Supporting Information

3-methyl-1,2,3-triazolium-1N-dinitromethylylide and the strategy of zwitterionic dinitromethyl groups in energetic materials design.

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X-Ray Crystallography

Figure S1. OTREP plot of **1**

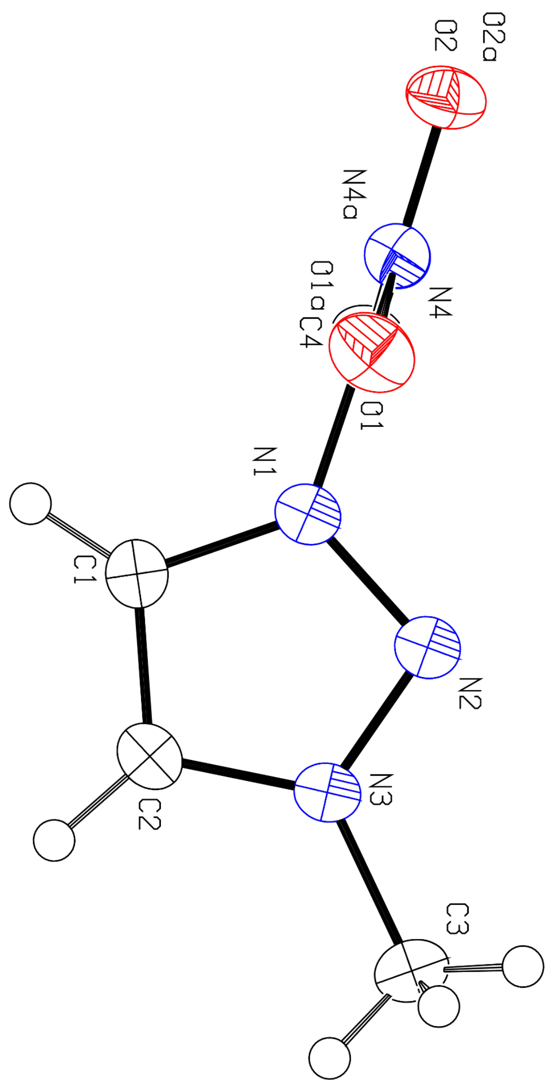

Figure S2. Figure of compound **1.**

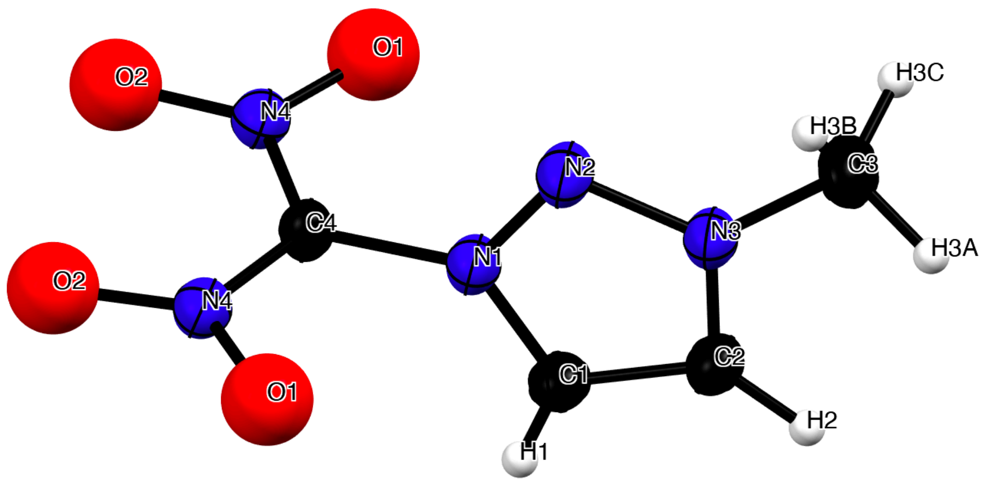

Table S1. Experimental details

	3-methyl-1,2,3-triazolium-1N-dinitromethylylide (**1**)
Crystal data	
Chemical formula	$C_4H_5N_5O_4$
M_r	187.13
Crystal system, space group	Orthorhombic, *Cmca*
Temperature (K)	150
a, *b*, *c* (Å)	7.7002 (7), 14.3978 (16), 12.7602 (11)
V (Å^3)	1414.7 (2)
Z	8
F(000)	768
D_x (Mg m^{-3})	1.757
Radiation type	Cu *K*α
No. of reflections for cell measurement	3719
θ range (°) for cell measurement	6.2–79.9
μ (mm^{-1})	1.38
Crystal shape	Plate
Colour	Colourless
Crystal size (mm)	0.16 × 0.15 × 0.02
Data collection	

Diffractometer	Bruker AXS D8 Quest diffractometer with PhotonIII_C14 charge-integrating and photon counting pixel array detector
Radiation source	I-mu-S microsource X-ray tube
Monochromator	Laterally graded multilayer (Goebel) mirror
Detector resolution (pixels mm^{-1})	7.4074
Scan method	ω and phi scans
Absorption correction	Multi-scan, *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10.
T_{min}, T_{max}	0.613, 0.754
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5056, 812, 741
R_{int}	0.037
θ values (°)	θ_{max} = 79.9, θ_{min} = 6.2
$(\sin \theta/\lambda)_{max}$ ($Å^{-1}$)	0.639
Range of *h*, *k*, *l*	*h* = -7→9, *k* = -18→17, *l* = -15→15
Refinement	
Refinement on	F^2
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.143, 1.16
No. of reflections	812
No. of parameters	72
No. of restraints	0
H-atom treatment	H-atom parameters constrained
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0842P)^2 + 0.8362P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$	< 0.001
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e $Å^{-3}$)	0.32, -0.25
Extinction method	*SHELXL2018*/3 (Sheldrick 2018), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient	0.0052 (11)

Detonation Properties

Table S2. Energetic properties of **1** compared to HMX and RDX

	1	**HMX**	**RDX**	**TNT**[26]
Formula	$C_4H_5N_5O_4$	$(CH_2NNO_2)_4$	$C_3H_6N_6O_6$	$C_6H_3CH_3$
FW / [g mol^{-1}]	187.13	296.16	222.12	227.13
IS / [J][a]	8	7	7.5	15
FS / [N][b]	144-160	112	120	240
N / [%][c]	36.74	37.84	37.84	0
Ω / [%][d]	-55.58	-21.61	-21.61	-73.96
T_{dec} / [°C][e]	150	275	205	295
ρ / [g·cm^{-3}][f]	1.757	1.905	1.858	1.65
ρ / [g·cm^{-3}][calc]	1.786	-	-	-
$\Delta_f H_m^o$ / [kJ mol^{-1}] [g]	224.2	74.8	86.3	-59.3
EXPLO6				
$-\Delta_{Ex}U°$ / [kJ kg^{-1}][h]	-5303	-5700	-5740	-5227
T_{det} / [K][i]	3525	4117	3745	3657
P_{CJ} / [kbar][j]	272	378	336	21.6
V_{det} / [m s^{-1}][k]	8162	9193	8801	7253
V_o / [L kg^{-1}][l]	739	763	783	574

[a] impact sensitivity (BAM drophammer (1 of 6)); [b] friction sensitivity (BAM friction tester (1 of 6)); [c] nitrogen content; [d] oxygen balance (Ω = (xO–2yC–1/2zH)M/1600); [e] decomposition temperature from DSC (β = 5 °C); [f] from X-ray diffraction; [g] calculated heat of formation; [h] energy of explosion; [i] explosion temperature; [j] detonation pressure; [k] detonation velocity; [l] volume of detonation gases (assuming only gaseous products).

NMR

Figure S3. ^{1}H NMR of **1** (DMSO-d_6)

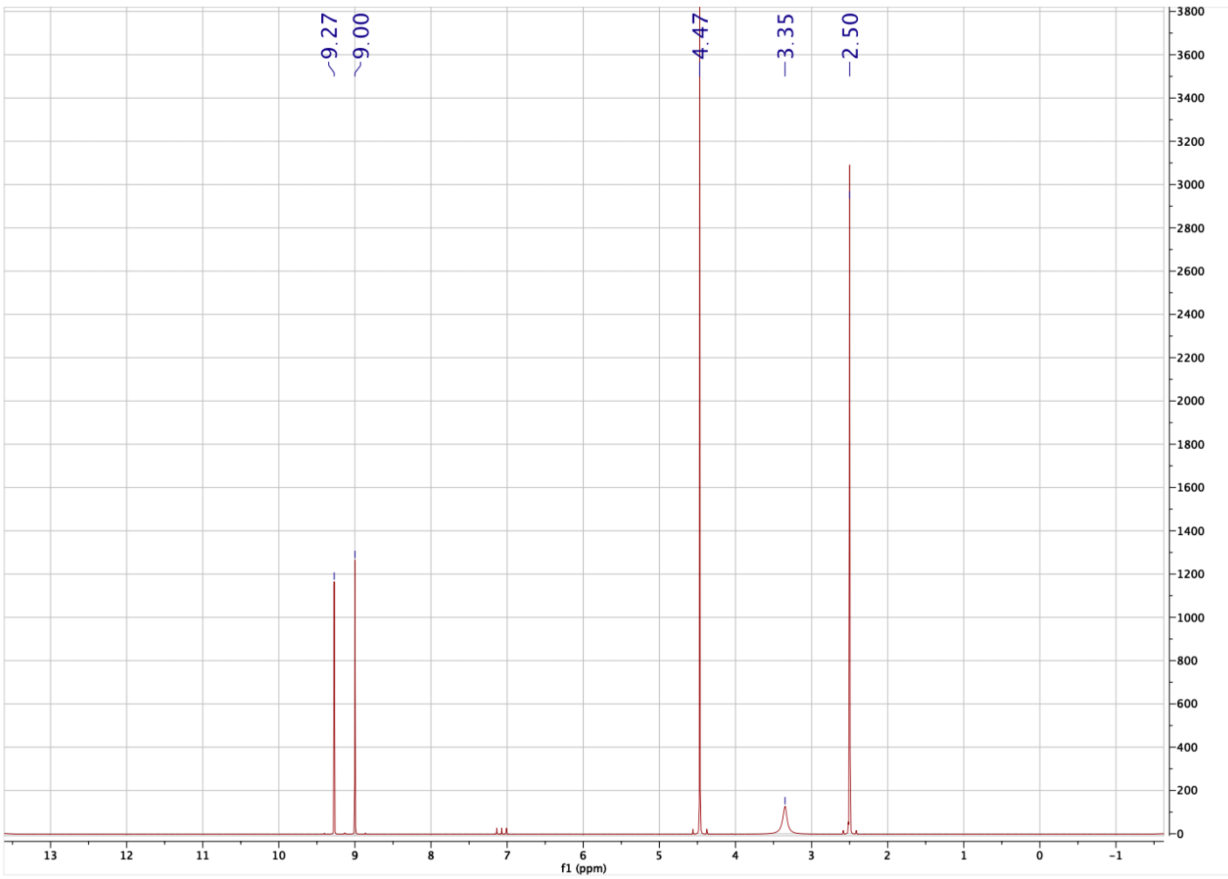

Figure S4. ^{13}C NMR **1** (DMSO-d_6)