Supplementary Information

Synthesis, Characterization and Properties of Nitrogen-rich compound based on Cyanuric Acid: A Promising Design in the Development of New Energetic Materials

Qiangqiang Liu[a,b], Bo Jin[b]*, Rufang Peng[ab]*, Zhicheng Guo[c], Jun Zhao[b], Qingchun Zhang[b], Yu Shang[b]

[a] Research Center of Laser Fusion, China Academy of Engineering Physics, Mianyang, 621010, China

[b] State Key Laboratory Cultivation Base for Nonmetal Composites and Functional Materials, Southwest University of Science and Technology, Mianyang 621010, China

[c]School of Nation Defence Science and Technology, Southwest University of Science and Technology, Mianyang 621010, China

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Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	3478(1)	7297(1)	3846(1)	14(1)
O(2)	5505(1)	1613(1)	2610(1)	15(1)
O(3)	1831(1)	1313(1)	4996(1)	13(1)
N(1)	2568(1)	4373(1)	4456(1)	11(1)
N(2)	4487(1)	4477(1)	3212(1)	11(1)
N(3)	3715(1)	1449(1)	3878(1)	10(1)
C(1)	3491(1)	5454(1)	3852(1)	10(1)
C(2)	4629(1)	2456(1)	3197(1)	10(1)
C(3)	2663(1)	2378(1)	4464(1)	9(1)
N(4)	6058(1)	7528(1)	536(1)	12(1)
N(5)	6303(1)	7416(1)	2070(1)	13(1)

Table S2. Bond lengths [Å] and angles [°] for **2**.

O(1)-C(1)	1.2388(12)
O(2)-C(2)	1.2306(11)
O(3)-C(3)	1.2477(11)
N(1)-C(3)	1.3437(12)
N(1)-C(1)	1.3528(11)
N(2)-C(2)	1.3657(12)
N(2)-C(1)	1.3903(11)
N(2)-H(2)	0.924(14)
N(3)-C(2)	1.3651(11)
N(3)-C(3)	1.3872(11)
N(3)-H(3)	0.882(16)
N(4)-N(5)	1.4573(11)
N(4)-H(4A)	0.904(14)
N(4)-H(4B)	0.910(14)
N(4)-H(4C)	0.931(14)
N(5)-H(5A)	0.870(14)
N(5)-H(5B)	0.886(13)
C(3)-N(1)-C(1)	119.37(7)
C(2)-N(2)-C(1)	123.44(7)
C(2)-N(2)-H(2)	120.2(9)
C(1)-N(2)-H(2)	116.3(9)
C(2)-N(3)-C(3)	123.19(8)
C(2)-N(3)-H(3)	118.5(7)
C(3)-N(3)-H(3)	118.0(7)
O(1)-C(1)-N(1)	122.18(8)
O(1)-C(1)-N(2)	118.46(8)
N(1)-C(1)-N(2)	119.35(8)
O(2)-C(2)-N(3)	122.82(8)
O(2)-C(2)-N(2)	122.64(8)
N(3)-C(2)-N(2)	114.53(7)
O(3)-C(3)-N(1)	121.90(8)
O(3)-C(3)-N(3)	118.16(8)
N(1)-C(3)-N(3)	119.94(7)
N(5)-N(4)-H(4A)	108.3(8)
N(5)-N(4)-H(4B)	108.0(8)
H(4A)-N(4)-H(4B)	107.7(11)
N(5)-N(4)-H(4C)	112.7(8)
H(4A)-N(4)-H(4C)	111.2(11)
H(4B)-N(4)-H(4C)	108.9(12)
N(4)-N(5)-H(5A)	104.7(8)
N(4)-N(5)-H(5B)	105.6(9)
H(5A)-N(5)-H(5B)	106.4(12)

Table S3. Anisotropic displacement parameters ($Å^2$ x 10^3) for **2.** The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$h^2 a^{*2} U^{11}$ + ... + 2 h k a* b* U^{12}]

	U11	U22	U33	U23	U13	U12
O(1)	18(1)	7(1)	17(1)	0(1)	4(1)	0(1)
O(2)	14(1)	12(1)	21(1)	-2(1)	10(1)	0(1)
O(3)	12(1)	10(1)	17(1)	1(1)	6(1)	-1(1)
N(1)	12(1)	8(1)	13(1)	-1(1)	4(1)	1(1)
N(2)	11(1)	8(1)	13(1)	1(1)	5(1)	-1(1)
N(3)	11(1)	6(1)	14(1)	0(1)	4(1)	0(1)
C(1)	10(1)	9(1)	9(1)	0(1)	0(1)	0(1)
C(2)	10(1)	10(1)	11(1)	-1(1)	1(1)	0(1)
C(3)	8(1)	11(1)	9(1)	0(1)	1(1)	0(1)
N(4)	12(1)	9(1)	14(1)	0(1)	6(1)	0(1)
N(5)	14(1)	12(1)	13(1)	0(1)	5(1)	1(1)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **2**.

	x	y	z	U(eq)
H(4A)	5099(16)	7426(19)	196(13)	20(3)
H(4B)	6491(14)	6460(20)	220(14)	21(3)
H(5A)	6010(14)	8560(20)	2330(13)	19(3)
H(3)	3732(12)	140(20)	3870(12)	21(3)
H(5B)	7252(15)	7399(19)	2357(14)	20(3)
H(4C)	6431(14)	8680(20)	217(14)	23(3)
H(2)	5099(14)	5280(20)	2820(13)	29(3)

Table S5. Torsion angles [°] for **2**.

C(3)-N(1)-C(1)-O(1)	-178.08(7)
C(3)-N(1)-C(1)-N(2)	2.08(11)
C(2)-N(2)-C(1)-O(1)	177.76(7)
C(2)-N(2)-C(1)-N(1)	-2.40(11)
C(3)-N(3)-C(2)-O(2)	-175.73(8)
C(3)-N(3)-C(2)-N(2)	3.95(11)
C(1)-N(2)-C(2)-O(2)	179.09(7)
C(1)-N(2)-C(2)-N(3)	-0.60(11)
C(1)-N(1)-C(3)-O(3)	-179.41(7)
C(1)-N(1)-C(3)-N(3)	1.11(11)
C(2)-N(3)-C(3)-O(3)	176.13(7)
C(2)-N(3)-C(3)-N(1)	-4.38(11)

Table S6. Hydrogen bonds for **2** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2)...N(5)	0.924(14)	2.053(15)	2.9696(11)	171.1(13)
N(4)-H(4C)...N(1)#1	0.931(14)	1.928(14)	2.8389(11)	165.6(12)
N(5)-H(5B)...O(2)#2	0.886(13)	2.181(14)	3.0228(11)	158.5(12)
N(3)-H(3)...O(1)#3	0.882(16)	1.924(16)	2.7996(11)	171.9(11)
N(5)-H(5A)...O(2)#4	0.870(14)	2.137(14)	2.9924(11)	167.4(12)
N(4)-H(4B)...O(3)#5	0.910(14)	1.910(14)	2.7609(11)	155.0(12)
N(4)-H(4A)...O(3)#6	0.904(14)	1.948(14)	2.8003(11)	156.6(12)

Symmetry transformations used to generate equivalent atoms:
#1 x+1/2,-y+3/2,z-1/2 #2 -x+3/2,y+1/2,-z+1/2 #3 x,y-1,z #4 x,y+1,z #5 x+1/2,-y+1/2,z-1/2 #6 -x+1/2,y+1/2,-z+1/2

Table S7. Atomic coordinates and B_{iso}/B_{eq} for **4**.

	x	y	z	B_{eq}
O1	0.34016(9)	0.73676(5)	0.87607(5)	1.097(8)
O2	0.21415(10)	1.09977(5)	1.06416(5)	1.343(9)
O3	0.28497(9)	1.09993(5)	0.67724(5)	1.147(8)
O4	0.30419(10)	0.80462(5)	0.56675(5)	1.236(9)
O5	0.21310(10)	1.16821(5)	0.36898(5)	1.403(9)
O6	0.24595(9)	0.80740(5)	0.18952(5)	1.090(8)
N1	0.25025(10)	1.10938(5)	0.87078(5)	0.966(9)
N2	0.27421(10)	0.91860(5)	0.97146(5)	0.916(9)
N3	0.30553(10)	0.91903(5)	0.77596(5)	0.916(9)
N4	0.25472(10)	0.98629(5)	0.46999(5)	0.880(8)
N5	0.22361(10)	0.98826(5)	0.27868(5)	0.898(8)
N6	0.26704(9)	0.79702(5)	0.37910(5)	0.854(8)
N7	-0.08173(10)	0.41294(6)	0.82308(6)	1.171(10)
N8	0.07826(10)	0.56838(5)	0.86693(6)	0.975(9)
N9	-0.08694(10)	0.65435(6)	0.83248(6)	1.144(9)
N10	0.22411(10)	0.36464(6)	0.89802(6)	1.060(9)
N11	0.38617(11)	0.40781(6)	0.93815(6)	1.285(10)
N12	0.21910(10)	0.56203(6)	0.58994(6)	1.086(9)
N13	0.50431(10)	0.45161(6)	0.66600(6)	1.082(9)
N14	0.58168(10)	0.55629(6)	0.68928(6)	1.170(10)
N15	0.28102(10)	0.34834(6)	0.60146(6)	1.039(9)
N16	0.10129(10)	0.34725(6)	0.55329(6)	1.012(9)
C1	0.30869(10)	0.85045(6)	0.87462(6)	0.804(9)
C2	0.24461(11)	1.04648(6)	0.97082(6)	0.870(9)
C3	0.27913(10)	1.04702(6)	0.77269(6)	0.821(9)
C4	0.27648(10)	0.85844(6)	0.47403(6)	0.823(9)
C5	0.22950(11)	1.05539(6)	0.37244(6)	0.875(9)
C6	0.24546(10)	0.86082(6)	0.28051(6)	0.781(9)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S8. Atomic coordinates and B_{iso} involving hydrogen atoms for **4.**

	x	y	z	B_{iso}
H1	0.268(2)	0.8839(13)	1.0387(12)	2.0(3)
H2	0.323(2)	0.8821(13)	0.7120(12)	2.0(3)
H3	0.269(2)	1.0217(13)	0.5341(12)	2.2(3)
H4	0.214(2)	1.0244(13)	0.2119(12)	2.0(3)
H5	-0.091(2)	0.3324(14)	0.8285(12)	2.3(3)
H6	-0.1778(19)	0.4748(12)	0.7997(11)	1.5(2)
H7	0.1856(18)	0.5898(11)	0.8873(10)	1.0(2)
H8	-0.121(2)	0.7186(13)	0.8817(12)	2.0(3)
H9	-0.047(2)	0.6889(13)	0.7606(12)	2.0(3)
H10	0.234(2)	0.2827(13)	0.8871(12)	1.9(2)
H11	0.389(2)	0.3831(12)	1.0135(12)	1.8(2)
H12	0.503(2)	0.3671(14)	0.8993(12)	2.2(3)
H13	0.267(2)	0.6337(12)	0.5875(11)	1.5(2)
H14	0.112(2)	0.5608(12)	0.5580(11)	1.7(2)
H15	0.590(2)	0.3832(14)	0.6596(12)	2.1(3)
H16	0.597(2)	0.6042(14)	0.6253(13)	2.4(3)
H17	0.499(2)	0.5995(13)	0.7435(12)	1.7(2)
H18	0.338(2)	0.2793(13)	0.6385(12)	2.0(3)
H19	0.015(2)	0.3230(13)	0.6079(12)	2.1(3)
H20	0.133(2)	0.2867(13)	0.4998(12)	1.7(2)

Table S9. Anisotropic displacement parameters for **4**. The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$.

	U11	U22	U33	U12	U13	U23
O1	0.0222(3)	0.00643(19)	0.0138(2)	-0.00364(17)	-0.00357(19)	-0.00003(16)
O2	0.0316(3)	0.0094(2)	0.0093(2)	-0.0014(2)	-0.0035(2)	-0.00187(17)
O3	0.0252(3)	0.0098(2)	0.0093(2)	-0.00457(18)	-0.00344(19)	0.00208(17)
O4	0.0284(3)	0.0108(2)	0.0092(2)	-0.00507(19)	-0.0061(2)	0.00179(17)
O5	0.0325(3)	0.0071(2)	0.0138(3)	-0.00230(19)	-0.0054(2)	-0.00044(17)
O6	0.0231(3)	0.0106(2)	0.0095(2)	-0.00573(18)	-0.00430(18)	-0.00140(16)
N1	0.0201(3)	0.0074(2)	0.0093(3)	-0.00234(19)	-0.0029(2)	-0.00001(18)
N2	0.0197(3)	0.0069(2)	0.0084(3)	-0.00268(19)	-0.0029(2)	0.00055(18)
N3	0.0203(3)	0.0070(2)	0.0080(3)	-0.00322(19)	-0.0027(2)	-0.00046(18)
N4	0.0177(3)	0.0075(2)	0.0086(3)	-0.00248(19)	-0.00280(19)	-0.00066(18)
N5	0.0185(3)	0.0073(2)	0.0088(3)	-0.00219(18)	-0.0042(2)	0.00015(18)
N6	0.0158(2)	0.0084(2)	0.0089(3)	-0.00316(18)	-0.00316(19)	0.00020(18)
N7	0.0163(3)	0.0104(2)	0.0196(3)	-0.0049(2)	-0.0051(2)	-0.0016(2)
N8	0.0153(2)	0.0066(2)	0.0162(3)	-0.00247(18)	-0.0051(2)	0.00029(19)
N9	0.0185(3)	0.0089(2)	0.0157(3)	0.00046(19)	-0.0053(2)	-0.0002(2)
N10	0.0170(3)	0.0080(2)	0.0158(3)	-0.00143(19)	-0.0053(2)	-0.00002(19)
N11	0.0161(3)	0.0156(3)	0.0179(3)	-0.0021(2)	-0.0067(2)	-0.0000(2)
N12	0.0182(3)	0.0085(2)	0.0158(3)	-0.00276(19)	-0.0071(2)	0.00134(19)
N13	0.0138(2)	0.0099(2)	0.0182(3)	-0.00169(19)	-0.0050(2)	-0.0020(2)
N14	0.0169(3)	0.0128(3)	0.0163(3)	-0.0052(2)	-0.0035(2)	-0.0029(2)
N15	0.0151(2)	0.0080(2)	0.0177(3)	-0.00263(18)	-0.0065(2)	0.00099(19)
N16	0.0152(3)	0.0111(2)	0.0136(3)	-0.00403(19)	-0.0047(2)	-0.00042(19)
C1	0.0135(3)	0.0077(2)	0.0101(3)	-0.00311(19)	-0.0026(2)	-0.00005(19)
C2	0.0157(3)	0.0073(2)	0.0101(3)	-0.0015(2)	-0.0028(2)	-0.0004(2)
C3	0.0143(3)	0.0074(2)	0.0099(3)	-0.00247(19)	-0.0026(2)	0.0003(2)
C4	0.0137(3)	0.0088(2)	0.0092(3)	-0.0027(2)	-0.0021(2)	0.0001(2)
C5	0.0154(3)	0.0083(3)	0.0095(3)	-0.0015(2)	-0.0024(2)	-0.0004(2)
C6	0.0119(2)	0.0084(2)	0.0099(3)	-0.00259(19)	-0.0026(2)	-0.0003(2)
C7	0.0136(3)	0.0083(2)	0.0088(3)	-0.00304(19)	-0.0008(2)	-0.00026(19)
C8	0.0129(3)	0.0090(2)	0.0083(3)	-0.00228(19)	-0.0009(2)	-0.00019(19)

Table S10. Bond lengths [Å] for **4**.

	distance		distance
O(1)-C(1)	1.2296(9)	N(10)-N(11)	1.4135(11)
O(3)-C(3)	1.2495(9)	N(12)-C(8)	1.3204(9)
O(5)-C(5)	1.2266(9)	N(13)-C(8)	1.3379(11)
N(1)-C(2)	1.3475(9)	N(15)-C(8)	1.3388(11)
N(2)-C(1)	1.3625(10)	N(2)-H(1)	0.868(14)
N(3)-C(1)	1.3656(9)	N(4)-H(3)	0.890(15)
N(4)-C(4)	1.3880(9)	N(7)-H(5)	0.902(16)
N(5)-C(5)	1.3659(10)	N(8)-H(7)	0.867(13)
N(6)-C(4)	1.3482(10)	N(9)-H(9)	0.944(14)
N(7)-C(7)	1.3314(11)	N(11)-H(11)	0.924(14)
N(8)-C(7)_	1.3303(10)	N(12)-H(13)	0.906(14)
N(10)-C(7)	1.3316(9)	N(13)-H(15)	0.853(14)
N(13)-N(14)	1.4051(11)	N(14)-H(17)	0.876(13)
N(15)-N(16)	1.4064(11)	N(16)-H(19)	0.879(14)
O(2)-C(2))	1.2439(10)	N(3)-H(2)	0.856(15)
O(4)-C(4)	1.2454(9)	N(5)-H(4)	0.875(14)
O(6)-C(6)	1.2458(10)	N(7)-H(6)	0.906(12)
N(1)-C(3)	1.3433(10)	N(9)-H(8)	0.909(14)
N(2)-C(2)	1.3847(9)	N(10)-H(10)	0.906(14)
N(3)-C(3)	1.3870(9)	N(11)-H(12)	0.899(13)
N(4)-C(5)	1.3691(9)	N(12)-H(14)	0.860(15)
N(5)-C(6)	1.3834(9)	N(14)-H(16)	0.911(15)
N(6)-C(6)	1.3482(9)	N(15)-H(18)	0.908(13)
N(8)-N(9)	1.4077(9)	N(16)-H(20)	0.912(14)

Table S11. Bond angles [°] for **4**.

	Angle		Angle
C(2)-N(1)-C(3)	119.34(6)	C(1)-N(2)-H(1)	121.6(10)
C(1)-N(3)-C(3)	123.55(6)	C(1)-N(3)-H(2)	119.2(10)
C(5)-N(5)-C(6)	123.29(6)	C(4)-N(4)-H(3)	115.9(9)
N(9)-N(8)-C(7)	118.38(7)	C(5)-N(5)-H(4)	120.6(10)
N(14)-N(13)-C(8)	123.84(6)	C(7)-N(7)-H(5)	118.9(10)
O(1)-C(1)-N(2)	122.75(7)	H(5)-N(7)-H(6)	125.2(13)
N(2)-C(1)-N(3)	114.35(6)	C(7)-N(8)-H(7)	118.6(7)
O(2)-C(2)-N(2)	118.14(6)	N(8)-N(9)-H(9)	109.9(8)
O(3)-C(3)-N(1)	122.44(6)	N(11)-N(10)-H(10)	119.9(9)
N(1)-C(3)-N(3)	119.52(6)	N(10)-N(11)-H(11)	108.2(9)
O(4)-C(4)-N(6)	122.38(6)	H(11)-N(11)-H(12)	106.1(12)
O(5)-C(5)-N(4)	123.10(7)	C(8)-N(12)-H(14)	119.5(9)
N(4)-C(5)-N(5)	114.41(6)	N(14)-N(13)-H(15)	116.5(11)
O(6)-C(6)-N(6)	121.39(6)	N(13)-N(14)-H(16)	110.8(11)
N(7)-C(7)-N(8)	119.70(6)	H(16)-N(14)-H(17)	110.0(12)
N(8)-C(7)-N(10)	120.09(7)	C(8)-N(15)-H(18)	119.9(10)
N(12)-C(8)-N(15)	120.88(7)	N(15)-N(16)-H(20)	106.7(9)
C(1)-N(2)-C(2)	123.30(6)	C(2)-N(2)-H(1)	115.2(10)
C(4)-N(4)-C(5)	123.36(6)	C(3)-N(3)-H(2)	117.2(10)
C(4)-N(6)-C(6)	119.12(6)	C(5)-N(4)-H(3)	120.5(9)
N(11)-N(10)-C(7)	117.70(7)	C(6)-N(5)-H(4)	115.9(10)
N(16)-N(15)-C(8)	119.28(6)	C(7)-N(7)-H(6)	115.5(9)
O(1)-C(1)-N(3)	122.90(7)	N(9)-N(8)-H(7)	123.0(7)
O(2)-C(2)-N(1)	121.99(6)	N(8)-N(9)-H(8)	109.7(9)
N(1)-C(2)-N(2)	119.87(6)	H(8)-N(9)-H(9)	105.8(12)
O(3)-C(3)-N(3)	118.03(6)	C(7)-N(10)-H(10)	121.8(9)
O(4)-C(4)-N(4)	117.93(7)	N(10)-N(11)-H(12)	106.7(11)
N(4)-C(4)-N(6)	119.69(6)	C(8)-N(12)-H(13)	120.8(8)
O(5)-C(5)-N(5)	122.49(7)	H(13)-N(12)-H(14)	118.1(12)
O(6)-C(6)-N(5)	118.54(6)	C(8)-N(13)-H(15)	116.1(11)
N(5)-C(6)-N(6)	120.06(6)	N(13)-N(14)-H(17)	109.9(10)
N(7)-C(7)-N(10)	120.20(7)	N(16)-N(15)-H(18)	118.5(10)
N(12)-C(8)-N(13)	122.75(7)	N(15)-N(16)-H(19)	106.4(10)
N(13)-C(8)-N(15)	116.38(6)	H(19)-N(16)-H(20)	106.7(13)

Table S12. Torsion Angles[°] for **4**. (Those having bond angles > 160 or < 20 degrees are excluded.)

	Angle		Angle
C(2)-N(1)-C(3)-O(3)	179.68(6)	C(2)-N(1)-C(3)-N(3)	-0.91(10)
C(3)-N(1)-C(2)-O(2)	-178.50(6)	C(3)-N(1)-C(2)-N(2)	1.80(10)
C(1)-N(2)-C(2)-O(2)	179.96(6)	C(1)-N(2)-C(2)-N(1)	-0.33(11)
C(2)-N(2)-C(1)-O(1)	178.02(6)	C(2)-N(2)-C(1)-N(3)	-1.92(10)
C(1)-N(3)-C(3)-O(3)	177.88(6)	C(1)-N(3)-C(3)-N(1)	-1.55(10)
C(3)-N(3)-C(1)-O(1)	-177.08(6)	C(3)-N(3)-C(1)-N(2)	2.86(10)
C(4)-N(4)-C(5)-O(5)	-178.98(6)	C(4)-N(4)-C(5)-N(5)	1.14(10)
C(5)-N(4)-C(4)-O(4)	178.06(6)	C(5)-N(4)-C(4)-N(6)	-1.99(10)
C(5)-N(5)-C(6)-O(6)	-177.21(6)	C(5)-N(5)-C(6)-N(6)	2.33(10)
C(6)-N(5)-C(5)-O(5)	178.82(6)	C(6)-N(5)-C(5)-N(4)	-1.30(10)
C(4)-N(6)-C(6)-O(6)	176.48(6)	C(4)-N(6)-C(6)-N(5)	-3.05(9)
C(6)-N(6)-C(4)-O(4)	-177.17(6)	C(6)-N(6)-C(4)-N(4)	2.88(9)
N(9)-N(8)-C(7)-N(7)	2.76(10)	N(9)-N(8)-C(7)-N(10)	-178.22(5)
N(11)-N(10)-C(7)-N(7)	179.02(5)	N(11)-N(10)-C(7)-N(8)	0.01(9)
N(14)-N(13)-C(8)-N(12)	-0.54(10)	N(14)-N(13)-C(8)-N(15)	179.60(6)
N(16)-N(15)-C(8)-N(12)	-0.67(10)	N(16)-N(15)-C(8)-N(13)	179.20(5)

Table S13. Hydrogen bonds for **4** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(1) ...O(6)#1	2.8104(10)	0.868(14)	1.942(14)	178.2(13)
N(3)-H(2) ...O(4)	2.8221(11)	0.856(15)	1.978(15)	168.6(13)
N(4)-H(3) ...O(3)	2.8444(11)	0.890(15)	1.955(15)	177.2(13)
N(5)-H(4) ...O(2)#2	2.7786(10)	0.875(14)	1.905(14)	175.9(13)
N(7)-H(5) ...O(6)#3	2.8729(11)	0.902(16)	2.052(16)	150.9(13)
N(7)-H(6) ...N(9)	2.6609(12)	0.906(12)	2.244(14)	107.5(11)
N(7)-H(6) ...N(14)#4	3.0843(11)	0.906(12)	2.247(13)	153.5(12)
N(8)-H(7) ...O(1)	2.8091(11)	0.867(13)	2.079(13)	141.4(10)
N(8)-H(7) ...N(9)	1.4077(9)	0.867(13)	2.016(12)	35.8(5)
N(8)-H(7) ...N(11)	2.6575(10)	0.867(13)	2.298(11)	105.0(9)
N(9)-H(8) ...O(2)#5	2.9400(11)	0.909(14)	2.076(14)	158.2(13)
N(9)-H(8) ...N(8)	1.4077(9)	0.909(14)	1.916(13)	43.8(6)
N(9)-H(9) ...N(8)	1.4077(9)	0.944(14)	1.944(14)	42.9(6)
N(10)-H(10) ...N(1)#6	2.8133(12)	0.906(14)	1.908(14)	177.6(12)
N(10)-H(10) ...N(11)	1.4135(11)	0.906(14)	2.024(16)	37.2(7)
N(11)-H(11) ...N(10)	1.4135(11)	0.924(14)	1.915(15)	44.5(7)
N(11)-H(12) ...N(10)	1.4135(11)	0.899(13)	1.881(16)	46.0(8)
N(12)-H(13) ...O(4)	2.8367(12)	0.906(14)	1.951(14)	165.3(12)
N(12)-H(13) ...N(14)	2.8352(12)	0.906(14)	2.563(13)	98.0(9)
N(12)-H(14) ...N(16)	2.7058(12)	0.860(15)	2.372(14)	103.6(10)
N(12)-H(14) ...N(16)3#	2.9212(11)	0.860(15)	2.159(14)	147.5(12)
N(13)-H(15) ...N(6)#7	2.9004(10)	0.853(14)	2.071(14)	163.7(15)
N(13)-H(15) ...N(14)	1.4051(11)	0.853(14)	1.943(15)	40.3(8)
N(14)-H(16) ...N(13)	1.4051(11)	0.911(15)	1.927(16)	43.0(8)
N(14)-H(17) ...N(13)	1.4051(11)	0.876(13)	1.893(14)	44.3(7)
N(15)-H(18) ...O(3)#6	2.8441(11)	0.908(13)	2.098(15)	138.8(13)
N(15)-H(18) ...N(16)	1.4064(11)	0.908(13)	2.005(14)	38.1(7)
N(16)-H(19) ...N(15)	1.4064(11)	0.879(14)	1.856(15)	46.6(8)
N(16)-H(20) ...O(5)#6	2.9192(11)	0.912(14)	2.012(14)	173.4(13)
N(16)-H(20) ...N(15)	1.4064(11)	0.912(14)	1.883(15)	45.7(7)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z+1 #2 x,y,z-1 #3 -x,-y+1,-z+1 #4 x-1,y,z #5 -x,-y+2,-z+2 #6 x,y-1,z #7 -x+1,-y+1,-z+1

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **9·H_2O**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	4217(3)	4258(2)	2780(2)	27(1)
O(2)	2959(3)	-627(2)	4313(2)	24(1)
O(3)	-899(3)	3223(2)	477(2)	24(1)
O(4)	2024(4)	6054(2)	5583(2)	35(1)
N(1)	3716(4)	1793(2)	3516(2)	22(1)
N(2)	998(4)	1287(2)	2395(2)	22(1)
N(3)	1774(4)	3757(2)	1550(2)	22(1)
N(4)	4913(4)	7629(2)	1083(2)	26(1)
N(5)	7660(4)	6971(2)	2891(2)	23(1)
N(6)	9042(4)	7741(2)	3198(2)	25(1)
N(7)	8622(4)	9140(2)	2250(2)	24(1)
N(8)	7003(4)	9347(2)	1312(2)	23(1)
C(1)	3291(4)	3333(3)	2621(3)	22(1)
C(2)	2580(4)	725(3)	3458(2)	21(1)
C(3)	536(4)	2788(2)	1407(2)	20(1)
C(4)	6428(4)	7970(3)	1738(2)	21(1)

Table S15. Bond lengths [Å] and angles [°] for **9·H_2O.**

O(1)-C(1)	1.228(3)	N(3)-C(3)	1.376(3)
O(2)-C(2)	1.224(3)	N(3)-H(2)	0.85(3)
O(3)-C(3)	1.221(3)	N(4)-C(4)	1.350(3)
O(4)-H(7)	0.87(4)	N(4)-H(4)	0.89(4)
O(4)-H(8)	0.90(4)	N(4)-H(5)	0.89(3)
N(1)-C(1)	1.372(3)	N(5)-C(4)	1.339(3)
N(1)-C(2)	1.381(3)	N(5)-N(6)	1.362(2)
N(1)-H(1)	0.99(3)	N(5)-H(6)	0.98(4)
N(2)-C(2)	1.365(3)	N(6)-N(7)	1.288(3)
N(2)-C(3)	1.372(3)	N(7)-N(8)	1.359(3)
N(2)-H(3)	0.78(3)	N(8)-C(4)	1.334(3)
N(3)-C(1)	1.367(3)		
H(7)-O(4)-H(8)	112(4)	N(7)-N(6)-N(5)	106.31(18)
C(1)-N(1)-C(2)	124.4(2)	N(6)-N(7)-N(8)	111.78(17)
C(1)-N(1)-H(1)	117.5(18)	C(4)-N(8)-N(7)	105.05(18)
C(2)-N(1)-H(1)	118.0(18)	O(1)-C(1)-N(3)	122.7(2)
C(2)-N(2)-C(3)	124.68(19)	O(1)-C(1)-N(1)	121.9(2)
C(2)-N(2)-H(3)	119(2)	N(3)-C(1)-N(1)	115.38(19)
C(3)-N(2)-H(3)	116(2)	O(2)-C(2)-N(2)	122.71(19)
C(1)-N(3)-C(3)	124.58(19)	O(2)-C(2)-N(1)	121.9(2)
C(1)-N(3)-H(2)	123(2)	N(2)-C(2)-N(1)	115.4(2)
C(3)-N(3)-H(2)	112(2)	O(3)-C(3)-N(2)	121.67(19)
C(4)-N(4)-H(4)	114(2)	O(3)-C(3)-N(3)	122.9(2)
C(4)-N(4)-H(5)	121.4(19)	N(2)-C(3)-N(3)	115.40(18)
H(4)-N(4)-H(5)	122(3)	N(8)-C(4)-N(5)	108.88(19)
C(4)-N(5)-N(6)	107.99(18)	N(8)-C(4)-N(4)	125.4(2)
C(4)-N(5)-H(6)	133(2)	N(5)-C(4)-N(4)	125.6(2)
N(6)-N(5)-H(6)	119(2)		

Table S16. Anisotropic displacement parameters ($Å^2$ x 10^3) for **9·H_2O**. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$h^2a^{*2}U_{11}$ + ... + 2hka*b*U_{12}].

	U11	U22	U33	U23	U13	U12
O(1)	39(1)	18(1)	35(1)	-7(1)	-15(1)	-16(1)
O(2)	32(1)	12(1)	30(1)	-2(1)	-12(1)	-12(1)
O(3)	31(1)	17(1)	30(1)	-5(1)	-14(1)	-12(1)
O(4)	45(1)	19(1)	48(1)	1(1)	-25(1)	-21(1)
N(1)	30(1)	16(1)	30(1)	-6(1)	-14(1)	-13(1)
N(2)	30(1)	16(1)	29(1)	-6(1)	-12(1)	-13(1)
N(3)	33(1)	12(1)	29(1)	-3(1)	-15(1)	-13(1)
N(4)	35(1)	18(1)	34(1)	-6(1)	-12(1)	-17(1)
N(5)	31(1)	14(1)	30(1)	-6(1)	-11(1)	-14(1)
N(6)	31(1)	18(1)	32(1)	-7(1)	-12(1)	-13(1)
N(7)	30(1)	18(1)	33(1)	-7(1)	-11(1)	-14(1)
N(8)	30(1)	15(1)	31(1)	-6(1)	-11(1)	-13(1)
C(1)	28(1)	17(1)	29(1)	-9(1)	-9(1)	-11(1)
C(2)	26(1)	18(1)	26(1)	-7(1)	-7(1)	-13(1)
C(3)	27(1)	15(1)	25(1)	-7(1)	-6(1)	-11(1)
C(4)	27(1)	16(1)	25(1)	-7(1)	-5(1)	-13(1)

Table S17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **9·H_2O**.

	x	y	z	U(eq)
H(1)	4810(50)	1450(30)	4300(30)	31(7)
H(2)	1410(50)	4670(40)	930(30)	32(7)
H(3)	300(50)	740(40)	2330(30)	22(6)
H(4)	4460(60)	6720(40)	1620(40)	33(7)
H(5)	4030(50)	8360(30)	370(30)	18(6)
H(6)	7710(60)	5880(50)	3490(40)	45(9)
H(7)	1470(70)	6700(50)	4750(40)	49(10)
H(8)	3320(70)	6320(50)	5770(40)	55(10)

Table S18. Torsion angles [°] for **9·H_2O**.

C(4)-N(5)-N(6)-N(7)	-0.1(3)
N(5)-N(6)-N(7)-N(8)	0.0(3)
N(6)-N(7)-N(8)-C(4)	0.0(2)
C(3)-N(3)-C(1)-O(1)	-174.7(2)
C(3)-N(3)-C(1)-N(1)	5.3(3)
C(2)-N(1)-C(1)-O(1)	175.2(2)
C(2)-N(1)-C(1)-N(3)	-4.8(3)
C(3)-N(2)-C(2)-O(2)	-179.4(2)
C(3)-N(2)-C(2)-N(1)	1.1(3)
C(1)-N(1)-C(2)-O(2)	-177.6(2)
C(1)-N(1)-C(2)-N(2)	1.8(3)
C(2)-N(2)-C(3)-O(3)	179.9(2)
C(2)-N(2)-C(3)-N(3)	-0.7(3)
C(1)-N(3)-C(3)-O(3)	176.7(2)
C(1)-N(3)-C(3)-N(2)	-2.7(3)
N(7)-N(8)-C(4)-N(5)	-0.1(2)
N(7)-N(8)-C(4)-N(4)	-178.2(2)
N(6)-N(5)-C(4)-N(8)	0.1(3)
N(6)-N(5)-C(4)-N(4)	178.2(2)

Table S19. Hydrogen bonds for **9·H_2O** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(2)#1	0.99(3)	1.84(3)	2.823(3)	174(3)
N(3)-H(2)...O(3)#2	0.85(3)	1.93(3)	2.772(3)	174(3)
N(2)-H(3)...N(7)#3	0.78(3)	2.05(4)	2.825(3)	176(3)
N(4)-H(4)...O(1)	0.89(4)	2.22(4)	3.097(3)	168(3)
N(4)-H(5)...N(8)#4	0.89(3)	2.18(3)	3.011(3)	156(2)
N(5)-H(6)...O(4)#5	0.98(4)	1.69(4)	2.668(3)	175(3)
O(4)-H(7)...N(6)#6	0.87(4)	2.03(4)	2.849(3)	157(3)
O(4)-H(8)...O(1)#5	0.90(4)	2.02(4)	2.803(3)	145(3)

Symmetry transformations used to generate equivalent atoms:

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

Table S20. Crystal data and structure refinement for $CA \cdot H_2O$.

	$CA \cdot H_2O$
Formula	$C_3H_7N_3O_5$
M(g/mol)	165.12
Crystal Color	colorless
Crystal System	Monoclinic
Space Group	C2/c
a [Å]	12.312(3)
b [Å]	6.7174(14)
c [Å]	8.707(2)
α [°]	90
β [°]	115.09(2)
γ [°]	90
V [Å^3]	652.2(3)
Z	4
T [k]	123
λ [Å]	0.71075
ρ_{calcd} [g/cm-3]	1.82
μ [mm^{-1}]	0.160
F (000)	344
crystal size [mm^3]	0.220×0.200×0.180
ϑ_{max} [°]	27.840
No. Refl. collected	3576
No. Indep. reflections	778
[R_{int}]	0.0898
GOF[a] on F^2	0.954
R_1 [b] [I>2σ(I)]	0.05654
wR_2 [c] [All refl.]	0.1360

Crystal of $CA \cdot H_2O$ was obtained when we cultured the crystal salt **5** by slow evaporation from water solution at room temperature and normal pressure. Its CCDC number is 1447126.

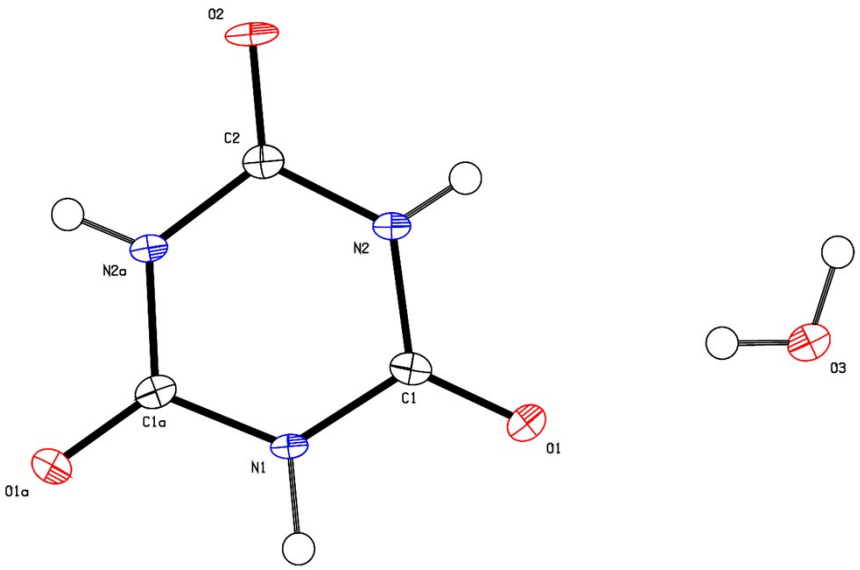


Figure S1 Molecular structure of CA·H_2O. Ellipsoids are drawn at the 50%probability level.

Table S21. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for CA·H_2O. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	3607(1)	950(2)	4738(2)	21(1)
O(2)	5000	6818(3)	7500	32(1)
O(3)	1966(2)	1728(3)	1371(2)	24(1)
N(1)	5000	924(4)	7500	14(1)
N(2)	4285(2)	3914(3)	6088(2)	16(1)
C(1)	4250(2)	1870(3)	6017(3)	15(1)
C(2)	5000	4995(5)	7500	19(1)

Table S22. Bond lengths [Å] and angles [°] for CA·H_2O.

O(1)-C(1)	1.225(3)	H(1)-O(3)-H(4)	106(3)
O(2)-C(2)	1.225(4)	C(1)#1-N(1)-C(1)	125.3(3)
O(3)-H(1)	0.85(4)	C(1)#1-N(1)-H(3)	117.36(13)
O(3)-H(4)	0.92(5)	C(1)-N(1)-H(3)	117.36(13)
N(1)-C(1)#1	1.383(2)	C(1)-N(2)-C(2)	124.3(2)
N(1)-C(1)	1.383(2)	C(1)-N(2)-H(2)	115(2)
N(1)-H(3)	0.98(4)	C(2)-N(2)-H(2)	120(2)
N(2)-C(1)	1.374(3)	O(1)-C(1)-N(2)	122.7(2)
N(2)-C(2)	1.377(3)	O(1)-C(1)-N(1)	122.3(2)
N(2)-H(2)	0.85(4)	N(2)-C(1)-N(1)	114.9(2)
C(2)-N(2)#1	1.377(3)	O(2)-C(2)-N(2)#1	121.82(13)
		O(2)-C(2)-N(2)	121.82(13)
		N(2)#1-C(2)-N(2)	116.4(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,-z+3/2

Table S22. Anisotropic displacement parameters ($Å^2$ x 10^3) for $CA \cdot H_2O$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2a^{*2} U_{11} + ... + 2hka^*b^*U_{12}]$.

	U11	U22	U33	U23	U13
O(1)	26(1)	12(1)	17(1)	-2(1)	1(1)
O(2)	49(2)	5(1)	30(2)	0	5(1)
O(3)	30(1)	13(1)	20(1)	-2(1)	2(1)
N(1)	19(1)	6(1)	14(1)	0	4(1)
N(2)	21(1)	7(1)	15(1)	1(1)	3(1)
C(1)	18(1)	10(1)	17(1)	2(1)	7(1)
C(2)	25(2)	11(2)	17(2)	0	5(1)

Table S23. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $CA \cdot H_2O$.

	x	y	z	U(eq)
H(1)	2570(40)	1830(60)	2320(60)	98(16)
H(2)	3790(30)	4500(50)	5210(40)	49(9)
H(3)	5000	-540(60)	7500	16(8)
H(4)	1850(30)	2970(80)	890(50)	107(16)

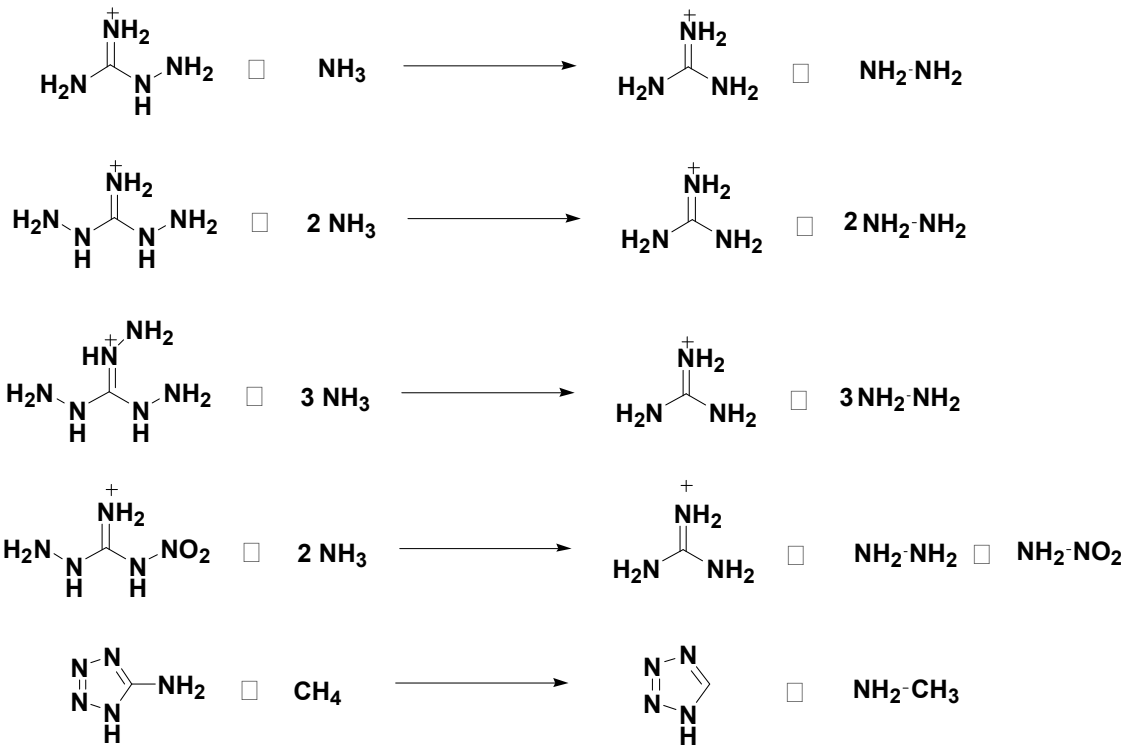
Table S24. Torsion angles [°] for $CA \cdot H_2O$.

C(2)-N(2)-C(1)-O(1)	-179.65(17)
C(2)-N(2)-C(1)-N(1)	0.0(2)
C(1)#1-N(1)-C(1)-O(1)	179.7(2)
C(1)#1-N(1)-C(1)-N(2)	-0.02(11)
C(1)-N(2)-C(2)-O(2)	179.98(13)
C(1)-N(2)-C(2)-N(2)#1	-0.02(13)

Symmetry transformations used to generate equivalent atoms:

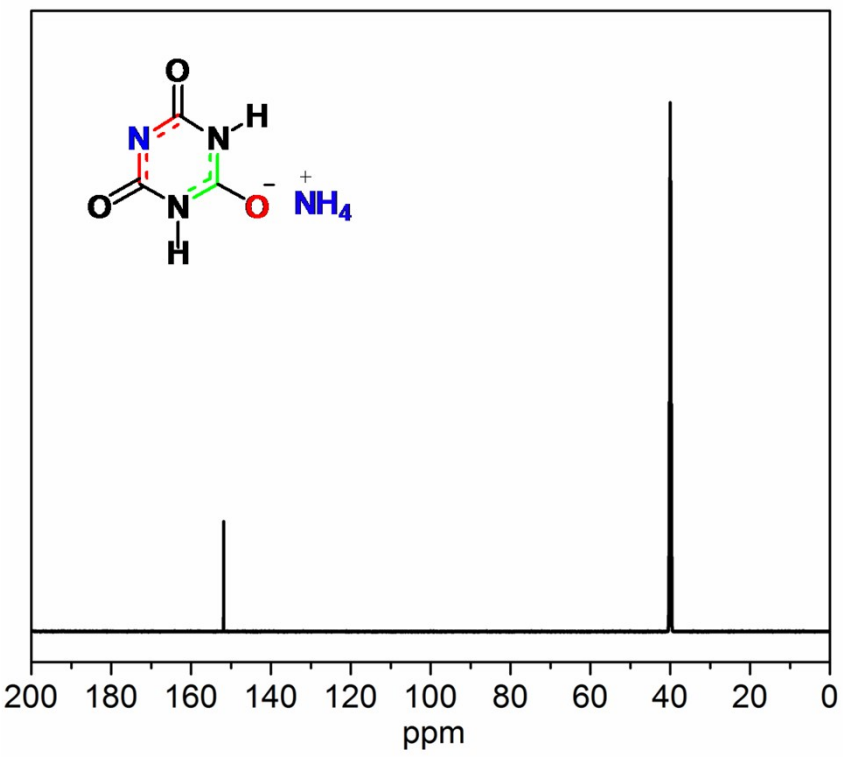
#1 -x+1,y,-z+3/2

Computational Details



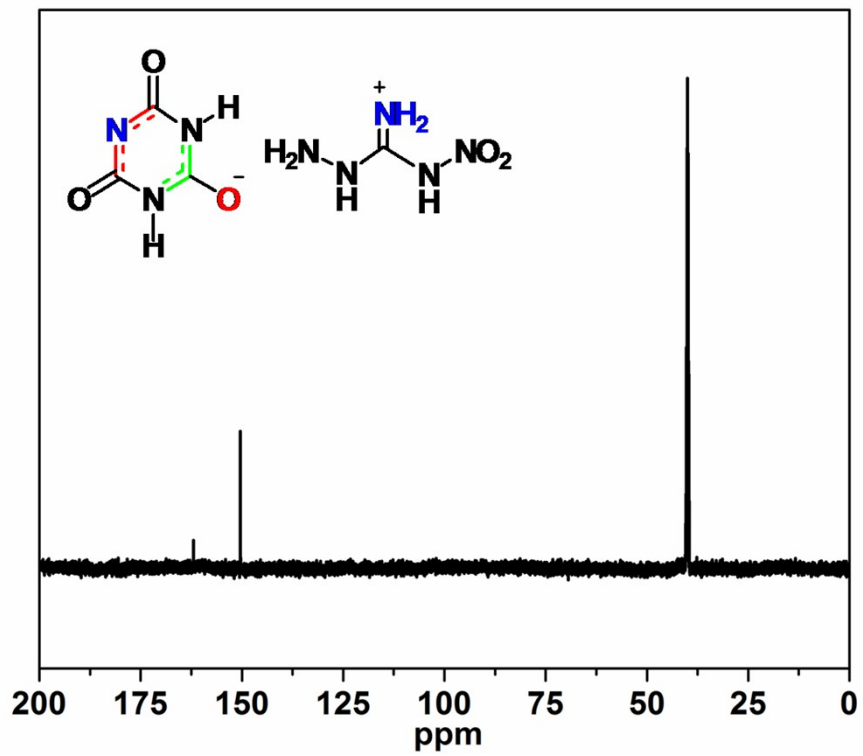
Scheme S1. Isodesmic reactions for **2, 4,5** and **6** cations and 5-amino-1*H*-tetrazole

Fig. S2 ^{13}C NMR spectra of salt **1**



In the ^{13}C NMR spectra, a single peak (~ 152 ppm) is due to the anion, indicating the anion ring tautomerism.

Fig. S3 ^{13}C NMR spectra of salt **6**.



In the 13C NMR spectra, there are two signals (~150 ppm and ~162 ppm). single peak at 150 ppm is due to the anion, and the other one at 162 ppm is associated with the cation.