Supporting Information

Belonging to the manuscript

Energetic Azolium Azolate Salts

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General experimental methods:

Crystals of compound **10** was removed from the flask and covered with a layer of hydrocarbon oil. A suitable crystal was selected, attached to a glass fiber and placed in the low-temperature nitrogen stream.Data for **10** were collected at 84(2) K using a Bruker/Siemens SMART APEX instrument (Mo Kα radiation, λ = 0.71073 Å) equipped with a Cryocool NeverIce low temperature device. Data were measured using omega scans of 0.3 ° per frame for 5 seconds, and a full sphere of data was collected. A total of 2132 frames were collected with a final resolution of 0.77 Å. The first 50 frames were recollected at the end of data collection to monitor for decay. Cell parameters were retrieved using SMART software and refined using SAINTPlus on all observed reflections. Data reduction and correction for Lp and decay were performed using the SAINTPlus software. Absorption corrections were applied using SADABS. The structure was solved by direct methods and refined by least squares method on F^2 using the SHELXTL program package. The structure was solved in the space group P2(1)/c (# 14) by analysis of systematic absences. No decomposition was observed during data collection. Details of the data collection and refinement are given in the following Tables.

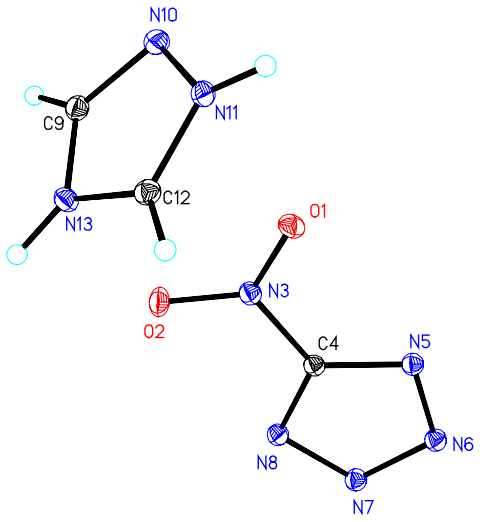

Figure 1. ORTEP drawing of compound **(10)**.

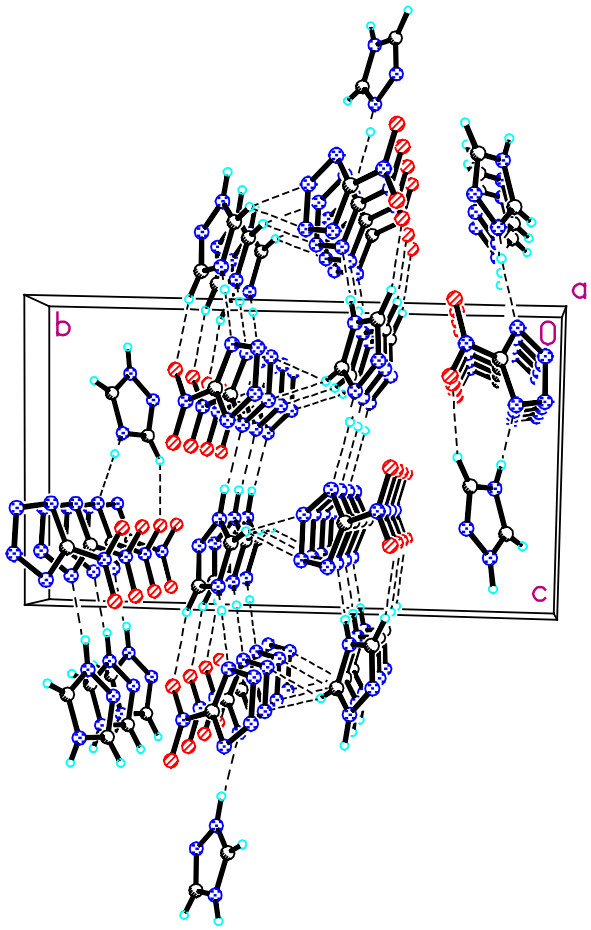

Figure 2. A diagram showing the components of the unit cell.

Table 1. Crystal data and structure refinement for 1, 2, 4-triazolium 5-nitro-tetrazolate (**10**).

Empirical formula	C3 H4 N8 O2	
Formula weight	184.14	
Temperature	86(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 4.9847(3) Å	α= 90°.
	b = 15.7812(10) Å	β= 100.128(1)°.
	c = 9.2339(6) Å	γ = 90°.
Volume	715.06(8) $Å^3$	
Z	4	
Density (calculated)	1.710 Mg/m^3	
Absorption coefficient	0.145 mm^{-1}	
F(000)	376	
Crystal size	0.33 x 0.21 x 0.16 mm^3	
Crystal color and habit	colorless block	
Diffractometer	Bruker/Siemens SMART APEX	
Theta range for data collection	2.58 to 25.39°.	
Index ranges	-6<=h<=6, -19<=k<=19, -11<=l<=11	
Reflections collected	7898	
Independent reflections	1302 [R(int) = 0.0203]	
Completeness to theta = 25.39°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9772 and 0.9538	
Solution method	XS, Bruker SHELXTL v. 6.12	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1302 / 0 / 118	
Goodness-of-fit on F^2	1.088	
Final R indices [I>2sigma(I)]	R1 = 0.0285, wR2 = 0.0697	
R indices (all data)	R1 = 0.0296, wR2 = 0.0705	
Largest diff. peak and hole	0.189 and -0.237 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound (**10**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4729(2)	7024(1)	2379(1)	19(1)
O(2)	6731(2)	6981(1)	4674(1)	23(1)
N(3)	6499(2)	6773(1)	3377(1)	16(1)
C(4)	8494(2)	6187(1)	3000(1)	14(1)
N(5)	8452(2)	5896(1)	1651(1)	16(1)
N(6)	10661(2)	5391(1)	1809(1)	17(1)
N(7)	11897(2)	5399(1)	3202(1)	17(1)
N(8)	10536(2)	5906(1)	3990(1)	16(1)
C(9)	1856(3)	8346(1)	4203(1)	16(1)
N(10)	317(2)	8299(1)	2914(1)	16(1)
N(11)	1793(2)	8719(1)	2023(1)	15(1)
C(12)	4107(3)	9000(1)	2763(1)	15(1)
N(13)	4201(2)	8775(1)	4157(1)	15(1)

Table 3. Bond lengths [Å] and angles [°] for compound (**10**).

O(1)-N(3)	1.2236(14)	N(11)-C(12)-N(13)	107.03(11)
O(2)-N(3)	1.2276(14)	N(11)-C(12)-H(12)	126.5
N(3)-C(4)	1.4448(16)	N(13)-C(12)-H(12)	126.5
C(4)-N(8)	1.3197(16)	C(12)-N(13)-C(9)	106.25(10)
C(4)-N(5)	1.3243(16)	C(12)-N(13)-H(13)	126.9
N(5)-N(6)	1.3458(15)	C(9)-N(13)-H(13)	126.9
N(6)-N(7)	1.3249(15)		
N(7)-N(8)	1.3435(15)		
C(9)-N(10)	1.2995(17)		
C(9)-N(13)	1.3576(17)		
C(9)-H(9)	0.9500		
N(10)-N(11)	1.3682(15)		
N(11)-C(12)	1.3096(16)		
N(11)-H(11)	0.8800		
C(12)-N(13)	1.3284(16)		
C(12)-H(12)	0.9500		
N(13)-H(13)	0.8800		

O(1)-N(3)-O(2)	125.48(11)
O(1)-N(3)-C(4)	117.45(10)
O(2)-N(3)-C(4)	117.07(10)
N(8)-C(4)-N(5)	114.67(11)
N(8)-C(4)-N(3)	121.88(11)
N(5)-C(4)-N(3)	123.45(11)
C(4)-N(5)-N(6)	103.10(10)
N(7)-N(6)-N(5)	109.37(10)
N(6)-N(7)-N(8)	109.78(10)
C(4)-N(8)-N(7)	103.09(10)
N(10)-C(9)-N(13)	111.87(11)
N(10)-C(9)-H(9)	124.1
N(13)-C(9)-H(9)	124.1
C(9)-N(10)-N(11)	103.29(10)
C(12)-N(11)-N(10)	111.56(10)
C(12)-N(11)-H(11)	124.2
N(10)-N(11)-H(11)	124.2

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound (**10**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	17(1)	21(1)	17(1)	1(1)	-1(1)	3(1)
O(2)	27(1)	27(1)	14(1)	-4(1)	3(1)	6(1)
N(3)	16(1)	17(1)	14(1)	0(1)	2(1)	-1(1)
C(4)	14(1)	14(1)	14(1)	0(1)	2(1)	-2(1)
N(5)	16(1)	16(1)	15(1)	0(1)	3(1)	0(1)
N(6)	17(1)	17(1)	16(1)	0(1)	3(1)	1(1)
N(7)	17(1)	18(1)	16(1)	0(1)	3(1)	1(1)
N(8)	16(1)	17(1)	15(1)	0(1)	2(1)	1(1)
C(9)	17(1)	17(1)	14(1)	0(1)	4(1)	1(1)
N(10)	15(1)	18(1)	16(1)	0(1)	4(1)	0(1)
N(11)	16(1)	17(1)	12(1)	1(1)	2(1)	1(1)
C(12)	15(1)	14(1)	17(1)	0(1)	3(1)	2(1)
N(13)	15(1)	17(1)	13(1)	-1(1)	-1(1)	1(1)

Table 5. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2 x\ 10^{\ 3}$) for compound (**10**).

	x	y	z	U(eq)
H(9)	1396	8108	5072	19
H(11)	1256	8792	1071	18
H(12)	5461	9307	2376	18
H(13)	5519	8882	4901	18

Table 6. Hydrogen bonds for compound (**10**) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(11)-H(11)...N(8)#1	0.88	1.95	2.8228(15)	170.5
N(13)-H(13)...N(5)#2	0.88	2.01	2.8897(15)	177.9
C(9)-H(9)...O(1)#2	0.95	2.47	3.0847(15)	122.4
C(12)-H(12)...N(6)#3	0.95	2.59	3.3788(16)	140.3
C(12)-H(12)...N(7)#3	0.95	2.29	3.2025(16)	161.4

Symmetry transformations used to generate equivalent atoms:

#1 x-1,-y+3/2,z-1/2 #2 x,-y+3/2,z+1/2 #3 -x+2,y+1/2,-z+1/2