheet for compounds **4**, **5** and **6**.

Comp.	**4**	**5**	**6**
Formula	$C_3H_3N_8O·NH_3OH$	$C_3H_2N_7O_2·NH_4$	$C_3H_2N_7O_2·N_2H_5$
Temperature	296(2) K	296(2) K	296(2) K
System Space group	Monoclinic P21/n	Monoclinic $P2_1$	Monoclinic $P2_1/c$

Dimensions	a = 7.7908(10) Å b = 15.457(2) Å c = 7.2605(11) Å a= 90° b= 114.635(4) ° g = 90°	a = 3.8698(2) Å b = 8.3310(5) Å c = 11.6487(8) Å α= 90 ° β= 95.015(2) ° γ = 90°	a = 25.649(5) Å b = 9.0726(16) Å c = 6.7690(14) Å a= 90° b= 92.424(6)° g = 90°
Volume/ Å^3	794.75(19)	374.11(4)	1573.8(5)
Z	4	2	8
Density / g·cm^{-3}	1.681	1.653	1.698
F(000)	416	192	832
Theta range / °	2.635 to 27.524	3.010 to 27.457	2.245 to 24.999
Index ranges	-9≤h≤9, -15≤k≤20, -9≤l≤9	-5≤h≤4, -10≤k≤10, -15≤l≤15	-30≤h≤29, -10≤k≤9, -8≤l≤8
Reflections collected	6393	3742	11860
Independent reflections	1803 [R(int) = 0.0395]	1548 [R(int) = 0.0216]	2712 [R(int) = 0.0616]
Data/restraints/ parameters	1803 / 0 / 139	1548 / 1 / 130	2712 / 0 / 257
Goodness-of-fit on F^2	1.075	1.109	1.078
Final R indices [I>2sigma(I)]	R1 = 0.0500, wR2 = 0.1125	R1 = 0.0322, wR2 = 0.0728	R1 = 0.0887, wR2 = 0.2414
R indices (all data)	R1 = 0.0769, wR2 = 0.1225	R1 = 0.0371, wR2 = 0.0758	R1 = 0.1017, wR2 = 0.2572
CCDC Num.	2268512	2217973	2217234

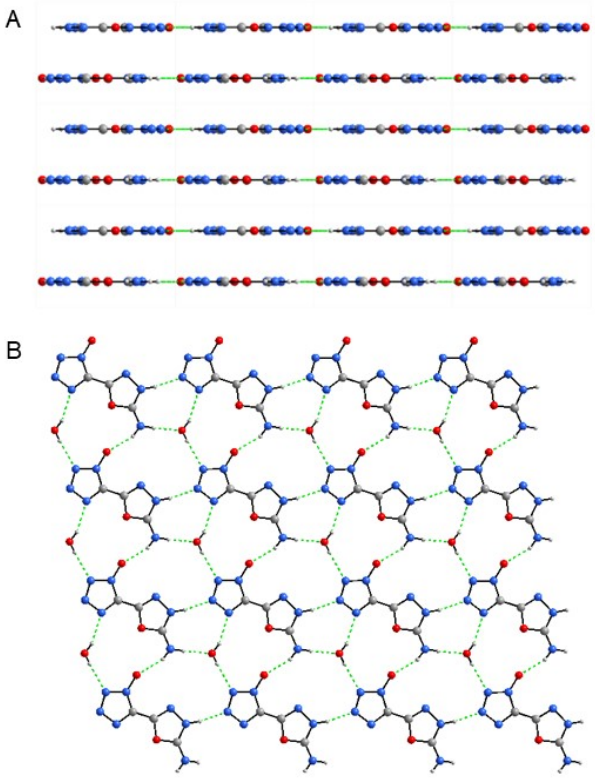

Figure S1 Interlayer (A) and intralayer (B) hydrogen bonding of **AOTO·H$_2$O** crystals (Green

dashed lines represent hydrogen bonds).

Table S3 Hydrogen Bond of Compound **AOTO·H_2O**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(3A)...N(4)#1	0.79(5)	2.10(6)	2.855(3)	160(5)
O(3)-H(3B)...N(2)	0.76(5)	2.10(5)	2.861(3)	177(5)
N(7)-H(7B)...O(3)#2	0.857(16)	1.858(17)	2.713(3)	177(3)
N(7)-H(7A)...O(2)#3	0.828(16)	1.974(17)	2.755(3)	157(3)
N(6)-H(6)...N(3)#4	0.92(3)	1.90(3)	2.808(3)	172(2)

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z #2 x-1,y,z+1 #3 x-1,y,z #4 x,y,z+1

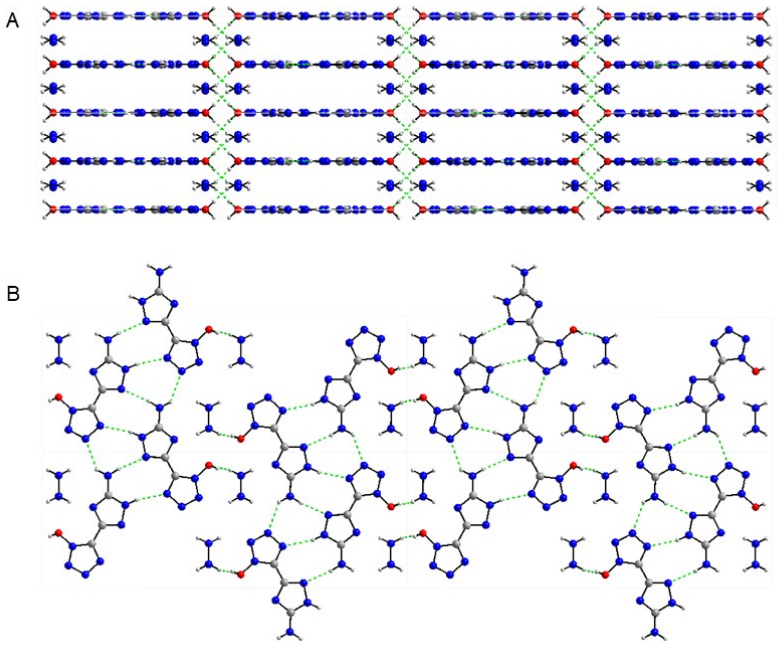

Figure S2 Interlayer (A) and intralayer (B) hydrogen bonding of **ATTO·N_2H_4** crystals (Green dashed lines represent hydrogen bonds).

Table S4 Hydrogen Bond of Compound **ATTO·N_2H_4**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(7)-H(7)...N(4)#3	0.86	2.13	2.976(7)	167.4
N(8)-H(8A)...N(6)#3	0.86	2.06	2.912(8)	171.8
N(8)-H(8B)...N(3)#4	0.86	2.26	2.952(8)	138.0
N(9)-H(9A)...O(1)#1	0.89	2.07	2.916(5)	158.0
N(9)-H(9B)...N(5)#5	0.89	2.20	3.056(5)	160.2
O(1)-H(1)...N(9)	0.82	2.69	3.414(5)	147.8
O(1)-H(1)...N(9)#1	0.82	2.10	2.916(5)	173.9

Symmetry transformations used to generate equivalent atoms:

#1 -x+3/2,y,-z+3/2 #2 -x+1,y,z #3 x,-y+1/2,z-1/2

#4 x,y,z-1 #5 x+1/2,-y+1,z+1/2

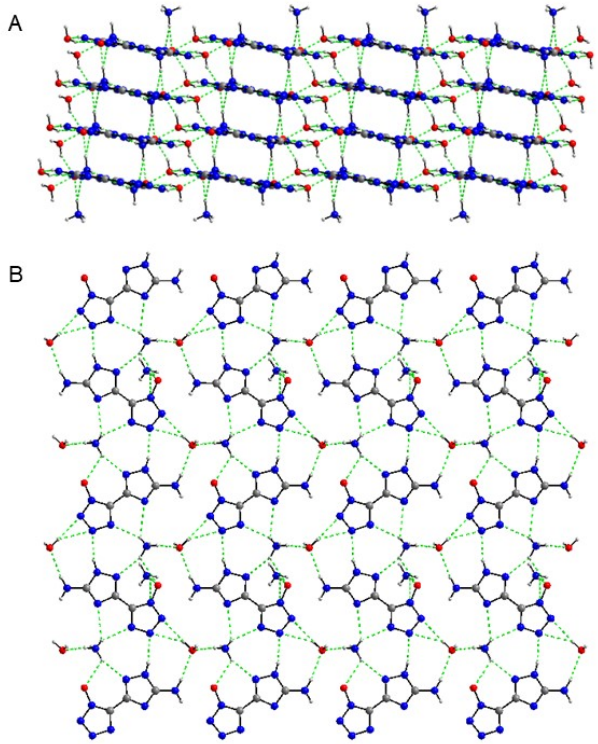

Figure S3 Interlayer (A) andintralayer (B) hydrogen bonding of **3** crystals (Green dashed lines represent hydrogen bonds).

Table S5 Hydrogen bond of compound **3**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(6)-H(6)...N(3)#1	0.84(3)	2.10(3)	2.921(3)	167(2)
N(8)-H(8B)...O(2)#2	0.86	2.23	3.075(3)	168.1
N(9)-H(9A)...O(2)#3	0.89(3)	2.00(3)	2.884(3)	170(2)
N(9)-H(9B)...N(1)#4	1.00(3)	2.50(3)	3.344(3)	142(2)
N(9)-H(9B)...O(1)#4	1.00(3)	1.84(3)	2.830(3)	172(2)
N(9)-H(9C)...N(4)#1	0.81(4)	2.27(4)	2.950(3)	141(4)
N(9)-H(9C)...N(7)#1	0.81(4)	2.58(4)	3.172(3)	130(3)
N(9)-H(9D)...N(5)	0.93(4)	2.17(4)	3.049(3)	158(3)
N(9)-H(9D)...O(1)	0.93(4)	2.35(4)	2.913(3)	119(3)
O(2)-H(2A)...N(1)	0.92(3)	2.70(3)	3.470(2)	141(2)
O(2)-H(2A)...O(1)	0.92(3)	1.85(3)	2.713(2)	156(3)
O(2)-H(2B)...N(2)#5	0.85(4)	2.27(4)	3.096(2)	164(4)
O(2)-H(2B)...N(3)#5	0.85(4)	2.48(4)	3.222(2)	146(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y+1/2,-z+1/2 #2 x-1,-y+3/2,z-1/2 #3 x,-y+3/2,z-1/2

#4 x,-y+3/2,z+1/2 #5 -x+2,-y+1,-z+1

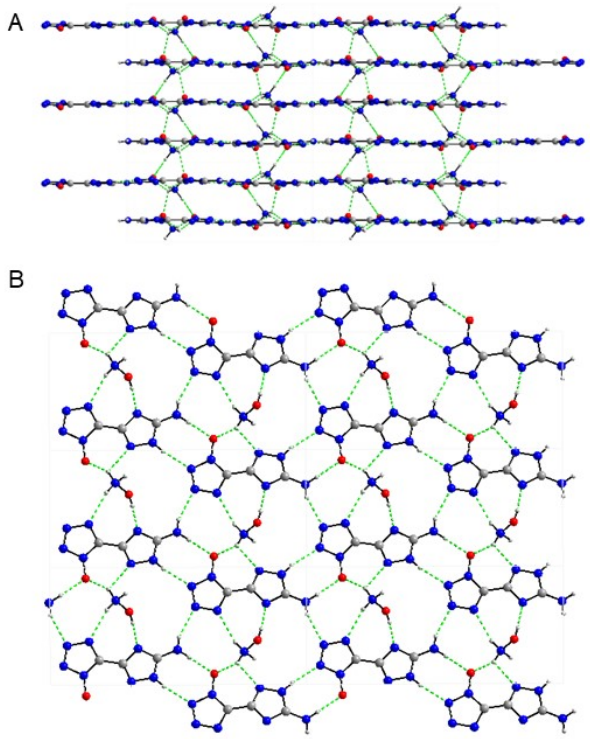

Figure S4 Interlayer (A) and intralayer (B) hydrogen bonding of **4** crystals (Green dashed lines represent hydrogen bonds).

Table S6 Hydrogen bond of compound **4**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(6)-H(6)...N(2)#1	0.86	2.11	2.967(2)	171.3
N(8)-H(8B)...O(1)#1	0.86	2.05	2.898(2)	169.4
N(8)-H(8A)...N(3)#2	0.86	2.20	3.013(2)	157.9
N(9)-H(9A)...N(4)	0.89(2)	2.18(2)	2.991(3)	151(2)
N(9)-H(9A)...O(2)#3	0.89(2)	2.36(2)	2.972(3)	125.7(18)
N(9)-H(9B)...N(7)#4	0.95(2)	2.39(2)	2.973(3)	118.9(16)
N(9)-H(9B)...O(1)#4	0.95(2)	1.95(2)	2.837(2)	152.7(19)
N(9)-H(9C)...N(1)#5	0.99(2)	2.59(2)	3.462(3)	147.8(17)
N(9)-H(9C)...O(1)#5	0.99(2)	1.84(2)	2.824(2)	175.2(19)
O(2)-H(2)...N(5)	0.82(3)	1.85(3)	2.662(2)	174(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,y+1/2,-z+3/2 #2 -x+1,y+1/2,-z+3/2 #3 x,-y+1/2,z-1/2

#4 x-1,y,z #5 x-1,-y+1/2,z-1/2

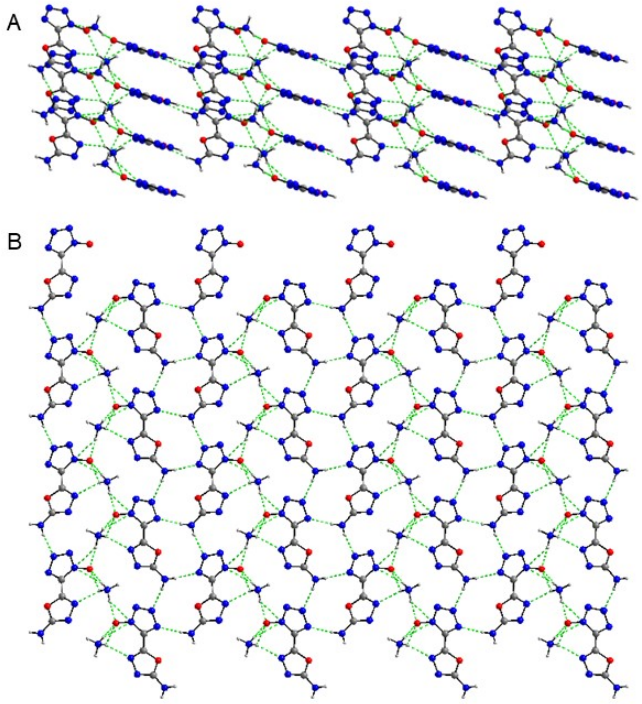

Figure S5 Interlayer (A) and intralayer (B) hydrogen bonding of **5** crystals (Green dashed lines represent hydrogen bonds).

Table S7 Hydrogen bond of compound **5**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(7)-H(7A)...N(5)#1	0.86	2.16	3.017(3)	171.6
N(7)-H(7B)...N(6)#2	0.86	2.13	2.984(3)	173.9
N(8)-H(8A)...N(3)#3	0.90(3)	2.55(3)	3.315(3)	143(2)
N(8)-H(8A)...O(2)#3	0.90(3)	1.92(3)	2.816(3)	173(2)
N(8)-H(8B)...N(3)	0.98(3)	2.56(3)	3.428(3)	148(2)
N(8)-H(8B)...O(2)	0.98(3)	1.83(3)	2.810(3)	177(2)
N(8)-H(8C)...N(2)#4	0.87(3)	2.32(3)	3.093(3)	148(3)
N(8)-H(8C)...O(2)#4	0.87(3)	2.29(3)	2.896(3)	127(3)
N(8)-H(8D)...N(1)#5	0.93(3)	2.07(3)	2.949(3)	156(2)

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y-1,z #2 -x+1,y-1/2,-z+2 #3 -x+1,y+1/2,-z+1

#4 -x+2,y+1/2,-z+1 #5 x,y+1,z

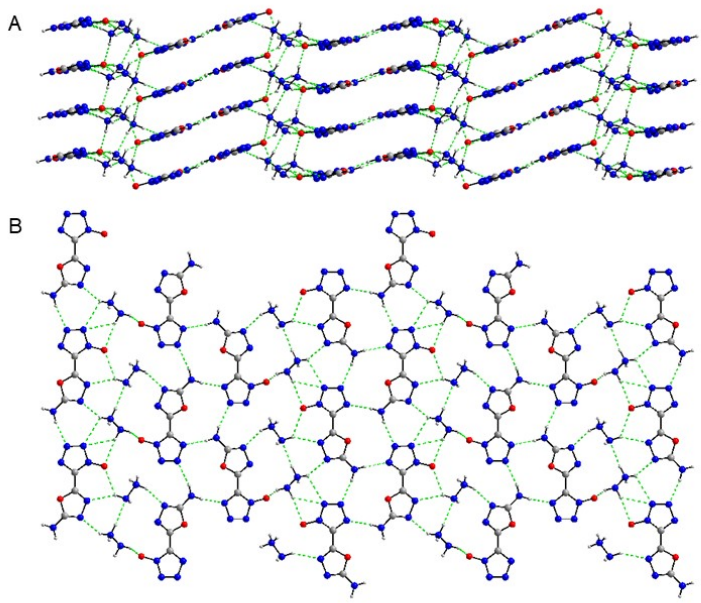

Figure S6 Interlayer (A) and intralayer (B) hydrogen bonding of **6** crystals (Green dashed lines represent hydrogen bonds).

Table S8 Hydrogen bond of compound **6**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(7)-H(7A)...N(3)#1	0.86	2.14	2.984(7)	166.6
N(7)-H(7B)...N(4)#2	0.86	2.10	2.951(6)	170.5
N(14)-H(14A)...N(10)#1	0.86	2.09	2.934(7)	168.5
N(14)-H(14B)...N(11)#3	0.86	2.10	2.954(7)	172.6
N(18)-H(18A)...N(16)#4	0.89	2.25	3.116(7)	163.1
N(18)-H(18B)...N(9)#5	0.89	2.59	3.051(7)	113.5
N(18)-H(18B)...N(13)#4	0.89	2.08	2.877(7)	148.4
N(18)-H(18C)...O(3)#6	0.89	1.84	2.731(8)	173.5
N(17)-H(17A)...O(3)#5	0.89	2.26	3.129(7)	166.8
N(17)-H(17A)...N(9)#5	0.89	2.54	3.179(7)	128.9
N(17)-H(17B)...O(1)	0.89	2.24	2.995(8)	142.8
N(16)-H(16A)...N(5)#7	0.89	2.52	3.160(7)	129.7
N(16)-H(16B)...O(3)	0.89	2.46	3.096(6)	129.1
N(16)-H(16B)...N(12)	0.89	2.32	3.117(6)	149.7
N(15)-H(15A)...N(17)	0.89	2.03	2.915(8)	174.0
N(15)-H(15B)...O(1)#7	0.89	1.91	2.802(6)	178.7
N(15)-H(15C)...N(6)#8	0.89	2.02	2.866(6)	159.1

Symmetry transformations used to generate equivalent atoms:

#1 x,y-1,z #2 -x+1,y-1/2,-z+3/2 #3 -x,y-1/2,-z+1/2

#4 x,-y+1/2,z+1/2 #5 x,-y+3/2,z+1/2 #6 x,y,z+1

#7 x,y,z-1 #8 x,-y+1/2,z-1/2

3 TG of compound 3, 4, 5, 6, AOTO, ATTO and ATTO-N_2H_4

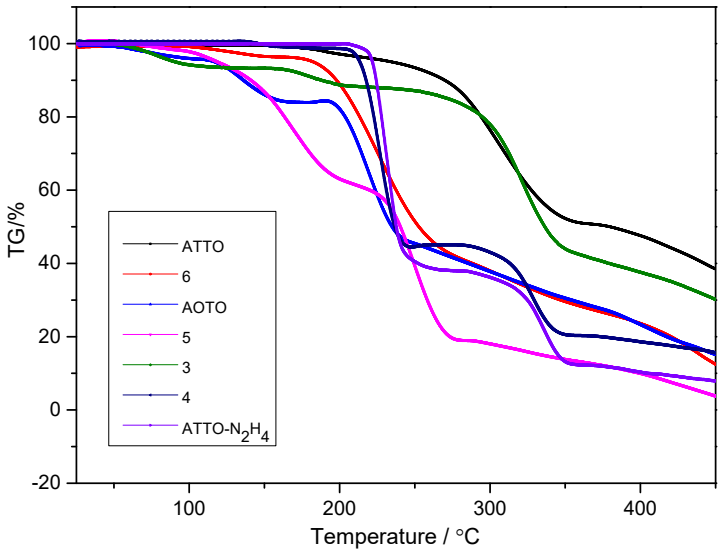

Figure S7 TG of **3, 4, 5, 6, AOTO, ATTO and ATTO-N_2H_4**.

4 IR and NMR spectrum

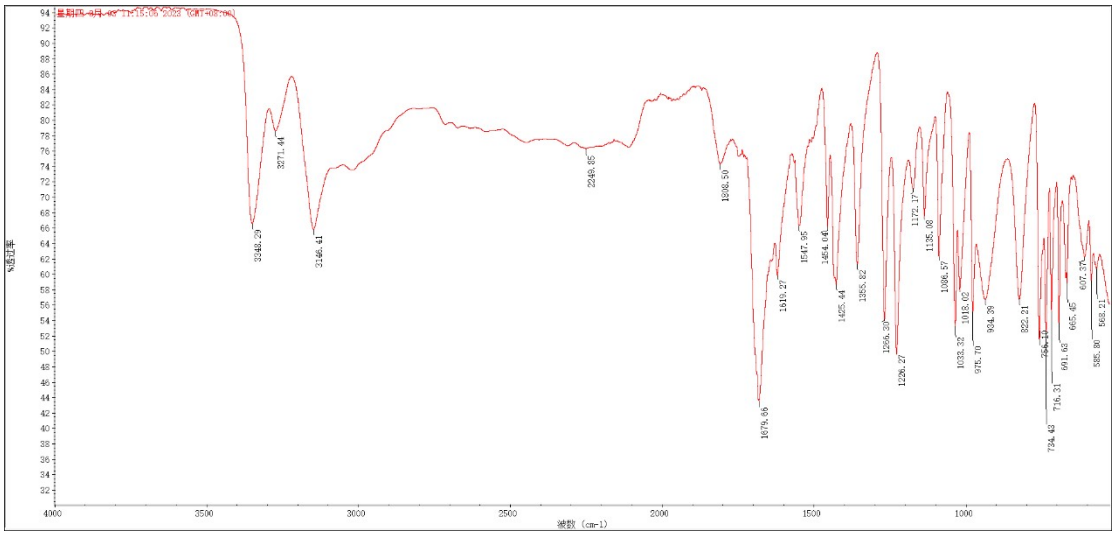

Figure S8 IR spectrum of **ATTO**.

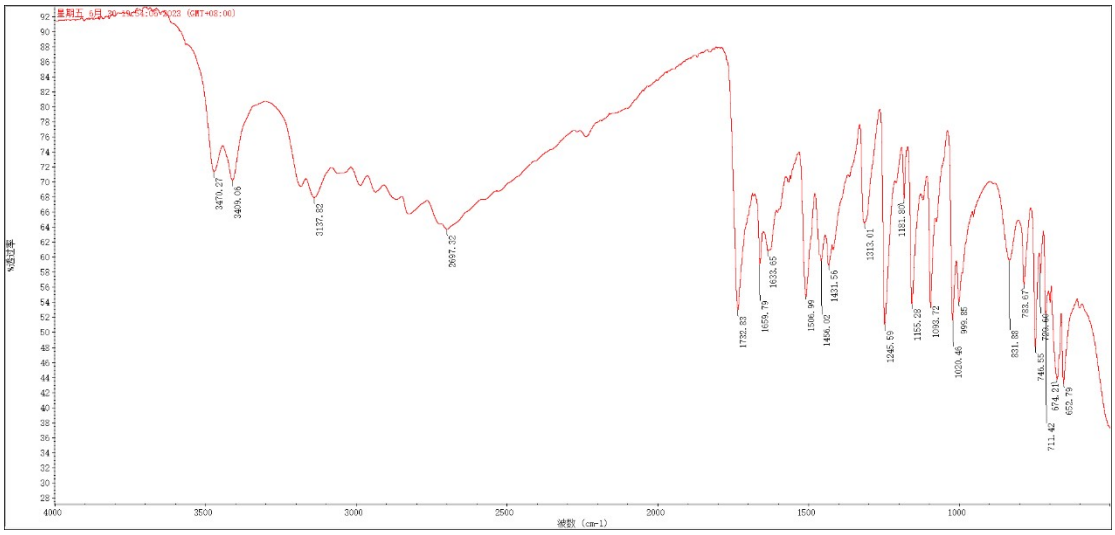

Figure S9 IR spectrum of **AOTO**.

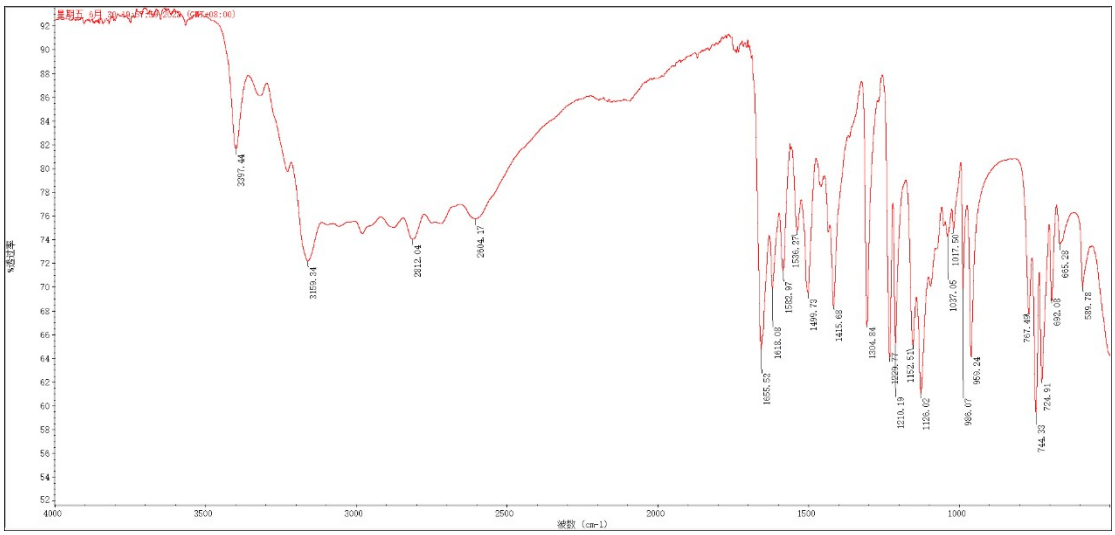

Figure S10 IR spectrum of **ATTO·N_2H_4**.

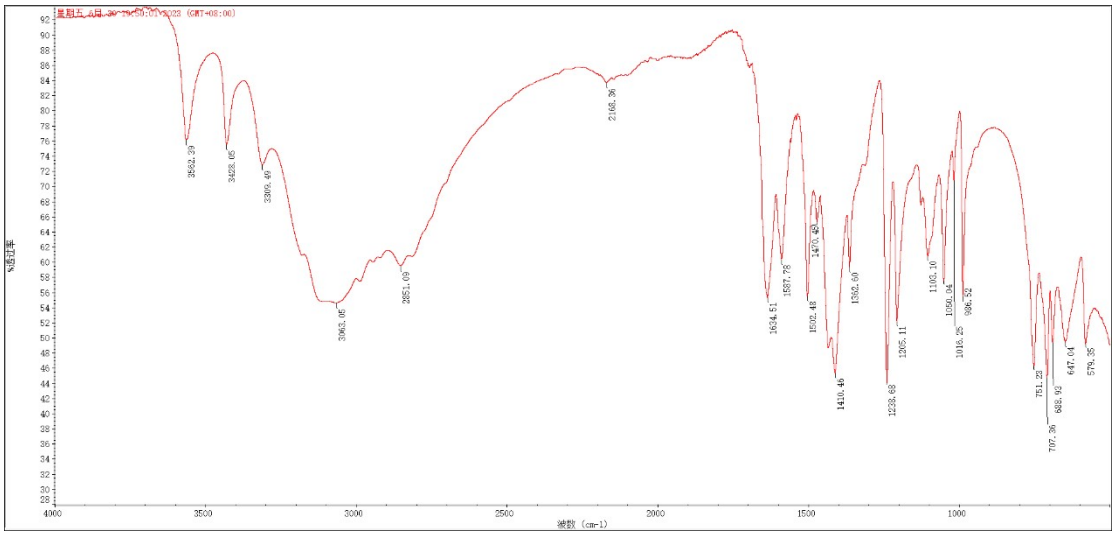

Figure S11 IR spectrum of **3**.

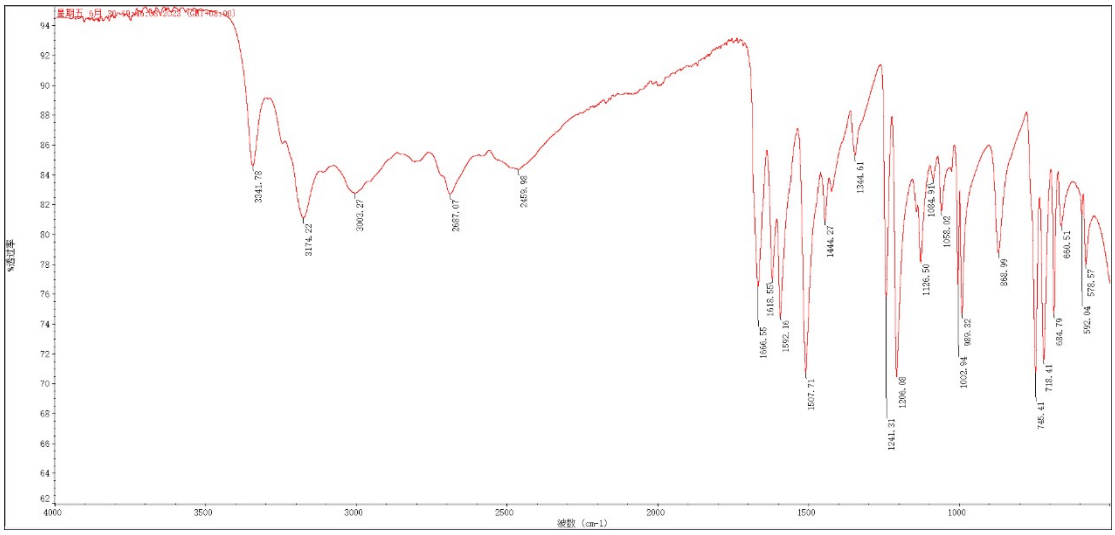

Figure S12 IR spectrum of **4**.

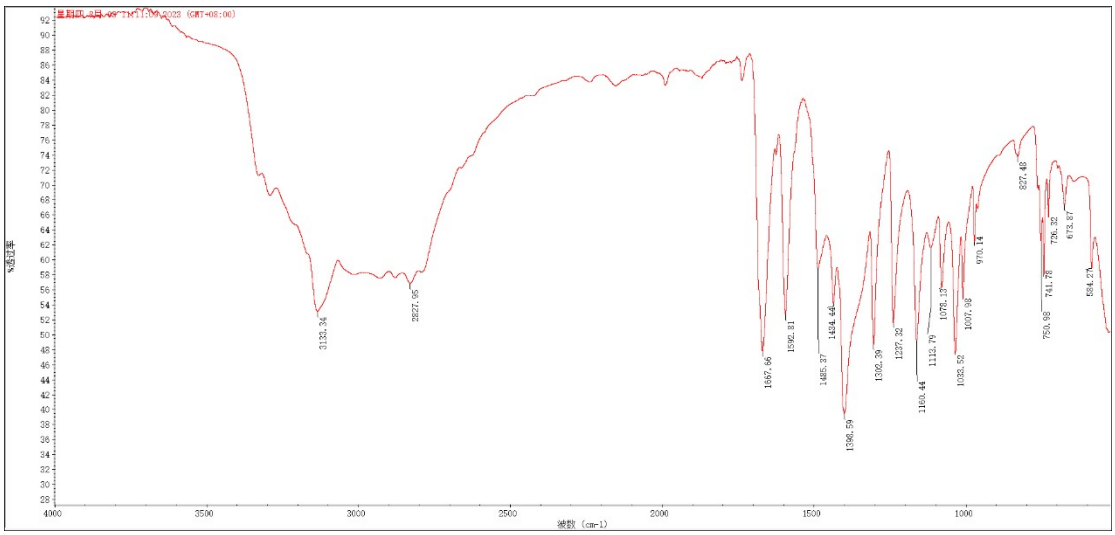

Figure S13 IR spectrum of **5**.

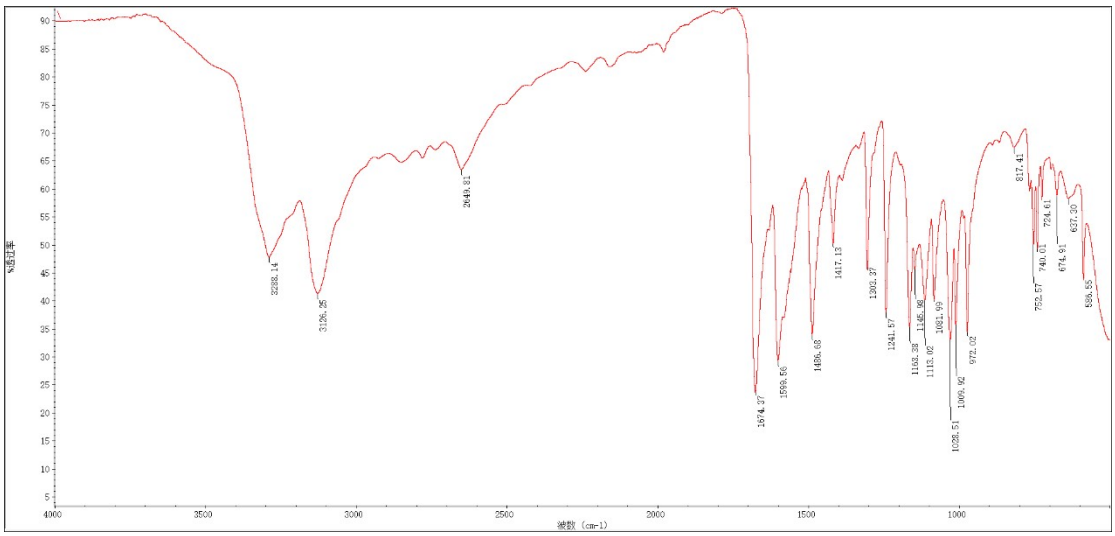

Figure S14 IR spectrum of **6**.

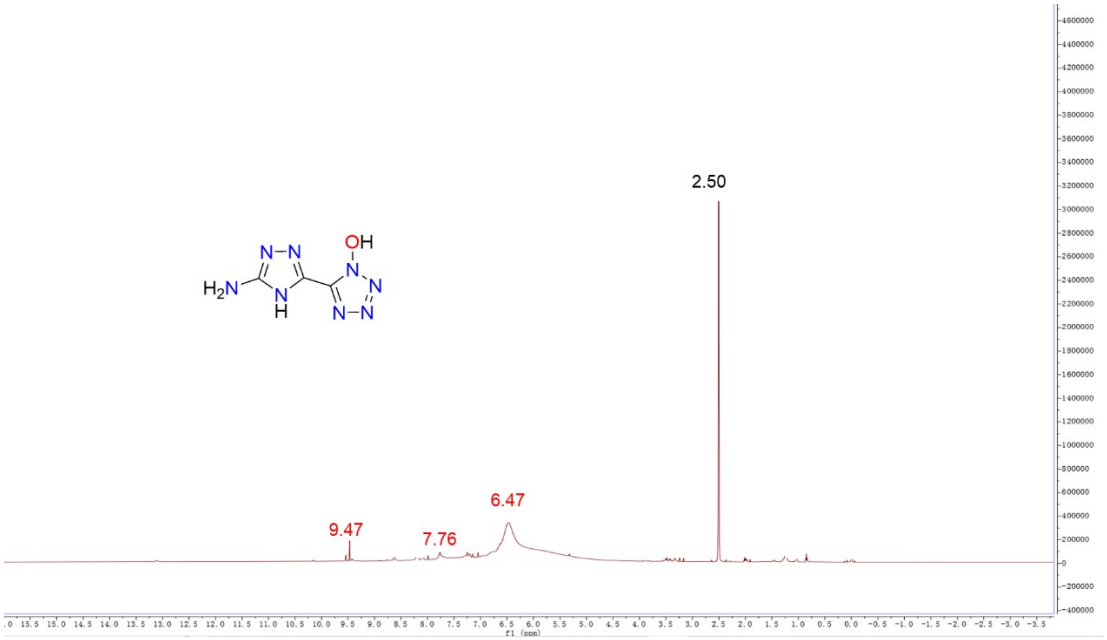

Figure S15 ^{1}H NMR spectrum of **ATTO** (DMSO-d_6).

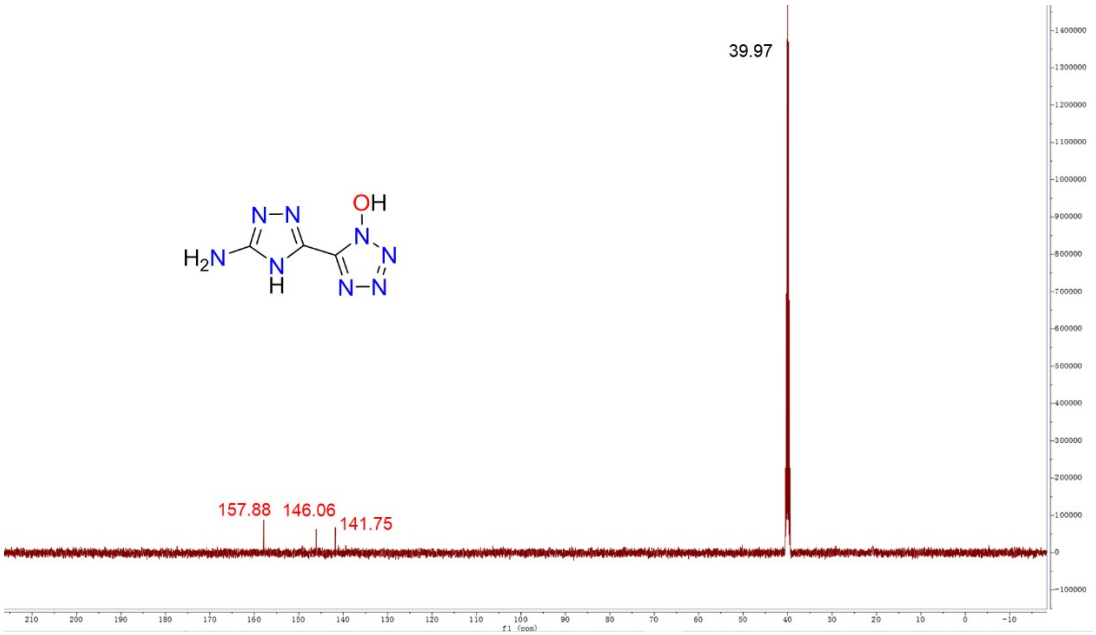

Figure S16 ^{13}C NMR spectrum of **ATTO** (DMSO-d_6).

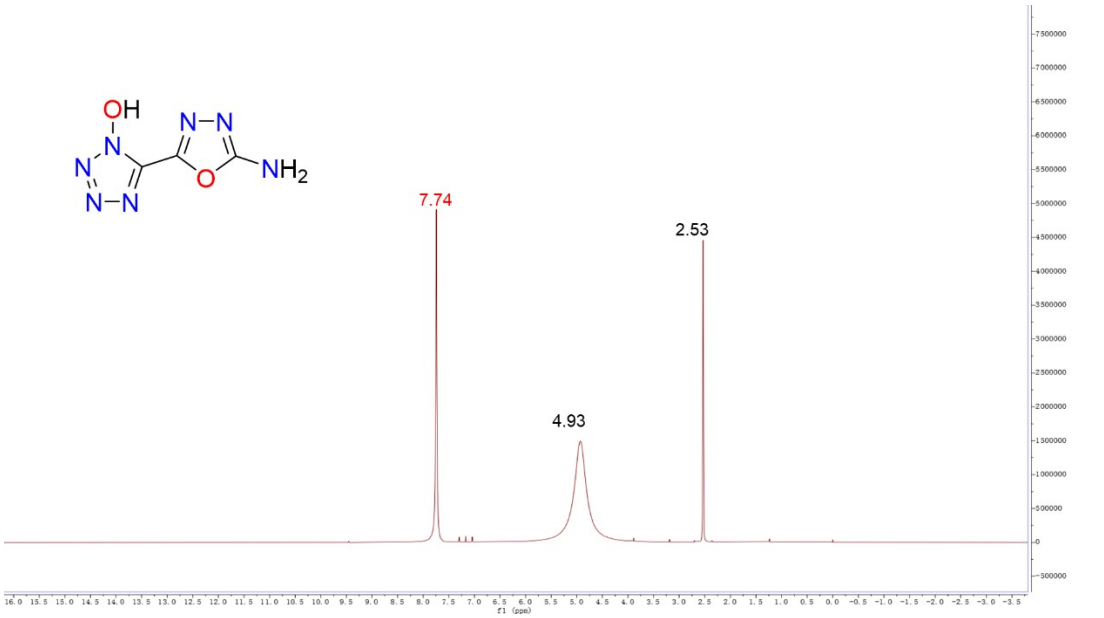

Figure S17 ^{1}H NMR spectrum of **AOTO** (DMSO-d_6).

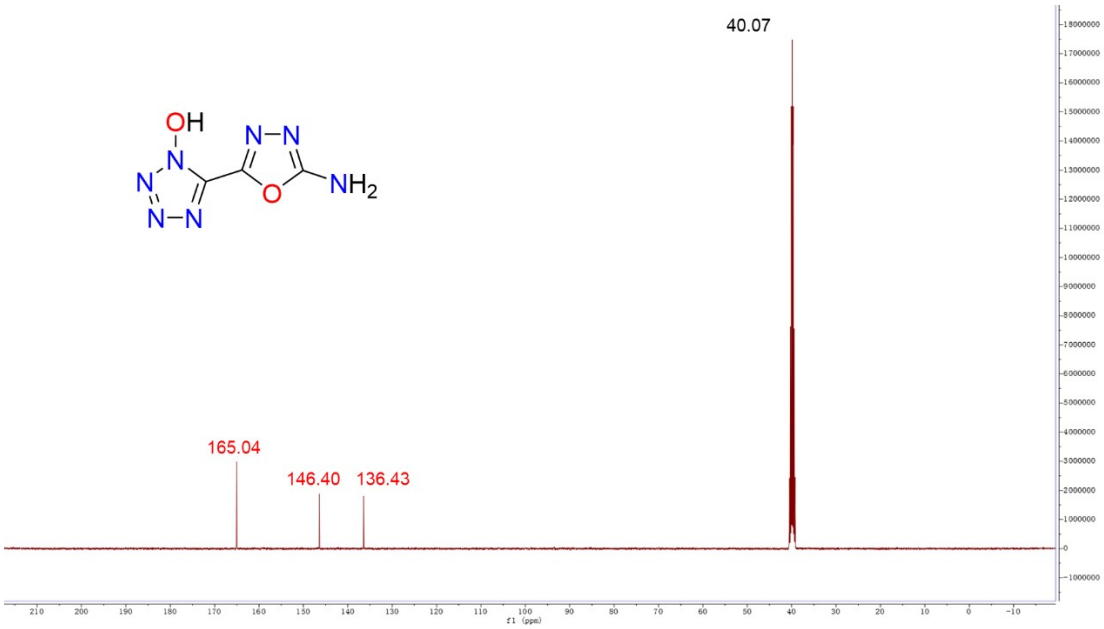

Figure S18 ^{13}C NMR spectrum of **AOTO** (DMSO-d_6).

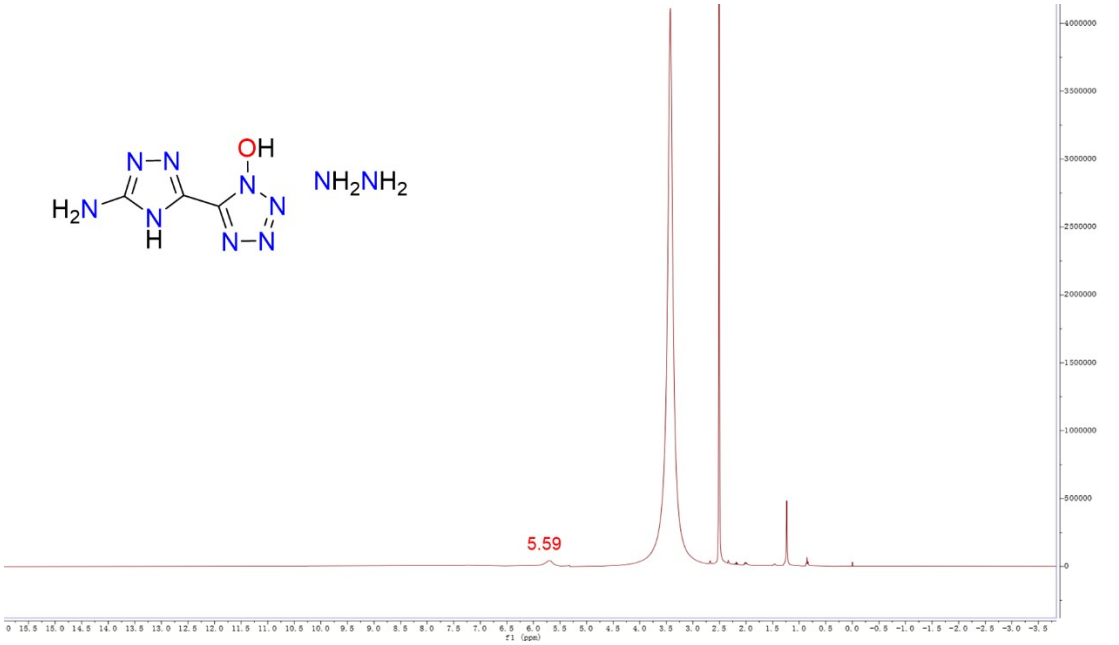

Figure S19 ^{1}H NMR spectrum of **ATTO-N_2H_4** (DMSO-d_6).

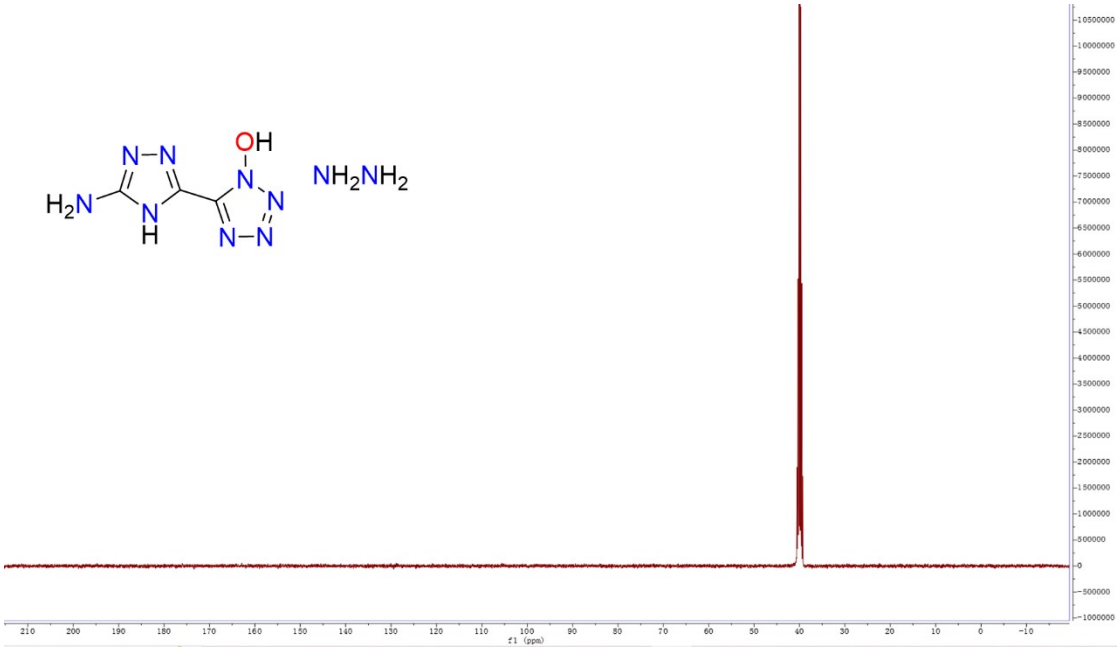

Figure S20 ^{13}C NMR spectrum of **ATTO-N_2H_4** (DMSO-d_6).

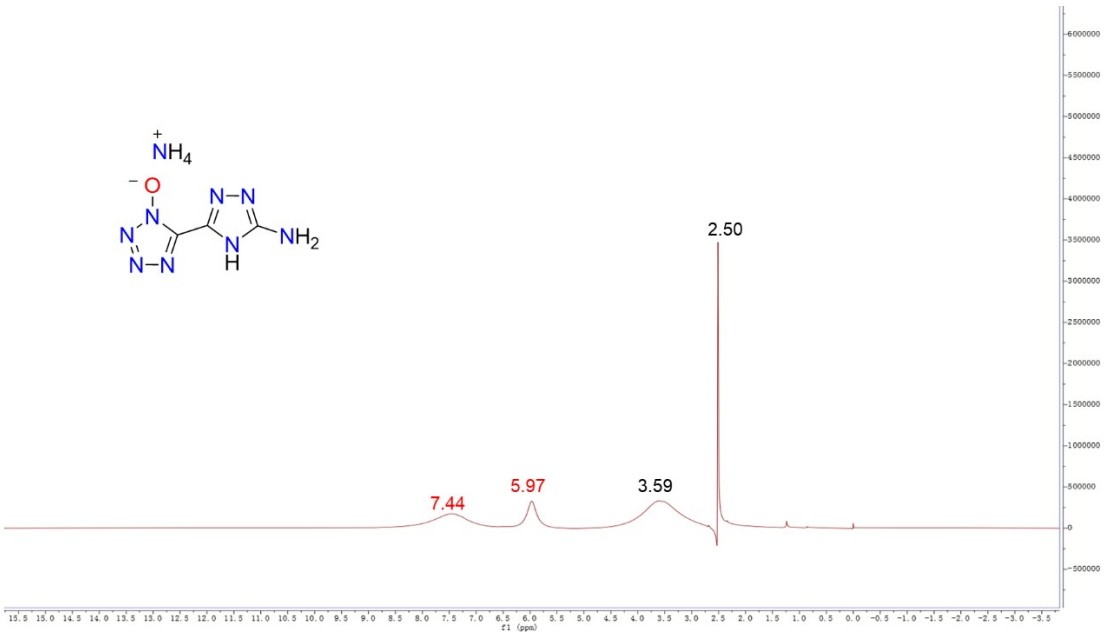

Figure S21 ^{1}H NMR spectrum of **3** (DMSO-d_6).

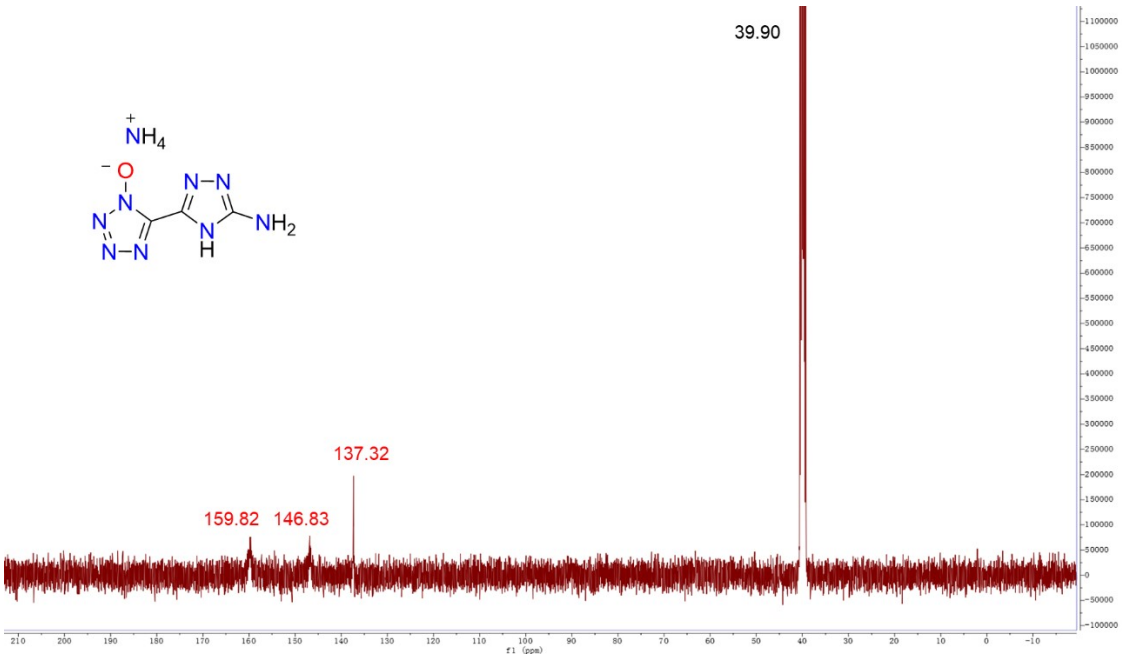

Figure S22 ^{13}C NMR spectrum of **3** (DMSO-d_6).

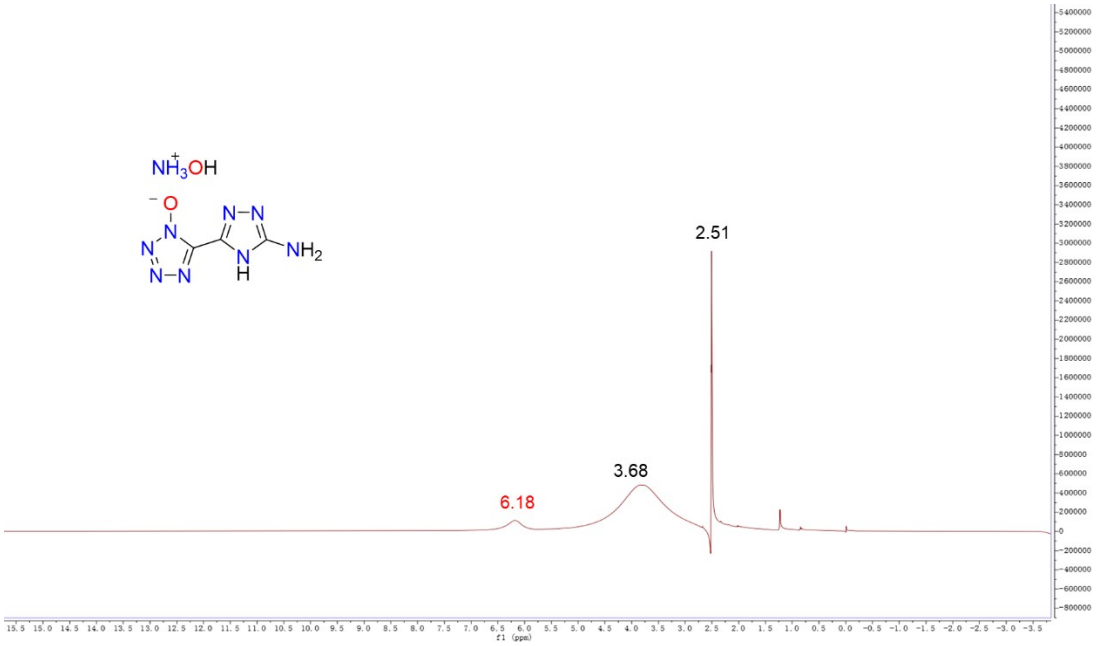

Figure S23 ^{1}H NMR spectrum of **4** (DMSO-d_6).

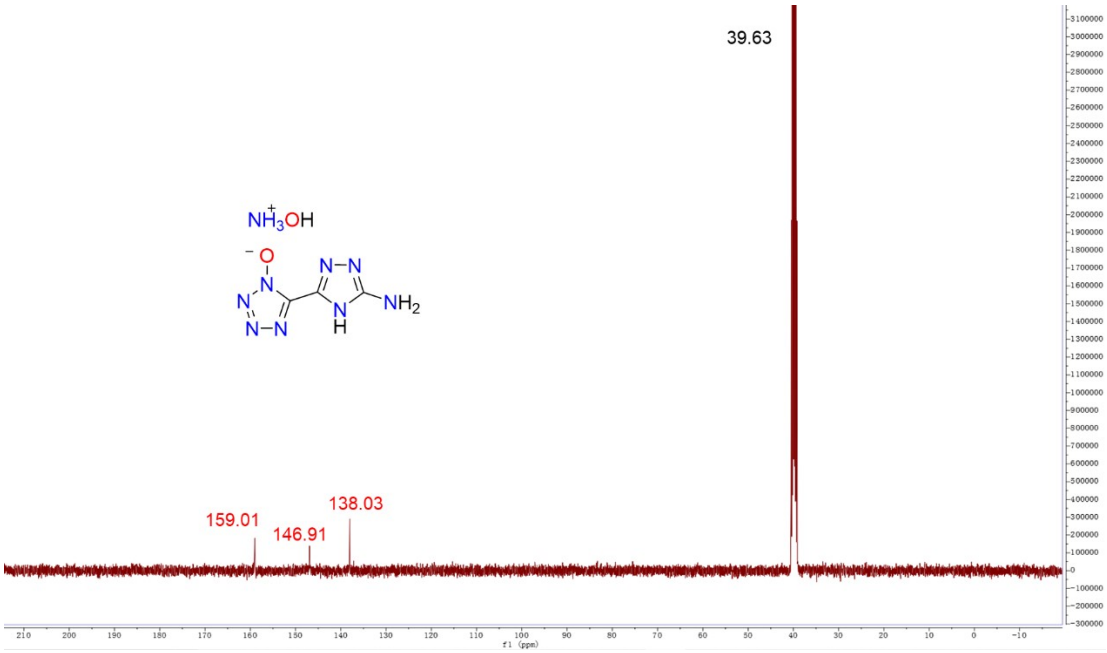

Figure S24 ^{13}C NMR spectrum of **4** (DMSO-d_6).

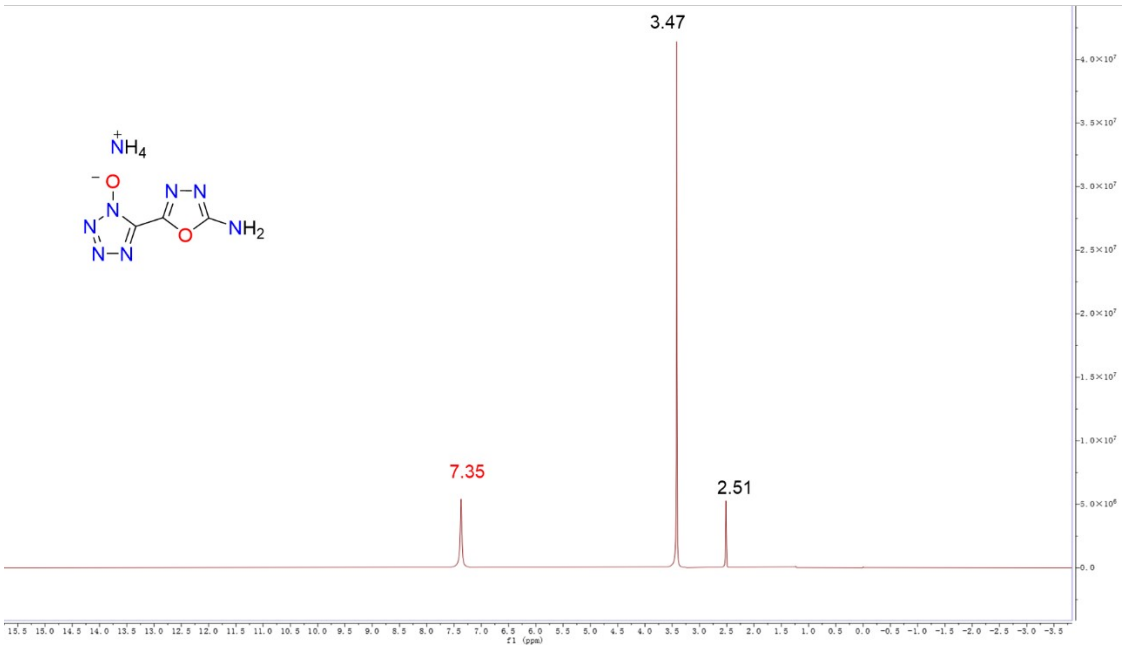

Figure S25 ^{1}H NMR spectrum of **5** (DMSO-d_6).

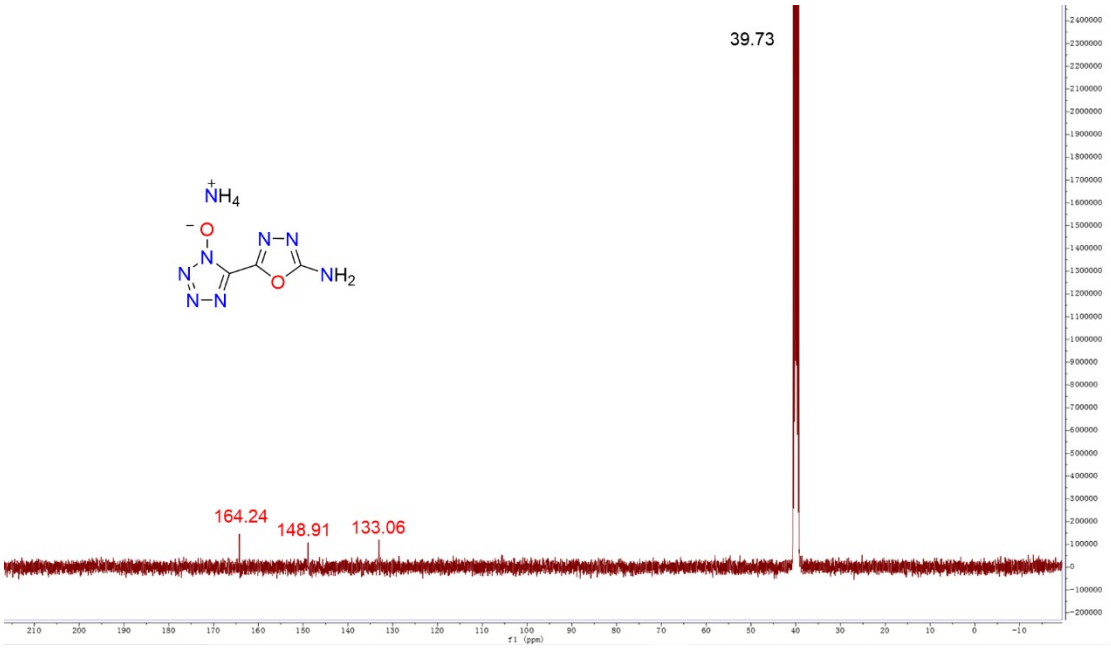

Figure S26 ^{13}C NMR spectrum of **4** (DMSO-d_6).

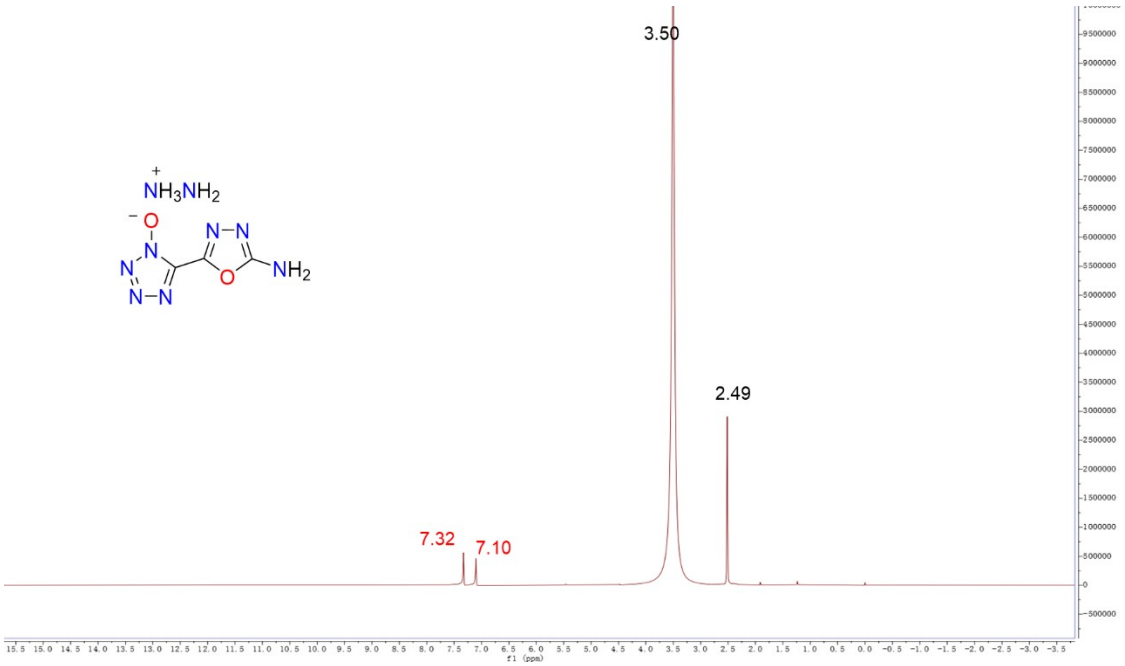

Figure S27 ^{1}H NMR spectrum of **6** (DMSO-d_6).

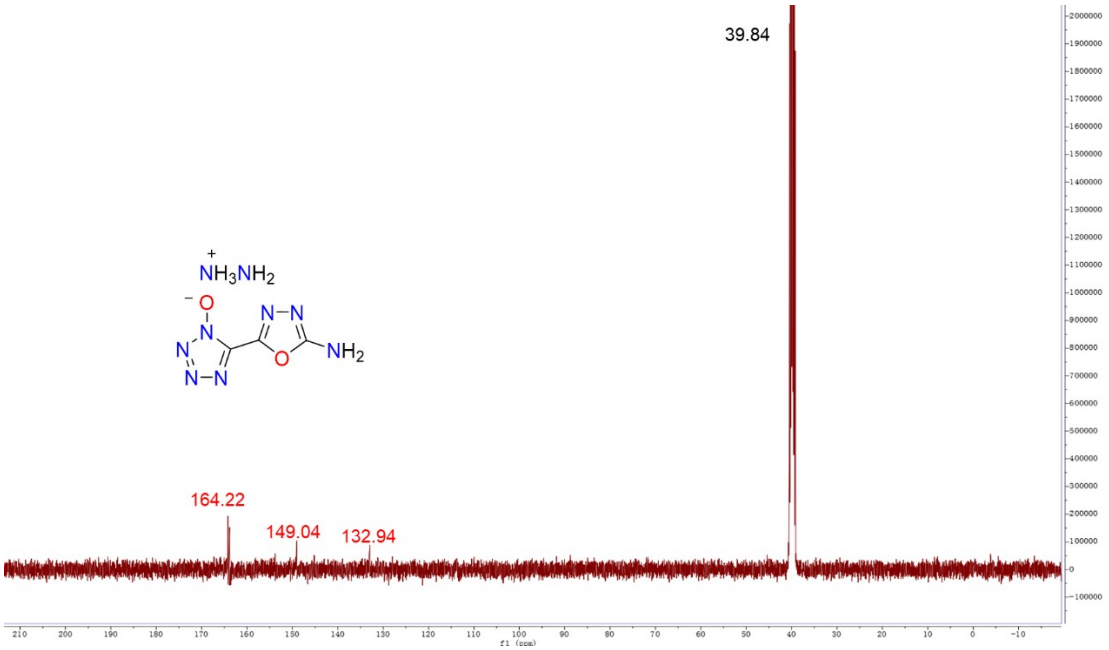

Figure S28 ^{13}C NMR spectrum of **6** (DMSO-d_6).

5 Calculation method and results

The geometric optimization and frequency analyses of all these compounds were based on available single-crystal structures by Gaussian 09 suite[1] of programs and using the B3LYP functional with the 6-31++G(d,p) basis set. The geometrical configurations were optimized with no constraints imposed under default convergence criteria. All of the optimized structures were characterized to be true local energy

minima on the potential energy surface without imaginary frequencies. Thermal corrections to enthalpy were computed at the same DFT level of theory. The gas phase heats of formation were calculated using isodesmic reactions (Figure S29). [2]

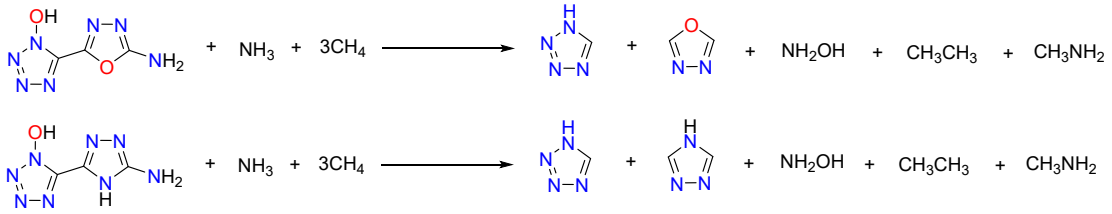

Figure S29 Isodesmic-reaction of **AOTO** and **ATTO**.

The enthalpy of sublimation can be represented as eq (1)[3] and on the basis of thepredicted electrostatic potential of a molecule.[4]

$$\Delta H_{sub} = a(SA)^2 + b\sqrt{\upsilon\sigma_{tot}^2} + c \qquad (1)$$

Here SA is the surface area of the 0.001 electrons bohr^{-3} isosurface of the electronic density of the compounds, $\upsilon\sigma_{tot}^2$ is derived from the molecular electrostatic potential calculation, and a, b, c are fitting parameters reported by Politzer et al.[4]

For energetic salts, the solid-phase heats of formation are calculated based on a Born-Haberenergy cycle (Figure S30).[5]

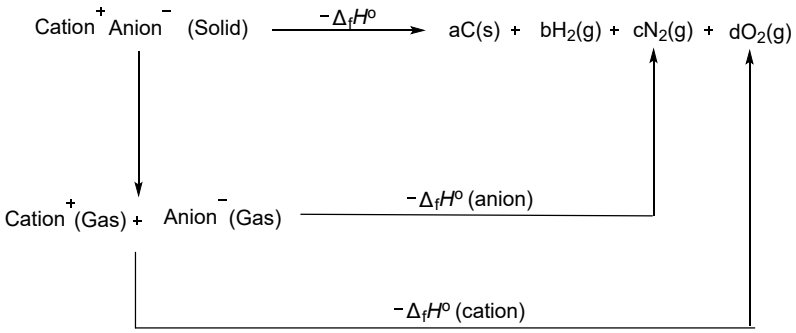

Figure S30 Born-Haber Cycle for the formation of energetic salts.

$$\Delta H_f^o \text{ (salt, 298 K)} = \Delta H_f^o \text{ (cation, 298K)} + \Delta H_f^o \text{ (anion, 298K)} - \Delta H_L \qquad (2)$$

where ΔH_L is the lattice energy of the salts, which could be predicted by using the formula suggested by Jenkins et al. [Eq. (3)]

$$\Delta H_L = U_{POT} + [p(n_M/2 - 2) + q(n_X/2 - 2)]RT \qquad (3)$$

where n_M and n_X represent the nature of the ions, $M_q^+$and X_p^-, and are equal to 3 for monatomic ions, 5 for linear polyatomicions, and 6 for nonlinear polyatomic ions. The equation for lattice potential energy U_{POT} is as the follow:

$$U_{POT} \text{ [kJ mol}^{-1}] = \gamma(\rho_m/M_m)^{1/3} + \delta \qquad (4)$$

where ρ_m (g cm^{-3}) is the density of the salt, M_m is the formula mass of the ionic compound, and values for γ (kJ mol^{-1} cm) and δ (kJ mol^{-1}) are assigned literature values.

The calculation of the enthalpy of cocrystal was based on the method in reference [6] and [7].

Table S9 Calculated total energy (E_0), zero-point energy (ZPE), thermal correction to enthalpy (ΔH_T), heats of formation ($\Delta_f H_{gas}$) in gas state, sublimation enthalpy (ΔH_{sub}) and heats of formation ($\Delta_f H_{sold}$) in gas state.

	E_0/Hartree	ZPE/Hartree	ΔH_T/Hartree	$\Delta_f H_{gas}$ (kJ/mol)	ΔH_{sub} (kJ/mol)	$\Delta_f H_{sold}$ (kJ/mol)
ATTO	-630.030082	0.107715	0.117976	631.36	139.16	492.2
AOTO	-649.8262892	0.093388	0.104059	634.97	160.57	474.4

Table S10 Calculated total energy (E_0), zero-point energy (ZPE), thermal correction to enthalpy (ΔH_T), and heats of formation ($\Delta_f H$) of ions.

	E_0/Hartree	ZPE/Hartree	ΔH_T/Hartree	$\Delta_f H$ (kJ/mol)
NH_4^+	-56.9219842	0.049481	0.053276	624.59
NH_3OH^+	-132.0866003	0.054499	0.058742	676.97
$N_2H_5^+$	-112.2529502	0.067866	0.072181	742.77
$ATTO^-$	-629.4769221	0.094356	0.1046	329.19
$AOTO^-$	-649.3412948	0.081531	0.091459	183.51
TO^-	-332.9670411	0.037808	0.04276	156.36
ATO^-	-388.3461172	0.054982	0.0613	147.28
BTO^{2-}	-664.6465108	0.0567	0.06581	579.25

Table S11 Calculated lattice energy (U_{pot}) and heats of formation ($\Delta_f H$) of ionic compounds.

	Upot (kJ/mol)	$\Delta_f H$ (kJ/mol)
ATTO-N_2H_4	517.16	554.8
3	515.68	438.1
4	510.86	495.3
5	519.00	289.1
6	512.18	414.1
$TO^-\cdot NH_3OH^+$	570.63	262.7
$ATO^-\cdot NH_3OH^+$	536.05	288.2
TKX-50	1482.39	450.8

Molecular surface properties

ATTO

Summary of surface analysis

Volume: 1130.68161 Bohr^3 (167.54973 Angstrom^3)

Estimated density according to mass and volume (M/V): 1.6662 g/cm^3

Minimal value: -47.93888 kcal/mol Maximal value: 61.34839 kcal/mol

Overall surface area: 627.58880 Bohr^2 (175.74276 Angstrom^2)

Positive surface area: 274.60824 Bohr^2 (76.89814 Angstrom^2)

Negative surface area: 352.98056 Bohr^2 (98.84462 Angstrom^2)
Overall average value: -0.00110349 a.u. (-0.69245 kcal/mol)
Positive average value: 0.03983103 a.u. (24.99437 kcal/mol)
Negative average value: -0.03294930 a.u. (-20.67602 kcal/mol)
Overall variance (sigma^2_tot): 0.00134546 a.u.^2 (529.80025 (kcal/mol)^2)
Positive variance: 0.00088960 a.u.^2 (350.29505 (kcal/mol)^2)
Negative variance: 0.00045586 a.u.^2 (179.50520 (kcal/mol)^2)
Balance of charges (nu): 0.22401996
Product of sigma^2_tot and nu: 0.00030141 a.u.^2 (118.68583 (kcal/mol)^2)
Internal charge separation (Pi): 0.03583621 a.u. (22.48758 kcal/mol)
Molecular polarity index (MPI): 0.97853432 eV (22.56556 kcal/mol)
Nonpolar surface area (|ESP| <= 10 kcal/mol): 52.30 Angstrom^2 (29.76 %)
Polar surface area (|ESP| > 10 kcal/mol): 123.44 Angstrom^2 (70.24 %)
Overall skewness: 0.7509464392
Positive skewness: 0.2654803808
Negative skewness: -0.2147186450

AOTO

Volume: 1091.28870 Bohr^3 (161.71230 Angstrom^3)
Estimated density according to mass and volume (M/V): 1.7364 g/cm^3
Minimal value: -59.12528 kcal/mol Maximal value: 97.45675 kcal/mol
Overall surface area: 614.08270 Bohr^2 (171.96067 Angstrom^2)
Positive surface area: 268.82501 Bohr^2 (75.27867 Angstrom^2)
Negative surface area: 345.25769 Bohr^2 (96.68200 Angstrom^2)
Overall average value: 0.00081990 a.u. (0.51449 kcal/mol)
Positive average value: 0.07739218 a.u. (48.56437 kcal/mol)
Negative average value: -0.05880092 a.u. (-36.89816 kcal/mol)
Overall variance (sigma^2_tot): 0.00232406 a.u.^2 (915.14312 (kcal/mol)^2)
Positive variance: 0.00166222 a.u.^2 (654.52949 (kcal/mol)^2)
Negative variance: 0.00066184 a.u.^2 (260.61363 (kcal/mol)^2)
Balance of charges (nu): 0.20367996
Product of sigma^2_tot and nu: 0.00047336 a.u.^2 (186.39632 (kcal/mol)^2)
Internal charge separation (Pi): 0.06704299 a.u. (42.07015 kcal/mol)
Molecular polarity index (MPI): 1.82151796 eV (42.00524 kcal/mol)
Nonpolar surface area (|ESP| <= 10 kcal/mol): 15.12 Angstrom^2 (8.80 %)
Polar surface area (|ESP| > 10 kcal/mol): 156.84 Angstrom^2 (91.20 %)
Overall skewness: 1.6266657918
Positive skewness: -0.0661089620
Negative skewness: 0.6501281806

Parameters at C-J point:								
Detonation parameters			**Composition of detonation products (23):**					
Heat of detonation =	-4128.57	kJ/kg	(per mol of expl.)		(per kg of	(Mol %)	(Mass %)	
Detonation temperature =	2891.65	K	N2	3.7268	22.16684	45.222	62.096	
Detonation pressure =	27.99422	GPa	C(d)	2.856676	16.99138	34.6637	20.4083	
Detonation velocity =	8681.37	m/s	H2O	0.922332	5.485992	11.1918	9.8832	
Particle velocity =	1781.56	m/s	NH3	0.542247	3.22526	6.5798	5.4929	
Sound velocity =	6899.81	m/s	H2	0.066999	0.398505	0.813	0.0803	
Density of products =	2.277349	g/cm3	CH4	0.058107	0.34562	0.7051	0.5545	
Specific volume of products =	0.439	cm3/g	CH2O2	0.026924	0.160142	0.3267	0.7371	
Exponent 'Gamma' =	3.873		C2H6	0.01591	0.094633	0.1931	0.2845	
Moles of gaseous products =	5.384	mol/mol EM	CO	0.01527	0.090822	0.1853	0.2544	
Moles of condensed products =	2.857	mol/mol EM	CO2	0.004245	0.025252	0.0515	0.1111	
Mean Mw of gas =	24.85	g/mol	HCN	0.003162	0.01881	0.0384	0.0508	
Mean Mw of condensed prod.	12.011	g/mol	C2H4	0.001868	0.01111	0.0227	0.0312	
Mean Mw of all prod. =	20.4	g/mol	N2H4	0.000482	0.002868	0.0059	0.0092	
Volume og gas at STP =	783.238	dm3/kg EM	CH3OH	5.91E-05	0.000352	0.0007	0.0011	
Internal energy of products =	5715.554	kJ/kg	NH2	2.54E-05	0.000151	0.0003	0.0002	
Compression energy =	1586.986	kJ/kg	H	8.52E-06	5.07E-05	0.0001	0	
Entropy of products) =	6.057	kJ/kg K	CH2O	1.33E-07	7.91E-07	0	0	
			CNO	3.68E-08	2.19E-07	0	0	
			N	3.52E-08	2.09E-07	0	0	
			HCNO	2.26E-08	1.34E-07	0	0	
			H2O2	1.57E-08	9.35E-08	0	0	
			N2O	7.64E-10	4.54E-09	0	0	
			C(gr)	2.23E-20	1.33E-19	0	0	

Figure S31 Calculation results of **ATTO** from EXPLO5.

Parameters at C-J point:								
Detonation parameters			**Composition of detonation products (23):**					
Heat of detonation =	-4161.97	kJ/kg	(per mol of expl.)		(per kg of	(Mol %)	(Mass %)	
Detonation temperature =	2638.28	K	N2	4.205886	21.01125	43.0635	58.8588	
Detonation pressure =	31.30505	GPa	C(d)	2.665573	13.31635	27.2925	15.9943	
Detonation velocity =	9305.52	m/s	NH3	1.584372	7.915015	16.2222	13.4801	
Particle velocity =	1919.07	m/s	H2O	0.97233	4.857449	9.9556	8.7508	
Sound velocity =	7386.45	m/s	CH4	0.159368	0.796153	1.6318	1.2773	
Density of products =	2.208446	g/cm3	H2	0.082063	0.409962	0.8402	0.0826	
Specific volume of products =	0.453	cm3/g	C2H6	0.076883	0.384081	0.7872	1.1549	
Exponent 'Gamma' =	3.849		CH2O2	0.011737	0.058635	0.1202	0.2699	
Moles of gaseous products =	7.101	mol/mol EM	CO	0.002883	0.014405	0.0295	0.0403	
Moles of condensed products =	2.666	mol/mol EM	C2H4	0.002332	0.011649	0.0239	0.0327	
Mean Mw of gas =	23.679	g/mol	HCN	0.001335	0.006668	0.0137	0.018	
Mean Mw of condensed prod.	12.011	g/mol	N2H4	0.001254	0.006263	0.0128	0.0201	
Mean Mw of all prod. =	20.494	g/mol	CO2	0.000638	0.003185	0.0065	0.014	
Volume og gas at STP =	867.576	dm3/kg EM	CH3OH	3.7E-05	0.000185	0.0004	0.0006	
Internal energy of products =	6003.393	kJ/kg	NH2	1.25E-05	6.24E-05	0.0001	0.0001	
Compression energy =	1841.426	kJ/kg	H	2.4E-06	1.2E-05	0	0	
Entropy of products) =	6.385	kJ/kg K	CH2O	1.15E-08	5.76E-08	0	0	
			N	5.12E-09	2.56E-08	0	0	
			CNO	1.92E-09	9.59E-09	0	0	
			H2O2	1.68E-09	8.38E-09	0	0	
			HCNO	1.04E-09	5.22E-09	0	0	
			N2O	4.3E-11	2.15E-10	0	0	
			C(gr)	1.34E-20	6.7E-20	0	0	

Figure S32 Calculation results of **ATTO·N_2H_4** from EXPLO5.

Parameters at C-J point:								
Detonation parameters			**Composition of detonation products (23):**					
Heat of detonation =	-5000.02	kJ/kg	(per mol of expl.)		(per kg of	(Mol %)	(Mass %)	
Detonation temperature =	3540.57	K	N2	3.450526	20.40428	45.0786	57.1585	
Detonation pressure =	28.83171	GPa	C(d)	2.421048	14.31658	31.6292	17.1956	
Detonation velocity =	8516.75	m/s	H2O	1.083291	6.40591	14.1524	11.5404	
Particle velocity =	1880.71	m/s	CH2O2	0.228655	1.352123	2.9872	6.2231	
Sound velocity =	6636.03	m/s	CO	0.203976	1.20619	2.6648	3.3785	
Density of products =	2.310137	g/cm3	CO2	0.127664	0.754925	1.6678	3.3224	
Specific volume of products =	0.433	cm3/g	NH3	0.089296	0.528043	1.1666	0.8993	
Exponent 'Gamma' =	3.528		H2	0.032518	0.192291	0.4248	0.0388	
Moles of gaseous products =	5.233	mol/mol EM	HCN	0.009289	0.054931	0.1214	0.1485	
Moles of condensed products =	2.421	mol/mol EM	CH4	0.006416	0.037938	0.0838	0.0609	
Mean Mw of gas =	26.755	g/mol	C2H4	0.000722	0.004271	0.0094	0.012	
Mean Mw of condensed prod.	12.011	g/mol	C2H6	0.000707	0.00418	0.0092	0.0126	
Mean Mw of all prod. =	22.092	g/mol	N2H4	0.000145	0.000857	0.0019	0.0027	
Volume og gas at STP =	756.844	dm3/kg EM	CH3OH	8.47E-05	0.000501	0.0011	0.0016	
Internal energy of products =	6768.573	kJ/kg	NH2	6.35E-05	0.000376	0.0008	0.0006	
Compression energy =	1768.554	kJ/kg	H	4.89E-05	0.000289	0.0006	0	
Entropy of products) =	6.395	kJ/kg K	CNO	5.36E-06	3.17E-05	0.0001	0.0001	
			CH2O	2.3E-06	1.36E-05	0	0	
			N	1.35E-06	7.98E-06	0	0	
			H2O2	1.13E-06	6.71E-06	0	0	
			HCNO	1E-06	5.91E-06	0	0	
			N2O	8.39E-08	4.96E-07	0	0	
			C(gr)	1.17E-18	6.91E-18	0	0	

Figure S33 Calculation results of **AOTO** from EXPLO5.

Parameters at C-J point:								
Detonation parameters			**Composition of detonation products (23):**					
Heat of detonation =	-3784.4	kJ/kg	(per mol of expl.)		(per kg of	(Mol %)	(Mass %)	
Detonation temperature =	2556.53	K	N2	3.926147	21.20442	43.4238	59.4	
Detonation pressure =	25.023	GPa	C(d)	2.574763	13.90584	28.4773	16.7023	
Detonation velocity =	8463.65	m/s	NH3	1.144611	6.18184	12.6596	10.5283	
Particle velocity =	1781.03	m/s	H2O	0.961159	5.191047	10.6306	9.3518	
Sound velocity =	6682.62	m/s	CH4	0.21322	1.151564	2.3583	1.8475	
Density of products =	2.102418	g/cm3	H2	0.102476	0.553456	1.1334	0.1116	
Specific volume of products =	0.476	cm3/g	C2H6	0.089803	0.48501	0.9932	1.4583	
Exponent 'Gamma' =	3.752		CH2O2	0.01405	0.07588	0.1554	0.3492	
Moles of gaseous products =	6.467	mol/mol EM	CO	0.007136	0.038541	0.0789	0.108	
Moles of condensed products =	2.575	mol/mol EM	C2H4	0.003664	0.019788	0.0405	0.0555	
Mean Mw of gas =	23.849	g/mol	HCN	0.002056	0.011103	0.0227	0.03	
Mean Mw of condensed prod.	12.011	g/mol	CO2	0.001764	0.009529	0.0195	0.0419	
Mean Mw of all prod. =	20.478	g/mol	N2H4	0.000513	0.00277	0.0057	0.0089	
Volume og gas at STP =	854.137	dm3/kg EM	CH3OH	7.68E-05	0.000415	0.0008	0.0013	
Internal energy of products =	5370.451	kJ/kg	NH2	1.3E-05	7.01E-05	0.0001	0.0001	
Compression energy =	1586.05	kJ/kg	H	3.13E-06	1.69E-05	0	0	
Entropy of products) =	6.381	kJ/kg K	CH2O	7.34E-08	3.96E-07	0	0	
			HCNO	8.65E-09	4.67E-08	0	0	
			CNO	3.37E-09	1.82E-08	0	0	
			N	2.83E-09	1.53E-08	0	0	
			H2O2	1.98E-09	1.07E-08	0	0	
			N2O	8.32E-11	4.49E-10	0	0	
			C(gr)	2.17E-20	1.17E-19	0	0	

Figure S34 Calculation results of **3** from EXPLO5.

Parameters at C-J point:								
Detonation parameters			**Composition of detonation products (23):**					
Heat of detonation =	-4753.02	kJ/kg	(per mol of expl.)		(per kg of	(Mol %)	(Mass %)	
Detonation temperature =	3093.63	K	N2	4.1064	20.414	42.0127	57.1858	
Detonation pressure =	27.24007	GPa	C(d)	2.677344	13.30979	27.392	15.9864	
Detonation velocity =	8630.71	m/s	H2O	1.789024	8.893716	18.3036	16.0223	
Particle velocity =	1877.55	m/s	NH3	0.777244	3.863885	7.952	6.5806	
Sound velocity =	6753.16	m/s	H2	0.138929	0.690651	1.4214	0.1392	
Density of products =	2.148362	g/cm3	CH4	0.109492	0.544314	1.1202	0.8732	
Specific volume of products =	0.465	cm3/g	CH2O2	0.07105	0.353208	0.7269	1.6256	
Exponent 'Gamma' =	3.597		CO	0.0453	0.225198	0.4635	0.6308	
Moles of gaseous products =	7.097	mol/mol EM	C2H6	0.033005	0.164074	0.3377	0.4933	
Moles of condensed products =	2.677	mol/mol EM	CO2	0.011685	0.058091	0.1196	0.2557	
Mean Mw of gas =	23.812	g/mol	HCN	0.008109	0.040314	0.083	0.109	
Mean Mw of condensed prod.	12.011	g/mol	C2H4	0.005403	0.026858	0.0553	0.0753	
Mean Mw of all prod. =	20.579	g/mol	N2H4	0.000884	0.004394	0.009	0.0141	
Volume og gas at STP =	862.815	dm3/kg EM	CH3OH	0.000204	0.001014	0.0021	0.0032	
Internal energy of products =	6515.642	kJ/kg	NH2	8.01E-05	0.000398	0.0008	0.0006	
Compression energy =	1762.617	kJ/kg	H	3.45E-05	0.000172	0.0004	0	
Entropy of products) =	6.83	kJ/kg K	CH2O	7.75E-07	3.85E-06	0	0	
			CNO	2.16E-07	1.08E-06	0	0	
			N	1.76E-07	8.75E-07	0	0	
			HCNO	1.25E-07	6.21E-07	0	0	
			H2O2	9.72E-08	4.83E-07	0	0	
			N2O	3.6E-09	1.79E-08	0	0	
			C(gr)	2.93E-20	1.46E-19	0	0	

Figure S35 Calculation results of **4** from EXPLO5.

Parameters at C-J point:								
Detonation parameters			**Composition of detonation products (23):**					
Heat of detonation =	-3933.82	kJ/kg	(per mol of expl.)		(per kg of	(Mol %)	(Mass %)	
Detonation temperature =	2780.13	K	N2	3.737901	20.08113	41.0803	56.2533	
Detonation pressure =	22.96423	GPa	C(d)	2.695128	14.47904	29.62	17.3908	
Detonation velocity =	7998.36	m/s	H2O	1.757277	9.440621	19.3129	17.0076	
Particle velocity =	1736.91	m/s	NH3	0.51911	2.788813	5.7051	4.7496	
Sound velocity =	6261.45	m/s	H2	0.110997	0.596311	1.2199	0.1202	
Density of products =	2.111537	g/cm3	CH4	0.099852	0.536436	1.0974	0.8606	
Specific volume of products =	0.474	cm3/g	CH2O2	0.073773	0.396333	0.8108	1.8241	
Exponent 'Gamma' =	3.605		CO	0.051754	0.278036	0.5688	0.7788	
Moles of gaseous products =	6.404	mol/mol EM	C2H6	0.02335	0.125442	0.2566	0.3772	
Moles of condensed products =	2.695	mol/mol EM	CO2	0.021626	0.116184	0.2377	0.5113	
Mean Mw of gas =	24.011	g/mol	HCN	0.004597	0.024697	0.0505	0.0667	
Mean Mw of condensed prod.	12.011	g/mol	C2H4	0.0032	0.017192	0.0352	0.0482	
Mean Mw of all prod. =	20.456	g/mol	N2H4	0.000232	0.001246	0.0025	0.004	
Volume og gas at STP =	841.374	dm3/kg EM	CH3OH	0.000168	0.000905	0.0019	0.0029	
Internal energy of products =	5442.255	kJ/kg	NH2	2.7E-05	0.000145	0.0003	0.0002	
Compression energy =	1508.436	kJ/kg	H	1.27E-05	6.8E-05	0.0001	0	
Entropy of products) =	6.5	kJ/kg K	CH2O	7.83E-07	4.2E-06	0	0	
			HCNO	1.32E-07	7.11E-07	0	0	
			CNO	6.73E-08	3.62E-07	0	0	
			H2O2	3.66E-08	1.96E-07	0	0	
			N	2.13E-08	1.15E-07	0	0	
			N2O	1.31E-09	7.05E-09	0	0	
			C(gr)	3.67E-20	1.97E-19	0	0	

Figure S36 Calculation results of **5** from EXPLO5.

Parameters at C-J point:								
Detonation parameters			**Composition of detonation products (23):**					
Heat of detonation =	-4361.08	kJ/kg	(per mol of expl.)		(per kg of	(Mol %)	(Mass %)	
Detonation temperature =	2901.36	K	N2	4.106509	20.41455	41.9238	57.1873	
Detonation pressure =	26.74077	GPa	C(d)	2.71088	13.47651	27.6757	16.1866	
Detonation velocity =	8584.26	m/s	H2O	1.821815	9.056725	18.5991	16.316	
Particle velocity =	1834.56	m/s	NH3	0.780937	3.882247	7.9727	6.6119	
Sound velocity =	6749.7	m/s	H2	0.120184	0.597467	1.227	0.1204	
Density of products =	2.159514	g/cm3	CH4	0.109337	0.543543	1.1162	0.872	
Specific volume of products =	0.463	cm3/g	CH2O2	0.062841	0.312399	0.6416	1.4378	
Exponent 'Gamma' =	3.679		CO	0.031904	0.158602	0.3257	0.4442	
Moles of gaseous products =	7.084	mol/mol EM	C2H6	0.031276	0.155481	0.3193	0.4675	
Moles of condensed products =	2.711	mol/mol EM	CO2	0.010227	0.05084	0.1044	0.2237	
Mean Mw of gas =	23.797	g/mol	HCN	0.004803	0.023877	0.049	0.0645	
Mean Mw of condensed prod.	12.011	g/mol	C2H4	0.003655	0.018172	0.0373	0.051	
Mean Mw of all prod. =	20.535	g/mol	N2H4	0.0006	0.002983	0.0061	0.0096	
Volume og gas at STP =	861.289	dm3/kg EM	CH3OH	0.000146	0.000724	0.0015	0.0023	
Internal energy of products =	6043.891	kJ/kg	NH2	4.05E-05	0.000201	0.0004	0.0003	
Compression energy =	1682.815	kJ/kg	H	1.6E-05	7.95E-05	0.0002	0	
Entropy of products) =	6.639	kJ/kg K	CH2O	3.72E-07	1.85E-06	0	0	
			CNO	6.92E-08	3.44E-07	0	0	
			HCNO	5.4E-08	2.68E-07	0	0	
			N	5.02E-08	2.5E-07	0	0	
			H2O2	4.21E-08	2.09E-07	0	0	
			N2O	1.27E-09	6.31E-09	0	0	
			C(gr)	2.56E-20	1.27E-19	0	0	

Figure S37 Calculation results of **6** from EXPLO5.

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