Electronic Supplementary Material (ESI) for Dalton Transactions.

Asymmetric nitrogen-riched energetic materials resulting from the combination of tetrazolyl, dinitromethyl and (1,2,4-oxadiazol-5- yl)nitroamino group with furoxan

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1. Crystal Structure Data

Table S1. Crystal data and structure refinement for **7**.

Identification code	**7**	
CCDC number	1860916	
Empirical formula	$C_4H_8N_{10}O_6$	
Formula weight	292.20	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 7.4560(3) Å	□= 73.599(2)°.
	b = 8.5912(3) Å	□= 83.431(2)°.
	c = 9.9008(4) Å	□ = 65.465(2)°.
Volume	553.46(4) $Å^3$	
Z	2	
Density (-123°C)	1.753 Mg/m^3	
Density (20°C)	1.717 Mg/m^3	
Absorption coefficient	1.416 mm^{-1}	
F(000)	300	
Crystal size	0.189 x 0.154 x 0.091 mm^3	
Theta range for data collection	4.656 to 74.406°.	
Index ranges	-9<=h<=7, -10<=k<=9, -12<=l<=9	
Reflections collected	3309	
Independent reflections	1795 [R_{int} = 0.0192]	
Completeness to theta = 67.679°	83.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7538 and 0.6533	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1795 / 18 / 206	
Goodness-of-fit on F^2	1.111	
Final R indices [I>2sigma(I)]	R_1 = 0.0381, wR_2 = 0.1015	
R indices (all data)	R_1 = 0.0422, wR_2 = 0.1096	
Extinction coefficient	0.026(2)	
Largest diff. peak and hole	0.426 and -0.310 $e.Å^{-3}$	

Table S2. Crystal data and structure refinement for **13**.

Identification code	**13**	
CCDC number	1860917	
Empirical formula	$C_5H_8N_{12}O_5$	
Formula weight	316.23	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.1220(7) Å	a= 76.121(6)°.
	b = 7.5186(9) Å	b= 74.829(6)°.
	c = 12.6185(17) Å	g = 67.346(5)°.
Volume	594.44(13) $Å^3$	
Z	2	
Density (20°C)	1.767 Mg/m^3	
Absorption coefficient	0.155 mm^{-1}	
F(000)	324	
Crystal size	0.210 x 0.107 x 0.030 mm^3	
Theta range for data collection	2.972 to 29.967°.	
Index ranges	-9<=h<=9, -10<=k<=10, -17<=l<=17	
Reflections collected	7147	
Independent reflections	3264 [R_{int} = 0.0289]	
Completeness to theta = 25.242°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7460 and 0.6808	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3264 / 16 / 223	
Goodness-of-fit on F^2	1.001	
Final R indices [I>2sigma(I)]	R_1 = 0.0437, wR_2 = 0.0928	
R indices (all data)	R_1 = 0.0917, wR_2 = 0.1124	
Largest diff. peak and hole	0.226 and -0.230 $e.Å^{-3}$	

Table S3. Crystal data and structure refinement for **20**.

Identification code	**20**	
CCDC number	1860918	
Empirical formula	$C_5K_2N_8O_9$	
Formula weight	394.33	
Temperature	293(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.2945(15) Å	a= 95.648(8)°.
	b = 7.6721(16) Å	b= 95.017(8)°.
	c = 12.581(3) Å	g = 117.937(8)°.
Volume	611.8(2) $Å^3$	
Z	2	
Density (20°C)	2.141 Mg/m^3	
Absorption coefficient	7.639 mm^{-1}	
F(000)	392	
Crystal size	0.315 x 0.246 x 0.086 mm^3	
Theta range for data collection	3.572 to 74.645°.	
Index ranges	-8<=h<=9, -9<=k<=9, -15<=l<=15	
Reflections collected	7674	
Independent reflections	2437 [R_{int} = 0.0410]	
Completeness to theta = 67.679°	98.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7538 and 0.4145	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2437 / 0 / 218	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R_1 = 0.0297, wR_2 = 0.0782	
R indices (all data)	R_1 = 0.0353, wR_2 = 0.0794	
Extinction coefficient	0.0214(12)	
Largest diff. peak and hole	0.232 and -0.406 $e.Å^{-3}$	

Table S4. Crystal data and structure refinement for **22**.

Identification code	**22**	
CCDC number	1860646	
Empirical formula	$C_5H_5KN_{10}O_9$	
Formula weight	388.29	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 7.7155(2) Å	a= 90°.
	b = 10.5198(2) Å	b=100.9850(10)°.
	c = 16.7965(4) Å	g = 90°.
Volume	1338.32(5) $Å^3$	
Z	4	
Density (20°C)	1.927 Mg/m^3	
Absorption coefficient	0.478 mm^{-1}	
F(000)	784	
Crystal size	0.208 x 0.119 x 0.082 mm^3	
Theta range for data collection	2.296 to 30.089°.	
Index ranges	-10<=h<=10, -14<=k<=14, -22<=l<=23	
Reflections collected	15653	
Independent reflections	3815 [R_{int} = 0.0199]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7460 and 0.7045	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3815 / 18 / 259	
Goodness-of-fit on F^2	1.030	
Final R indices [I>2sigma(I)]	R_1 = 0.0303, wR_2 = 0.0775	
R indices (all data)	R_1 = 0.0414, wR_2 = 0.0834	
Largest diff. peak and hole	0.308 and -0.202 $e.Å^{-3}$	

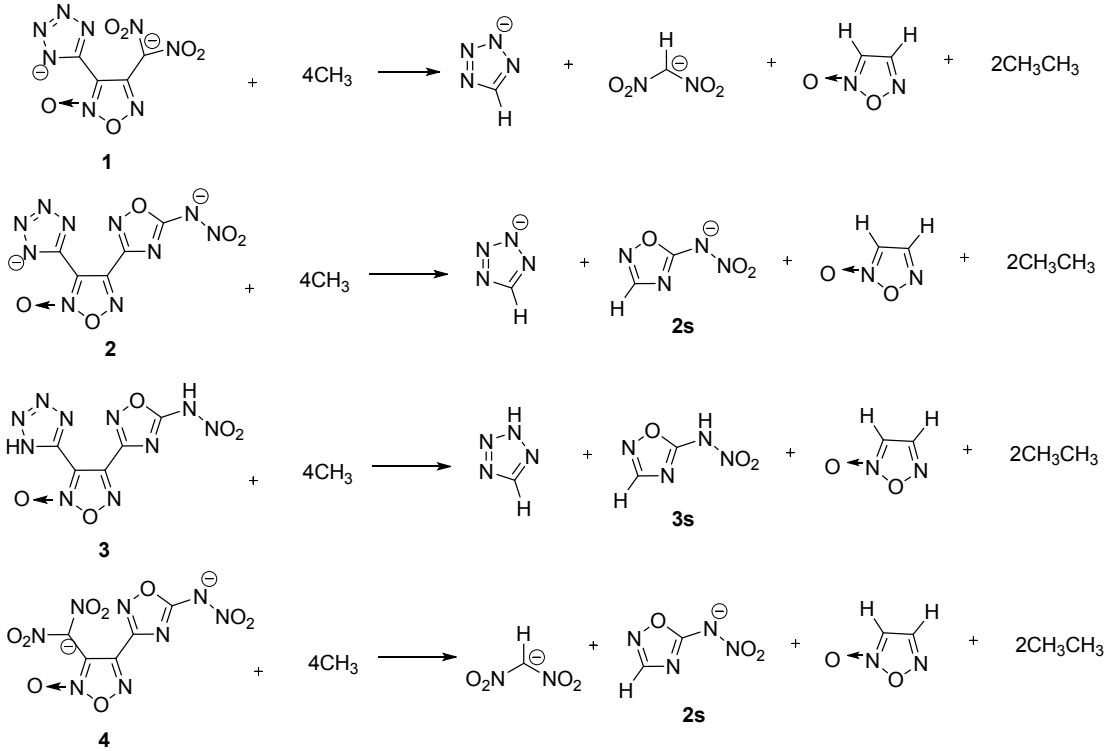
Table S5. Hydrogen bonds for **7** [Å and °]

	x	y	z	U(eq)
H(19A)	9350(30)	1340(20)	7870(20)	26
H(19B)	10020(30)	420(30)	6703(17)	26
H(19C)	7970(20)	1030(30)	7110(20)	26
H(19D)	9470(30)	-459(17)	8086(18)	26
H(20A)	7170(30)	6000(20)	3580(20)	30
H(20B)	7740(40)	5110(30)	2399(15)	30
H(20C)	9200(20)	5360(30)	3040(30)	30
H(20D)	8400(30)	4066(18)	3868(19)	30

Table S6. Hydrogen bonds for **13** [Å and °]

	x	y	z	U(eq)
H(22A)	2990(30)	2540(20)	6031(16)	59
H(22B)	1470(30)	1880(30)	5759(16)	59
H(22C)	3260(30)	424(17)	6190(18)	59
H(22D)	1650(30)	1730(30)	6946(10)	59
H(23A)	7980(30)	2170(30)	9250(10)	44
H(23B)	5784(16)	2480(30)	9819(17)	44
H(23C)	7420(30)	758(15)	10231(14)	44
H(23D)	7300(30)	2730(20)	10366(13)	44

2 Theoretical Calculations



Scheme S1. Isodesmic reactions for the anions of **1**, **2** and **4**; neutral molecule **3.**

Table S7. Calculated zero point energy (*ZPE*), values of the correction (*H*r), total energy (*E*0) and heats of formation (*HOF*)

Species	*ZPE*	*H*r	*E*0	corrected *E*0	*HOF*(kJ mol^{-1})
1	0.083423	0.098429	-1039.21499	-1039.11990	310.9900346
2	0.09611	0.112039	-1111.458895	-1111.35070	452.3509563
3	0.122524	0.138947	-1112.547643	-1112.41360	515.3611076
4	0.102014	0.120703	-1302.365758	-1302.24914	37.60963931
Tetrazole anion	0.033827	0.038051	-257.12423	-257.08754	181.58
Dinitromethyl anion	0.039727	0.046604	-448.0309171	-447.98590	-232.98
furoxan	0.049513	0.054822	-336.4521391	-336.39930	198.5
CH_3CH_3	0.07461	0.079038	-79.5716305	-79.49558	-84
2s	0.052589	0.060234	-520.2639482	-520.20582	-63.035
Tetrazole	0.046862	0.051291	-257.6538692	-257.60445	255.1030899
3s	0.06575	0.073758	-520.7812403	-520.71011	35.89633344

[a] Data obtained from G2.

[b] Data are from Ref. [D. R. Lide, ed., CRC Handbook of Chemistry and Physics, 88th Edition (Internet Version 2008), CRC Press/Taylor and Francis, Boca Raton, FL.].

Table S8. Calculated solid state heat of formation (*HOF*)

Compound	$\triangle H_L$ (kJ mol^{-1})	$\triangle H_f^{Cation}$ (kJ mol^{-1})	$\triangle H_f^{Anion}$ (kJ mol^{-1})	$\triangle H_f$ (kJ mol^{-1})
e-1	1347.671628	626.4	311.0	216.1283716
e-2	1220.034877	575.9	311.0	242.7651228
e-3	1164.925417	684.4	311.0	514.8745831
f-1				441.2891
f-2	1309.0303	626.4	425.4	369.1196999
f-3	1262.402442	770.0	425.4	702.9475582
f-4	1288.550473	669.5	425.4	475.7995266
f-6	1143.407707	684.4	425.4	650.7422931
g-1	1416.727949	501.1	37.6	-376.91831