Supplementary Material (ESI) for New Journal of Chemistry
This journal is (c) The Royal Society of Chemistry and
The Centre National de la Recherche Scientifique, 2009

Supporting Information to Paper:

New Energetic Compounds Based on the Nitrogen-rich 5,5´-Azotetrazolate Anion ($[C_2N_{10}]^{2-}$)

Thomas M. Klapötke* and Carles Miró Sabaté

Table S1 Crystal structure solution and refinement for 5,5´-azotetrazolate salts **2** and **4**.

Parameter	**2**	**4**
Formula	$C_8H_{28}N_{20}O_6$	$C_4H_{16}N_{16}O_4$
Formula weight [g mol^{-1}]	500.51	352.33
Crystal size	0.17*x*0.12*x*0.06	0.29*x*0.13*x*0.07
T / K	200(2)	100(2)
Crystal system	Monoclinic	Triclinic
Space group	$P2_1/n$	$P\bar{1}$
a / Å	9.3101(3)	4.563(5)
b / Å	6.5383(2)	7.362(5)
c / Å	19.5637(5)	11.334(5)
α / °	90	105.125(5)
β / °	90.48(1)	90.933(5)
γ / °	90	102.871(5)
Volume / Å^3	1190.84(6)	357.2(5)
Z	2	1
ρ (g cm^{-3})	1.396	1.638
λ (Mo Kα, Å)	0.71073	0.71073
μ (mm^{-1})	0.169	0.140
reflns collected	5078	2480
indep. reflns	1861	1311
R_{int}	0.0292	0.0193
obsd. reflns.	2709	1164
F(000)	528	184
GOOF	1.039	1.071
n°. parameters	210	141
R_1 / wR_2 [$I > 2\sigma(I)$]	0.0459, 0.1199	0.0530, 0.1323
R_1 / wR_2 (all data)	0.0720, 0.1356	0.0590, 0.1378

$R_1 = \Sigma \, ||F_o| - |F_c|| \, / \, \Sigma \, |F_o|$; $R_w = [\Sigma \, (F_o^2 - F_c^2) \, / \, \Sigma \, w \, (F_o)^2]^{1/2}$; $w = [\sigma_c^2 \, (F_o^2) + (xP)^2 + yP]^{-1}$, $P = (F_o^2 - 2F_c^2) \, / \, 3$.

Table S2 Primary level (diagonal) and secondary level (off-diagonal) graph-sets found in the crystal structure of compound **2**.

	A	B	C	D	E	F	G	H
O2–H22•••O3^{iv} (A)	D1,1(2)							
O1–H12•••O2 (B)	D2,2(4)	D1,1(2)						
O1–H11•••O2^{ii} (C)	D2,2(4)	C1,2(4)	D1,1(2)					
O3–H32•••N6 (D)	D2,2(4)	–	–	D1,1(2) [D2,2(8)]				
O2–H21•••N9 (E)	D2,2(5)	D2,2(4)	D2,2(4)	D2,2(5) [D2,2(8)]	D1,1(2) [D2,2(8)]			
O3–H31•••N7^{iii} (F)	D2,2(4)	–	–	R4,4(10) [C2,2(10)]	D2,2(5) [D2,2(9)]	D1,1(2) [D2,2(10)]		
N1–H1B•••O1^{ii} (G)	–	D2,2(4)	D2,2(4)	–	–	–	D1,1(2)	
N1–H1A•••N8^{i} (H)	–	–	–	D2,2(5) [D2,2(9)]	D2,2(4) [D2,2(9)]	D2,2(4) [D2,2(10)]	D2,2(5)	D1,1(2) [D2,2(10)]

Symmetry codes: (i) 0.5–x, –0.5+y, 0.5–z; (ii) 1.5–x, –0.5+y, 0.5–z; (iii) –x, 1–y, 1–z; (iv) 1–x, 1–y, 1–z.

Table S3 Primary level (diagonal) and secondary level (off-diagonal) graph-sets found in the crystal structure of compound **4**.

	A	B	C	D	E	F	G	H	I
O2–H2A•••O1^{vi} (A)	D1,1(2)								
O2–H2B•••N3^{iv} (B)	D2,2(5)	D1,1(2) [D2,2(10)]							
N8–H8B•••O2 (C)	R4,4(14)	D2,2(4)	D1,1(2)						
N8–H8A•••O1^{v} (D)	D2,3(8)	–	D3,3(10)	C1,1(5)					
N8–H8A•••O1^{iv} (E)	D2,3(8)	–	D3,3(10)	R4,4(20) [R2,2(4)]	R2,2(10)				
N6–H6B•••N1^{i} (F)	D2,2(6)	D2,2(5) [D2,2(9)]	D2,2(8)	C3,3(16)	C3,3(16)	D1,1(2) [D2,2(8)]			
N7–H7•••N5^{ii} (G)	D2,2(6)	D2,2(6) [D2,2(7)]	D2,2(6)	C3,3(10)	C3,3(10)	R4,4(16) [R2,2(9)]	D1,1(2) [D2,2(4)]		
N6–H6A•••N2^{iii} (H)	D2,2(6)	D2,2(4) [D2,2(10)]	D2,2(8)	C3,3(18)	C3,3(18)	R4,4(10) [C2,2(10)]	C2,2(9) [R4,4(20)]	D1,1(2) [D2,2(10)]	
N8–H8C•••N4^{ii} (I)	D2,2(7)	D2,2(4) [D2,2(9)]	D2,2(5)	C3,3(14)	C3,3(14)	R4,4(18) [R2,2(12)]	R2,2(7) [R4,4(16)]	C2,2(9) [R4,4(26)]	D1,1(2) [D2,2(8)]

Symmetry codes: (i) 1–x, –y, 1–z; (ii) –1+x, –1+y, z; (iii) 1+x, y, z; (iv) 1–x, –y, 2–z; (v) –1+x, y, z; (vi) 2–x, –y, 2–z.

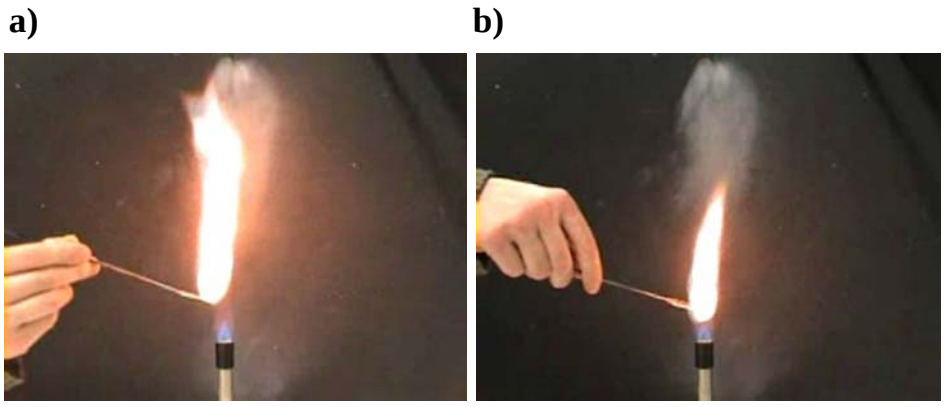

Figure S1 Smokeless deflagration in the "flame test" for 5,5′-azotetrazolate salts **1** (a) and **2** (b).

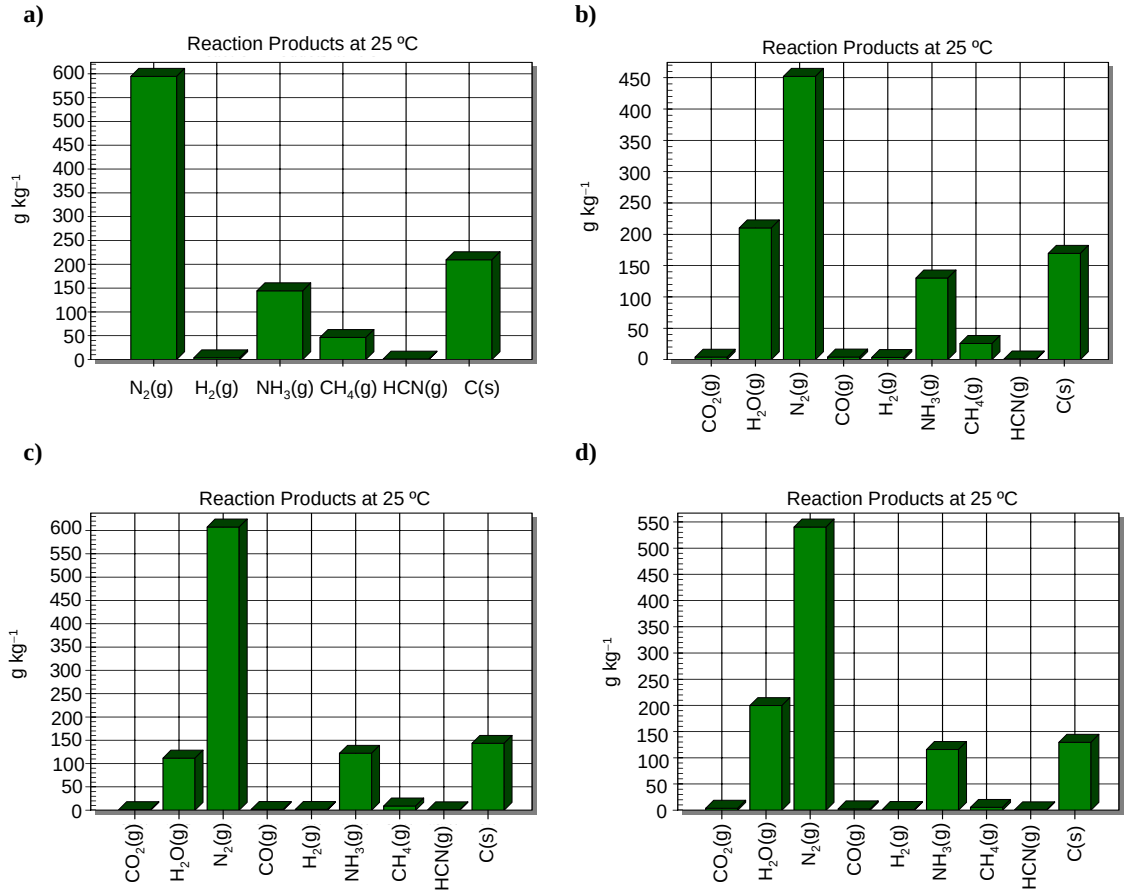

Figure S2 Predicted decomposition gases (computed using the ICT code) of 5,5′-azotetrazolate salts a) **1**, b) **2**, c) **3** and d) **4**.