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Electronic Supplementary Information

Tetrazolyl and dinitromethyl groups with 1,2,3-triazole lead to polyazole energetic materials

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1. Crystal Structure Data

Table S1. Crystal data and structure refinement for **5**.

Identification code	**5**	
CCDC number	1884770	
Empirical formula	$C_5H_3KN_6O_4$	
Formula weight	250.23	
Temperature	293(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 13.4341(3) Å	a= 90°.
	b = 8.8483(2) Å	b= 90°.
	c = 15.6056(3) Å	g = 90°.
Volume	1855.02(7) $Å^3$	
Z	8	
Density (20°C)	1.792 Mg/m^3	
Absorption coefficient	5.221 mm^{-1}	
F(000)	1008	
Crystal size	0.160 x 0.093 x 0.040 mm^3	
Theta range for data collection	5.670 to 74.520°.	
Index ranges	-15<=h<=12, -11<=k<=8, -19<=l<=18	
Reflections collected	10436	
Independent reflections	1866 [R_{int} = 0.0256]	
Completeness to theta = 67.679°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7538 and 0.5741	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1866 / 0 / 147	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R_1 = 0.0278, wR_2 = 0.0720	
R indices (all data)	R_1 = 0.0303, wR_2 = 0.0740	
Extinction coefficient	0.0049(3)	
Largest diff. peak and hole	0.291 and -0.215 $e.Å^{-3}$	

Table S2. Crystal data and structure refinement for **6**.

Identification code	**6**	
CCDC number	1884589	
Empirical formula	$C_5H_{15}N_{11}O_6$	
Formula weight	325.28	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.5623(11) Å	α= 97.880(2)°.
	b = 10.2596(15)Å	β= 91.529(2)°.
	c = 19.026(3) Å	γ = 109.537(2)°.
Volume	1373.9(3) $Å^3$	
Z	4	
Density (173(2)K)	1.573 Mg/m^3	
Crystal size	0.23×0.15×0.10 mm^3	
Radiation type	MoK□	
Θmin/°	1.084	
Θmax/°	25.344	
Measured Refl.	18302	
Independent Refl.	4997	
Reflections Used	3847	
Rint	0.0439	
Parameters	485	
Restraints	24	
Largest Peak	0.506	
Deepest Hole	-0.429	
GooF	1.075	
wR2 (all data)	0.2425	
wR2	0.2307	
R1 (all data)	0.0832	
R1	0.0681	

Table S3. Crystal data and structure refinement for **8**.

Identification code	**8**	
CCDC number	1884771	
Empirical formula	$C_5H_{13}N_{13}O_4$	
Formula weight	319.28	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 7.4845(2) Å	α= 90°.
	b = 12.8712(4) Å	β= 91.3270(10)°.
	c = 13.3363(4) Å	γ = 90°.
Volume	1284.40(7) $Å^3$	
Z	4	
Density (20°C)	1.651 Mg/m^3	
Absorption coefficient	0.140 mm^{-1}	
F(000)	664	
Crystal size	0.243 x 0.155 x 0.106 mm^3	
Theta range for data collection	2.199 to 30.025°.	
Index ranges	-10<=h<=10, -15<=k<=18, -18<=l<=18	
Reflections collected	15040	
Independent reflections	3657 [R_{int} = 0.0238]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7460 and 0.6957	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3657 / 8 / 215	
Goodness-of-fit on F^2	1.029	
Final R indices [I>2sigma(I)]	R_1 = 0.0458, wR_2 = 0.1218	
R indices (all data)	R_1 = 0.0634, wR_2 = 0.1351	
Largest diff. peak and hole	0.582 and -0.360 $e.Å^{-3}$	

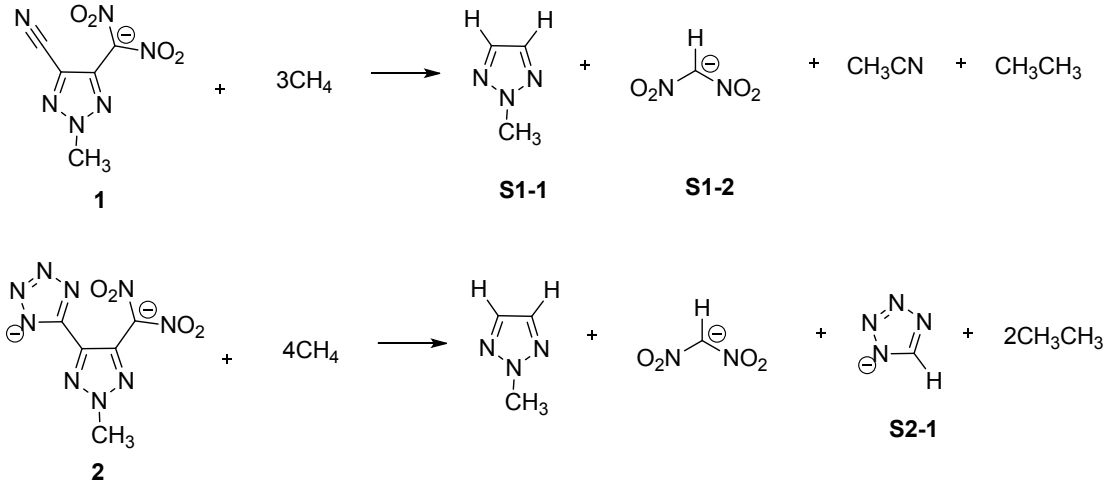
Table S4. Hydrogen bonds for **6** [Å and °]

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
N4C	H4CA	O3S[1]	0.96(3)	2.50(7)	3.024(6)	114(5)
N4C	H4CB	N2B	0.97(3)	2.08(4)	2.959(5)	150(5)
N4C	H4CC	O3A[1]	0.96(3)	2.14(5)	2.983(5)	146(6)
N4C	H4CD	O2B[2]	0.97(3)	2.37(8)	2.855(5)	110(6)
N4C	H4CD	O4B[2]	0.97(3)	2.19(7)	2.975(5)	137(7)
N3C	H3CA	N1B	0.84(3)	2.23(5)	2.942(5)	142(6)
N3C	H3CB	O1B[3]	0.84(3)	2.03(3)	2.846(5)	164(6)
N3C	H3CC	O2B[2]	0.84(3)	2.13(4)	2.892(5)	151(6)
N3C	H3CD	O3A	0.84(3)	2.04(5)	2.832(5)	158(10)
N2C	H2CA	O1A	0.89(3)	2.26(5)	2.940(5)	133(5)
N2C	H2CB	N3B	0.89(3)	2.05(3)	2.932(5)	168(5)
N2C	H2CC	O2S[4]	0.89(3)	1.96(3)	2.850(6)	176(6)
N2C	H2CD	N1A[5]	0.90(3)	2.01(3)	2.908(6)	173(6)
N1C	H1CA	O3B[6]	0.88(3)	2.14(3)	3.001(5)	168(6)
N1C	H1CB	O3S	0.89(3)	1.92(3)	2.796(6)	170(5)
N1C	H1CC	O4A	0.88(3)	2.17(5)	2.872(5)	136(5)
N1C	H1CD	O4S	0.88(3)	2.01(4)	2.840(6)	156(6)
O1S	H1SA	N4B[2]	0.87	2.05	2.914(5)	170.6
O1S	H1SB	O4S	0.87	2.16	2.993(6)	160.7
O4S	H4SA	O2A[2]	0.97(7)	1.97(7)	2.870(6)	153(6)
O4S	H4SB	N2A[7]	0.71(8)	2.30(8)	3.001(6)	169(7)
O2S	H2SA	N3A[1]	0.79(7)	2.13(7)	2.851(6)	151(7)
O2S	H2SB	N2A[7]	0.83(8)	2.24(8)	3.033(5)	158(6)
O3S	H3SA	O1S[8]	0.87	2.10	2.833(6)	141.5
O3S	H3SA	O2S[8]	0.87	2.40	3.027(5)	129.4
O3S	H3SB	N4A	0.87	1.94	2.806(5)	171.7

Table S5. Hydrogen bonds for **8** [Å and °]

D-H...A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
N(19)-H(19A)...O(7)#4	0.900(16)	2.37(3)	2.991(2)	126(2)
N(19)-H(19B)...N(12)#5	0.918(16)	2.371(18)	3.236(2)	157(2)
N(20)-H(20A)...O(1)#3	0.89	2.31	2.956(2)	129.5
N(20)-H(20A)...O(2)#3	0.89	2.25	3.046(2)	148.3
N(20)-H(20B)...N(16)#6	0.89	2.04	2.843(2)	149.3
N(20)-H(20B)...N(17)#6	0.89	2.62	3.369(2)	142.2
N(20)-H(20C)...O(2)	0.89	2.18	2.7515(19)	121.7
N(20)-H(20C)...O(6)	0.89	2.10	2.912(2)	151.1
N(21)-H(21B)...O(1)#7	0.874(15)	2.191(16)	2.935(2)	143(2)
N(22)-H(22A)...N(17)#3	0.89	2.32	2.899(2)	122.9
N(22)-H(22B)...N(15)#5	0.89	2.00	2.875(2)	166.1
N(22)-H(22C)...N(19)	0.89	2.05	2.893(2)	158.8

2 Theoretical Calculations



Scheme S1. Isodesmic reactions for the anions of **1** and **2.**

Table S6. 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	0.105432	0.11966	-819.7465378	-819.63110	190.795018
2	0.120875	0.136725	-983.5792442	-983.44735	476.1431758
S1-1	0.087307	0.093495	-280.8412053	-280.75120	299.4666839
S1-2	0.039727	0.046604	-448.0309171	-447.98590	-232.9813495
S2-1	0.033827	0.038051	-257.12423	-257.08754	181.5783287
CH_4	0.044793	0.048605	-40.3796224	-40.33281	-74.6
CH_3CN	0.045278	0.049841	-132.4107856	-132.36276	74.0
CH_3CH_3	0.07461	0.079038	-79.5716305	-79.49558	-84.0

[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 S7. 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})
5	490.7605398	501.1	190.795018	201.1344782
6	1320.374376	626.4	476.1	408.5688001
7	1297.901236	669.5	476.1	517.1987641
8	1277.918077	770.0	476.1	738.1819234
9	1098.401162	883.6	476.1	1144.898838