

Supporting Information

Nitrogen-rich 4-R-5-nitro-1,2,3-triazolate salts (R = -CH₃, -NH₂, -NO₂, -N₃ and -NHNO₂) as Energetic Materials

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Figure S1. (a) Thermal ellipsoid plot (30%) of **3a**. Hydrogen atoms are included but unlabeled for clarity. (b) Ball and stick packing diagram of **3a** viewed down the *b* axis. Dashed lines indicate hydrogen bonding.

Figure S2. (a) Thermal ellipsoid plot (30%) of **3e**. Hydrogen atoms are included but unlabeled for clarity.

Figure S3. (a) Thermal ellipsoid plot (30%) of **3f**. Hydrogen atoms are included but unlabeled for clarity. (b) Ball and stick packing diagram of **3f** viewed down the *b* axis. Dashed lines indicate hydrogen bonding.

Figure S4. Thermal ellipsoid plot (30%) of **4d**. Hydrogen atoms are included but unlabeled for clarity.

Figure S5. Thermal ellipsoid plot (30%) of **5a**. Hydrogen atoms are included but unlabeled for clarity.

Figure S6. (a) Thermal ellipsoid plot (30%) of **5b**. Hydrogen atoms are included but unlabeled for clarity. (b) Ball and stick packing diagram of **5b** viewed down the *a* axis. Dashed lines indicate hydrogen bonding.

Table S1. Selected Hydrogen Bonds for **3a**, **3e**, **3f**, **4d**, **5a** and **5b** (Å and °)

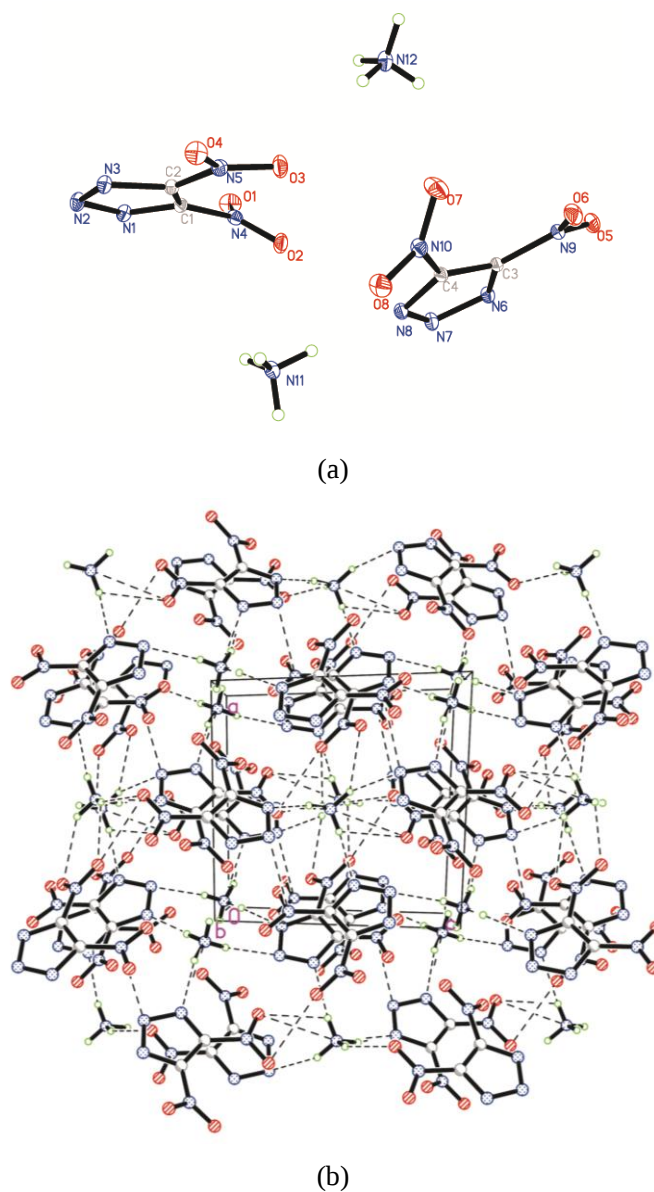


Figure S1. (a) Thermal ellipsoid plot (30%) of **3a**. Hydrogen atoms are included but unlabeled for clarity. (b) Ball and stick packing diagram of **3a** viewed down the *b* axis. Dashed lines indicate hydrogen bonding.

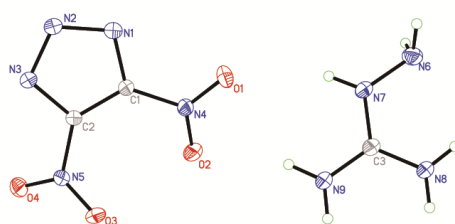
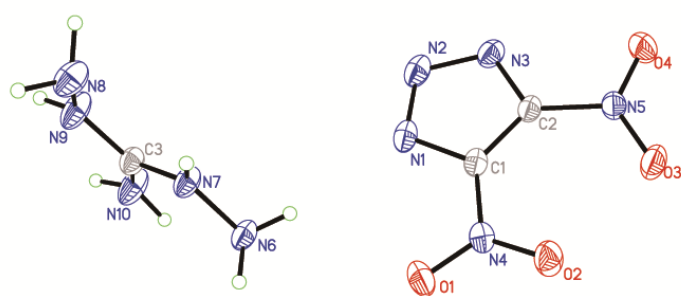
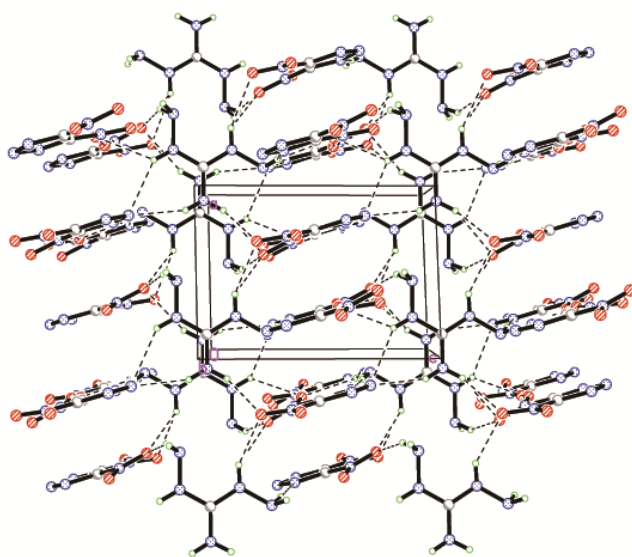


Figure S2. (a) Thermal ellipsoid plot (30%) of **3e**. Hydrogen atoms are included but unlabeled for clarity.



(a)



(b)

Figure S3. (a) Thermal ellipsoid plot (30%) of **3f**. Hydrogen atoms are included but unlabeled for clarity. (b) Ball and stick packing diagram of **3f** viewed down the *b* axis. Dashed lines indicate hydrogen bonding.

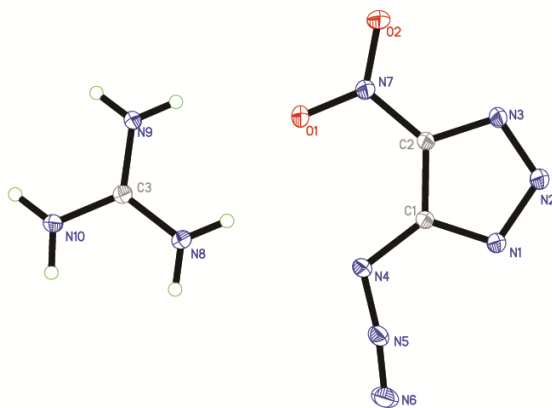


Figure S4. Thermal ellipsoid plot (30%) of **4d**. Hydrogen atoms are included but unlabeled for clarity.

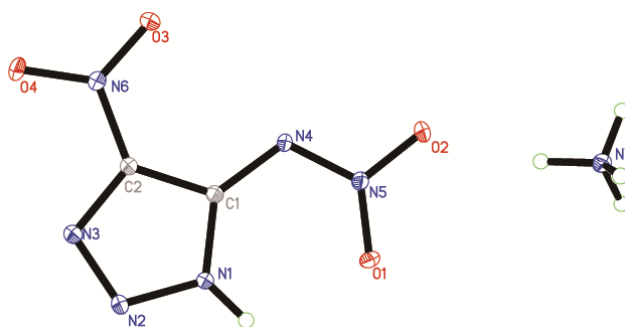


Figure S5. Thermal ellipsoid plot (30%) of **5a**. Hydrogen atoms are included but unlabeled for clarity.

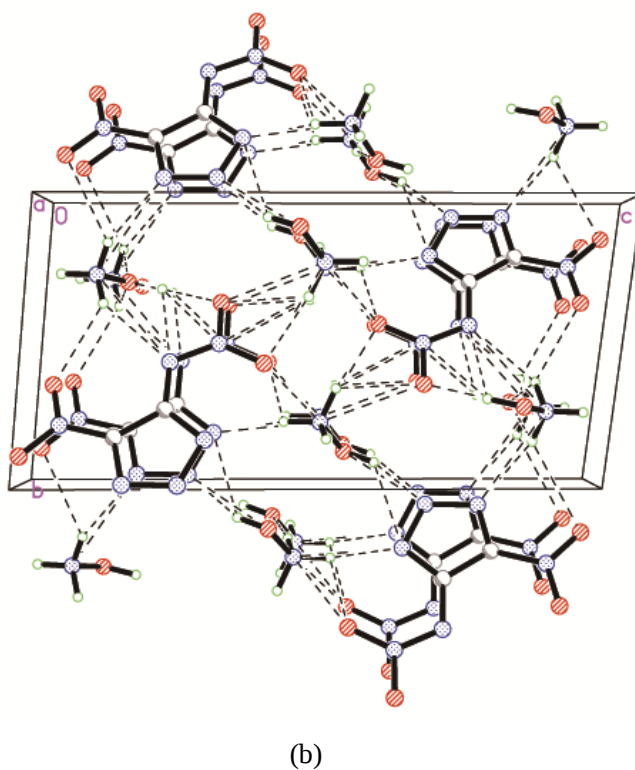
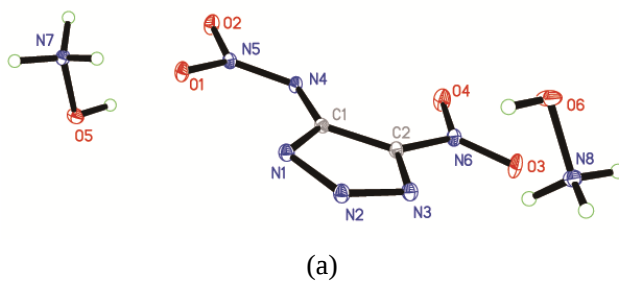


Figure S6. (a) Thermal ellipsoid plot (30%) of **5b**. Hydrogen atoms are included but unlabeled for clarity. (b) Ball and stick packing diagram of **5b** viewed down the *a* axis. Dashed lines indicate hydrogen bonding.

Table S1. Selected Hydrogen Bonds for **3a**, **3e**, **3f**, **4d**, **5a** and **5b** (Å and °)

D-H...A	Symm.	d(D-H) [Å]	d(H...A) [Å]	d(D...A) [Å]	<(DHA) [°]
3a					
N(12)-H(12A)...O(4)	1-x, 1-y, 1-z	0.846(19)	2.532(16)	2.9598(13)	112.4(13)
N(12)-H(12B)...N(1)	1-x, -y, 2-z	0.936(16)	1.943(17)	2.8638(14)	167.5(16)
N(12)-H(12C)...O(8)	1-x, 1-y, 1-z	0.919(19)	2.50(2)	3.1769(16)	130.8(14)
N(12)-H(12D)...O(7)	1-x, 1-y, 1-z	0.900(19)	2.485(19)	3.0953(16)	125.5(16)
3e					
N(7)-H(7)...O(1)		0.870(17)	2.444(16)	2.2303(15)	150.6(14)
N(7)-H(7)...O(1)	-1+x, y, z	0.870(17)	2.285(16)	2.8683(14)	124.5(12)
N(8)-H(8A)...N(1)	x, 0.5-y, -0.5+z	0.857(15)	2.297(15)	3.1406(15)	168.1(13)
N(8)-H(8B)...N(3)	-1+x, 0.5-y, -0.5+z	0.855(15)	2.242(15)	3.0538(15)	158.6(14)
N(9)-H(9A)...N(2)	x, 0.5-y, -0.5+z	0.871(16)	2.091(16)	2.9399(15)	164.4(14)
N(9)-H(9B)...O(1)		0.889(17)	2.494(17)	3.2742(15)	146.8(13)
N(9)-H(9B)...O(2)		0.889(17)	2.397(17)	3.2484(15)	160.5(15)
3f					
N(6)-H(6A)...N(1)		0.877(14)	2.413(14)	3.2723(18)	166.3(12)
N(6)-H(6B)...O(4)	x, 1+y, z	0.926(14)	2.430(14)	3.2577(17)	148.8(12)
N(6)-H(6B)...N(3)	x, 1+y, z	0.926(14)	2.469(14)	3.2741(18)	145.4(12)
N(7)-H(7)...O(2)	1-x, 1-y, 1-z	0.860(13)	2.338(14)	2.9881(16)	132.7(12)
N(7)-H(7)...O(3)	1-x, 1-y, 1-z	0.860(13)	2.541(14)	3.2302(17)	137.8(12)
N(10)-H(10A)...O(2)	-x, 1-y, 1-z	0.855(15)	2.480(15)	3.2526(17)	150.6(13)
N(10)-H(10A)...O(3)	-x, 1-y, 1-z	0.855(15)	2.516(15)	3.1629(17)	133.1(13)
4d					
N(8)-H(8A)...O(1)		0.861(18)	2.248(19)	3.0102(19)	147.6(17)
N(8)-H(8A)...N(4)		0.861(18)	2.521(18)	3.2159(18)	138.3(16)
N(8)-H(8B)...O(2)	-1+x, 1-y, 0.5-z	0.88(2)	2.222(19)	3.0044(18)	148.2(17)
N(9)-H(9A)...O(1)		0.834(18)	2.236(18)	2.9802(18)	148.7(17)
N(10)-H(10B)...N(3)	-1+x, 1-y, 0.5-z	0.863(19)	2.193(19)	3.0445(19)	169.1(17)
5a					
N(7)-H(7A)...O(2)	-x, -0.5+y, 0.5-z	0.907(16)	2.548(16)	2.9514(15)	107.6(12)
N(7)-H(7A)...O(3)	-x, -0.5+y, 0.5-z	0.907(16)	2.569(16)	3.1591(15)	123.3(12)
N(7)-H(7A)...N(4)	-x, -0.5+y, 0.5-z	0.907(16)	2.068(16)	2.9462(15)	162.6(14)
N(7)-H(7B)...O(2)		0.934(17)	1.907(17)	2.8229(14)	166.6(15)
N(7)-H(7C)...O(1)	x, 0.5-y, -0.5+z	0.906(16)	2.291(16)	2.9896(15)	133.7(13)
N(7)-H(7C)...O(4)	x, 1.5-y, -0.5+z	0.906(16)	2.387(16)	2.8931(15)	115.4(12)
N(7)-H(7D)...O(3)	x, -1+y, z	0.890(19)	2.200(19)	3.0566(15)	161.2(15)
N(7)-H(7D)...O(4)	x, -1+y, z	0.890(19)	2.550(17)	3.1895(16)	129.3(14)
5b					
O(5)-H(5)...N(2)	-1+x, -1+y, z	0.88(2)	1.80(2)	2.6405(17)	161(2)
O(6)-H(6)...O(2)	1+x, 1+y, z	0.93(2)	1.70(2)	2.6164(16)	172.5(19)
O(6)-H(6)...N(4)	1+x, 1+y, z	0.93(2)	2.57(2)	3.0929(19)	116.7(16)
O(6)-H(6)...N(5)	1+x, 1+y, z	0.93(2)	2.49(2)	3.3052(19)	146.5(17)

N(7)-H(7B)...O(1)		0.94(2)	1.97(2)	2.9020(17)	170.6(16)
N(7)-H(7B)...O(2)		0.94(2)	2.370(18)	2.8976(18)	115.3(14)
N(7)-H(7B)...N(5)		0.94(2)	2.479(19)	3.2733(19)	142.5(15)
N(7)-H(7C)...N(1)	1-x, 1-y, 1-z	0.937(18)	1.871(18)	2.7992(18)	170.2(14)
