Supplementary Material

Energetic salts based on nitroiminotetrazole-containing acetic acid

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Crystal structure information

Table 1. Crystal data and structure refinement for compound 4•H2O.

Identification code	SHRV72	
Empirical formula	$C_3H_6N_6O_5$	
Formula weight	206.14	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbcn	
Unit cell dimensions	a = 23.1690(14) Å	α=90°.
	b = 8.6022(5) Å	β= 90°.
	c = 8.0337(5) Å	$\gamma = 90^{\circ}$.
Volume	1601.15(17)Å ³	
Ζ	8	
Density (calculated)	1.710 Mg/m^3	
Absorption coefficient	0.159 mm^{-1}	
F(000)	848	
Crystal size	$0.57 \ge 0.53 \ge 0.49 \text{ mm}^3$	
Theta range for data collection	1.76 to 28.29°.	
Index ranges	-28<=h<=30, -11<=k<=11	, - 10<=l<=10
Reflections collected	16419	
Independent reflections	1996 $[R_{int} = 0.0199]$	
Completeness to theta = 28.29°	100.0 %	
Absorption correction	Semi-empirical from equiv	valents
Max. and min. transmission	1.000 and 0.833	
Refinement method	Full-matrix least-squares of	on F^2
Data / restraints / parameters	1996 / 3 / 140	
Goodness-of-fit on F^2	1.032	
Final R indices [I>2sigma(I)]	$R_1 = 0.0332, wR_2 = 0.092$	7
R indices (all data)	$R_1 = 0.0360, wR_2 = 0.0954$	4
Extinction coefficient	0.044(2)	
Largest diff. peak and hole	$0.284 \text{ and } -0.196 \text{ e.}\text{Å}^{-3}$	

	Х	у	Z	U(eq)	
N(1)	3568(1)	6448(1)	1475(1)	32(1)	
N(2)	3788(1)	5035(1)	1852(1)	40(1)	
N(3)	4197(1)	5239(1)	2886(1)	41(1)	
N(4)	4245(1)	6780(1)	3207(1)	34(1)	
C(5)	3852(1)	7562(1)	2317(1)	30(1)	
C(6)	3054(1)	6630(1)	463(1)	33(1)	
C(7)	2520(1)	6412(1)	1522(1)	33(1)	
O(8)	2057(1)	6897(1)	737(1)	50(1)	
O(9)	2529(1)	5866(1)	2887(1)	50(1)	
N(10)	3705(1)	9050(1)	2093(1)	36(1)	
N(11)	4029(1)	10082(1)	2906(1)	37(1)	
O(12)	3900(1)	11468(1)	2688(1)	49(1)	
O(13)	4435(1)	9705(1)	3823(1)	53(1)	
O(1S)	5123(1)	7237(1)	5266(1)	52(1)	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å²x 10^3) for 4•H2O. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

N(1)-C(5)	1.3455(14)
N(1)-N(2)	1.3521(14)
N(1)-C(6)	1.4512(14)
N(2)-N(3)	1.2734(14)
N(3) - N(4)	1.3550(14)
N(4)-C(5)	1 3382(14)
N(4)-H(4)	0.8600
C(5)-N(10)	1 3365(15)
C(6)-C(7)	1 5117(16)
C(6)-U(7)	0.9700
C(6) H(6R)	0.9700
$C(0) - \Pi(0B)$	1.1020(14)
C(7) - O(9)	1.1929(14) 1.2140(14)
C(7) - O(8)	1.3140(14)
O(8)-H(8)	0.841(9)
N(10)-N(11)	1.3340(14)
N(11) - O(13)	1.2388(13)
N(11)-O(12)	1.2415(14)
O(1S)-H(1SA)	0.833(9)
O(1S)-H(1SB)	0.842(9)
	110.10(0)
C(5)-N(1)-N(2)	110.12(9)
C(5)-N(1)-C(6)	127.34(10)
N(2)-N(1)-C(6)	122.11(9)
N(3)-N(2)-N(1)	107.58(10)
N(2)-N(3)-N(4)	108.68(10)
C(5)-N(4)-N(3)	109.56(9)
C(5)-N(4)-H(4)	125.2
N(3)-N(4)-H(4)	125.2
N(10)-C(5)-N(4)	136.64(10)
N(10)-C(5)-N(1)	119.29(10)
N(4)-C(5)-N(1)	104.06(9)
N(1)-C(6)-C(7)	110.04(9)
N(1)-C(6)-H(6A)	109.7
C(7)-C(6)-H(6A)	109.7
N(1)-C(6)-H(6B)	109.7
C(7)-C(6)-H(6B)	109.7
H(6A)-C(6)-H(6B)	108.2
O(9)-C(7)-O(8)	125.41(11)
O(9)-C(7)-C(6)	123.56(11)
O(8)-C(7)-C(6)	111.03(9)
C(7)-O(8)-H(8)	107.8(14)
N(11)-N(10)-C(5)	115.30(9)
O(13)-N(11)-O(12)	121.21(10)
O(13)-N(11)-N(10)	123 00(10)
O(12)-N(11)-N(10)	115 79(10)
H(1SA) - O(1S) - H(1SR)	107 8(18)
II(10/1)-0(10)-11(10D)	107.0(10)

Table 3.Bond lengths [Å] and angles [°] for 4•H2O.

	U^{11}	U ²²	U ³³	U ²³	U^{13}	U^{12}	
N(1)	28(1)	30(1)	38(1)	-2(1)	-3(1)	-1(1)	
N(2)	39(1)	31(1)	50(1)	-2(1)	-7(1)	1(1)	
N(3)	40(1)	31(1)	51(1)	0(1)	-9(1)	2(1)	
N(4)	32(1)	30(1)	40(1)	-1(1)	-7(1)	0(1)	
C(5)	25(1)	33(1)	33(1)	-2(1)	-1(1)	-1(1)	
C(6)	28(1)	40(1)	32(1)	-1(1)	-4(1)	-3(1)	
C(7)	31(1)	33(1)	35(1)	-3(1)	-2(1)	-2(1)	
O(8)	29(1)	71(1)	50(1)	18(1)	1(1)	2(1)	
O(9)	44(1)	68(1)	39(1)	12(1)	2(1)	4(1)	
N(10)	31(1)	29(1)	47(1)	-2(1)	-9(1)	0(1)	
N(11)	33(1)	30(1)	48(1)	-3(1)	-8(1)	1(1)	
O(12)	46(1)	27(1)	75(1)	-3(1)	-20(1)	2(1)	
O(13)	50(1)	37(1)	73(1)	-7(1)	-32(1)	4(1)	
O(1S)	51(1)	41(1)	65(1)	-2(1)	-29(1)	0(1)	

Table 4. Anisotropic displacement parameters (Å²x 10³) for 4•H2O. The anisotropic displacement factor exponent takes the form: $-2\pi^{2}$ [h² a*²U¹¹ + ... + 2 h k a* b* U¹²]

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å²x 10^3) for 4•H2O.

	Х	у	Z	U(eq)	
H(4)	4490	7193	3879	41	
H(6A)	3056	5870	-428	40	
H(6B)	3050	7658	-32	40	
H(1SA)	5272(8)	6577(18)	5890(20)	71(6)	
H(1SB)	5224(8)	8122(14)	5600(20)	68(6)	
H(8)	1768(6)	6640(20)	1310(20)	75(6)	
11(0)	1700(0)	00+0(20)	1510(20)	/3(0)	

C(5)-N(1)-N(2)-N(3)	-0.32(13)
C(6)-N(1)-N(2)-N(3)	-173.32(10)
N(1)-N(2)-N(3)-N(4)	0.67(13)
N(2)-N(3)-N(4)-C(5)	-0.79(14)
N(3)-N(4)-C(5)-N(10)	-178.29(13)
N(3)-N(4)-C(5)-N(1)	0.56(12)
N(2)-N(1)-C(5)-N(10)	178.94(10)
C(6)-N(1)-C(5)-N(10)	-8.53(17)
N(2)-N(1)-C(5)-N(4)	-0.16(12)
C(6)-N(1)-C(5)-N(4)	172.38(10)
C(5)-N(1)-C(6)-C(7)	-89.82(13)
N(2)-N(1)-C(6)-C(7)	81.90(13)
N(1)-C(6)-C(7)-O(9)	-13.86(16)
N(1)-C(6)-C(7)-O(8)	166.30(10)
N(4)-C(5)-N(10)-N(11)	2.2(2)
N(1)-C(5)-N(10)-N(11)	-176.52(10)
C(5)-N(10)-N(11)-O(13)	-0.73(17)
C(5)-N(10)-N(11)-O(12)	179.05(11)

Table 6.Torsion angles [°] for 4•H2O.

	0
Table 7.	Hydrogen bonds for 4•H2O [Å and °].

D-HA	d(D-H)	d(HA)	d(DA)	<(DHA)	
N(4)-H(4)O(1S)	0.86	1.84	2.6506(13)	156.0	
O(1S)-H(1SA)N(3)	#1 0.833(9)	2.218(10)	3.0372(14)	167.8(19)	
O(1S)-H(1SB)O(13	3)#20.842(9)	2.080(10)	2.9166(14)	171.9(19)	
O(8)-H(8)O(12)#3	0.841(9)	1.910(10)	2.7398(13)	168.9(19)	

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+1 #2 -x+1,-y+2,-z+1 #3 -x+1/2,y-1/2,z

Table 1.	Crystal	data and	structure refinement	for	compound 9.
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Identification code	SHRV125	
Empirical formula	$C_7H_{12}N_{14}O_4$	
Formula weight	356.31	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 5.4438(8) Å	α= 90°.
	b = 16.020(2) Å	β= 92.374(2)°.
	c = 17.071(3) Å	$\gamma = 90^{\circ}$.
Volume	$1487.5(4) \text{ Å}^3$	
Ζ	4	
Density (calculated)	1.591 Mg/m^3	
Absorption coefficient	0.132 mm^{-1}	
F(000)	736	
Crystal size	$0.47 \ge 0.04 \ge 0.03 \text{ mm}^3$	
Theta range for data collection	1.74 to 25.87°.	
Index ranges	-6<=h<=6, -19<=k<=19, -	20<=l<=20
Reflections collected	12677	
Independent reflections	$2842 [R_{int} = 0.0241]$	
Completeness to theta = 25.87°	98.4 %	
Absorption correction	Semi-empirical from equi	valents
Max. and min. transmission	0.9960 and 0.9404	
Refinement method	Full-matrix least-squares of	on F^2
Data / restraints / parameters	2842 / 0 / 238	
Goodness-of-fit on F^2	1.051	
Final R indices [I>2sigma(I)]	$R_1 = 0.0354, wR_2 = 0.0890$	0
R indices (all data)	$R_1 = 0.0486, wR_2 = 0.096$	8
Largest diff. peak and hole	$0.223 \text{ and } -0.249 \text{ e.Å}^{-3}$	

	Х	у	Z	U(eq)	
		-			
N(1)	-2053(2)	9304(1)	2832(1)	34(1)	
N(2)	-3157(3)	9702(1)	3415(1)	44(1)	
N(3)	-2022(3)	9475(1)	4056(1)	46(1)	
N(4)	-161(3)	8930(1)	3912(1)	40(1)	
C(5)	-197(3)	8839(1)	3137(1)	31(1)	
C(6)	-2758(3)	9418(1)	2015(1)	39(1)	
C(7)	-843(3)	9883(1)	1566(1)	38(1)	
O(8)	-921(3)	9819(1)	851(1)	65(1)	
O(9)	684(2)	10322(1)	1963(1)	50(1)	
N(10)	1137(2)	8406(1)	2609(1)	38(1)	
N(11)	3090(2)	8012(1)	2899(1)	38(1)	
O(12)	3708(2)	8015(1)	3608(1)	55(1)	
O(13)	4347(2)	7628(1)	2414(1)	55(1)	
N(14A)	-1200(3)	6556(1)	4686(1)	42(1)	
C(15A)	-1916(3)	6815(1)	3963(1)	47(1)	
N(16A)	-432(3)	6549(1)	3442(1)	50(1)	
N(17A)	1312(3)	6102(1)	3867(1)	45(1)	
C(18A)	841(3)	6104(1)	4604(1)	44(1)	
N(19A)	-2510(4)	6731(1)	5365(1)	63(1)	
N(14B)	-5354(2)	11408(1)	3849(1)	35(1)	
C(15B)	-3565(3)	11928(1)	3624(1)	45(1)	
N(16B)	-1947(3)	12057(1)	4190(1)	51(1)	
N(17B)	-2763(3)	11584(1)	4789(1)	44(1)	
C(18B)	-4789(3)	11204(1)	4586(1)	42(1)	
N(19B)	-7417(3)	11084(1)	3430(1)	51(1)	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å²x 10^3) for compound 9. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

N(1)-C(5)	1.3428(19)	N(1)-N(2)	1.3439(18)
N(1)-C(6)	1.4429(18)	N(2)-N(3)	1.285(2)
N(3)-N(4)	1.3671(19)	N(4)-C(5)	1.3307(19)
C(5)-N(10)	1.3697(19)	C(6)-C(7)	1.515(2)
C(6)-H(6A)	0.9700	C(6)-H(6B)	0 9700
C(7)-O(8)	1 2239(19)	C(7) - O(9)	1 2649(19)
N(10)-N(11)	1 3159(19)	N(11)-O(12)	1.2019(17) 1.2428(17)
N(11)-O(13)	1 2569(17)	N(14A)-C(18A)	1.2120(17) 1.338(2)
N(14A) - C(15A)	1.2369(17) 1.346(2)	$N(14\Delta)-N(19\Delta)$	1.550(2) 1.413(2)
C(15A)-N(16A)	1.546(2)	C(15A) - H(15A)	0.9300
N(16A) - N(17A)	1.298(2) 1.3724(10)	N(17A) - C(18A)	1.293(2)
N(17A) H(17A)	0.8600	C(18A) H(18A)	0.0300
N(10A) H(10A)	0.8000	V(10A) + H(10R)	0.9300
N(14D) C(19D)	(0.94(2))	N(14R) - H(15R) N(14R) - C(15R)	0.93(2)
N(14D) - C(10D)	1.3221(19)	N(14D)-C(15D)	1.550(2)
N(14B)-N(19B)	1.406(2)	V(15B)-N(10B) N(1(D) N(17D)	1.297(2)
C(15B)-H(15B)	0.9300	N(10B)-N(17B)	1.3609(19)
N(1/B)-C(18B)	1.295(2)	N(1/B)-H(1/B)	0.8600
C(18B)-H(18B)	0.9300	N(19B)-H(19C)	0.85(2)
N(19B)-H(19D)	0.83(2)		
C(5) N(1) N(2)	100.18(12)	C(5) N(1) C(6)	127 62(13)
N(2)-N(1)-C(6)	109.18(12) 123 14(13)	N(3)-N(2)-N(1)	127.02(13) 106 37(13)
N(2) N(2) N(4)	123.14(13) 111.21(12)	$\Gamma(5) - \Gamma(2) - \Gamma(1)$ $\Gamma(5) - \Gamma(4) - \Gamma(2)$	100.57(13) 105.51(12)
N(4) C(5) N(1)	111.21(12) 107.71(12)	V(3) - IN(4) - IN(5) N(4) - C(5) - N(10)	105.31(12) 126.20(14)
N(4)-C(5)-N(1) N(1)-C(5)-N(10)	107.71(13) 115.80(12)	N(4)-C(5)-N(10) N(1)-C(6)-C(7)	130.39(14) 112.09(12)
N(1) - C(3) - N(10)	113.89(12)	N(1)-C(0)-C(7)	112.96(15)
N(1) - C(0) - H(0A)	109.0	C(7) - C(0) - H(0A)	109.0
N(1)-C(0)-H(0B)	109.0	C(7) - C(0) - H(0B)	109.0
H(0A)-C(0)-H(0B)	107.8	O(8) - C(7) - O(9)	125.17(10)
O(8)-C(7)-C(6)	117.89(15)	O(9)-C(7)-C(6)	116.91(13)
N(11)-N(10)-C(5)	115.90(12)	O(12)-N(11)-O(13)	120.77(14)
O(12)-N(11)-N(10)	123.14(13)	O(13)-N(11)-N(10)	116.08(13)
C(18A)-N(14A)-C(15A)	106.27(15)	C(18A)-N(14A)-N(19A)	130.08(15)
C(15A)-N(14A)-N(19A)	123.62(15)	N(16A)-C(15A)-N(14A)	111.23(15)
N(16A)-C(15A)-H(15A)	124.4	N(14A)-C(15A)-H(15A)	124.4
C(15A)-N(16A)-N(17A)	104.24(14)	C(18A)-N(17A)-N(16A)	110.62(15)
C(18A)-N(17A)-H(17A)	124.7	N(16A)-N(17A)-H(17A)	124.7
N(17A)-C(18A)-N(14A)	107.63(15)	N(17A)-C(18A)-H(18A)	126.2
N(14A)-C(18A)-H(18A)	126.2	N(14A)-N(19A)-H(19A)	105.3(14)
N(14A)-N(19A)-H(19B)	108.2(15)	H(19A)-N(19A)-H(19B)	106(2)
C(18B)-N(14B)-C(15B)	106.32(14)	C(18B)-N(14B)-N(19B)	122.88(14)
C(15B)-N(14B)-N(19B)	130.76(14)	N(16B)-C(15B)-N(14B)	111.15(14)
N(16B)-C(15B)-H(15B)	124.4	N(14B)-C(15B)-H(15B)	124.4
C(15B)-N(16B)-N(17B)	103.84(15)	C(18B)-N(17B)-N(16B)	111.15(14)
C(18B)-N(17B)-H(17B)	124.4	N(16B)-N(17B)-H(17B)	124.4
N(17B)-C(18B)-N(14B)	107.54(14)	N(17B)-C(18B)-H(18B)	126.2
N(14B)-C(18B)-H(18B)	126.2	N(14B)-N(19B)-H(19C)	106.7(15)
N(14B)-N(19B)-H(19D)	107.4(16)	H(19C)-N(19B)-H(19D)	113(2)

Table 3.Bond lengths [Å] and angles [°] for compound 9.

	U^{11}	U ²²	U ³³	U ²³	U^{13}	U ¹²	
N(1)	36(1)	38(1)	29(1)	6(1)	4(1)	7(1)	
N(2)	45(1)	45(1)	42(1)	6(1)	13(1)	11(1)	
N(3)	54(1)	51(1)	34(1)	3(1)	12(1)	12(1)	
N(4)	46(1)	44(1)	28(1)	2(1)	2(1)	8(1)	
C(5)	34(1)	32(1)	27(1)	3(1)	1(1)	1(1)	
C(6)	38(1)	45(1)	34(1)	7(1)	-6(1)	1(1)	
C(7)	46(1)	39(1)	28(1)	3(1)	-3(1)	-2(1)	
O(8)	84(1)	84(1)	26(1)	-3(1)	1(1)	-27(1)	
O(9)	60(1)	57(1)	34(1)	1(1)	-5(1)	-20(1)	
N(10)	39(1)	43(1)	31(1)	-2(1)	0(1)	10(1)	
N(11)	36(1)	35(1)	45(1)	-6(1)	2(1)	2(1)	
O(12)	51(1)	67(1)	46(1)	-7(1)	-14(1)	22(1)	
O(13)	45(1)	53(1)	67(1)	-20(1)	12(1)	10(1)	
N(14A)	37(1)	40(1)	49(1)	-2(1)	0(1)	2(1)	
C(15A)	40(1)	43(1)	58(1)	6(1)	-8(1)	8(1)	
N(16A)	46(1)	50(1)	52(1)	5(1)	-7(1)	7(1)	
N(17A)	40(1)	44(1)	52(1)	-4(1)	-5(1)	11(1)	
C(18A)	42(1)	42(1)	48(1)	0(1)	-9(1)	6(1)	
N(19A)	55(1)	75(1)	60(1)	-3(1)	10(1)	7(1)	
N(14B)	41(1)	37(1)	28(1)	0(1)	4(1)	5(1)	
C(15B)	52(1)	54(1)	30(1)	10(1)	3(1)	-3(1)	
N(16B)	55(1)	61(1)	37(1)	7(1)	1(1)	-9(1)	
N(17B)	54(1)	52(1)	27(1)	2(1)	-2(1)	4(1)	
C(18B)	52(1)	43(1)	30(1)	6(1)	7(1)	2(1)	
N(19B)	47(1)	56(1)	48(1)	-5(1)	-6(1)	1(1)	

Table 4. Anisotropic displacement parameters ($Å^2 x \ 10^3$) for compound **9**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2}U^{11} + ... + 2h k a^{*} b^{*} U^{12}]$

Table 5. Hydrogen coordinates $(x \ 10^4)$ and isotropic displacement parameters $(\text{\AA}^2 x \ 10^3)$ for compound **9**.

	X	У	Z	U(eq)	
H(6A)	-4294	9725	1976	47	
H(6B)	-3036	8875	1776	47	
H(15A)	-3295	7143	3850	56	
H(17A)	2547	5855	3671	54	
H(18A)	1755	5839	5003	53	
H(19A)	-3050(50)	6208(15)	5545(13)	75	
H(19B)	-1410(50)	6930(15)	5748(14)	75	
H(15B)	-3501	12164	3127	54	
H(17B)	-2028	11543	5243	53	
H(18B)	-5685	10853	4900	50	
H(19C)	-8060(40)	11488(14)	3175(12)	61	
H(19D)	-6930(40)	10711(13)	3140(12)	61	

C(5)-N(1)-N(2)-N(3)	-0.78(17)
C(6)-N(1)-N(2)-N(3)	-178.00(14)
N(1)-N(2)-N(3)-N(4)	0.08(18)
N(2)-N(3)-N(4)-C(5)	0.63(19)
N(3)-N(4)-C(5)-N(1)	-1.09(17)
N(3)-N(4)-C(5)-N(10)	179.03(18)
N(2)-N(1)-C(5)-N(4)	1.18(17)
C(6)-N(1)-C(5)-N(4)	178.25(14)
N(2)-N(1)-C(5)-N(10)	-178.90(13)
C(6)-N(1)-C(5)-N(10)	-1.8(2)
C(5)-N(1)-C(6)-C(7)	-66.4(2)
N(2)-N(1)-C(6)-C(7)	110.28(17)
N(1)-C(6)-C(7)-O(8)	160.71(16)
N(1)-C(6)-C(7)-O(9)	-20.8(2)
N(4)-C(5)-N(10)-N(11)	-6.1(3)
N(1)-C(5)-N(10)-N(11)	173.99(13)
C(5)-N(10)-N(11)-O(12)	0.8(2)
C(5)-N(10)-N(11)-O(13)	-178.58(13)
C(18A)-N(14A)-C(15A)-N(16A)	0.0(2)
N(19A)-N(14A)-C(15A)-N(16A)	-178.04(17)
N(14A)-C(15A)-N(16A)-N(17A)	-0.3(2)
C(15A)-N(16A)-N(17A)-C(18A)	0.58(19)
N(16A)-N(17A)-C(18A)-N(14A)	-0.59(19)
C(15A)-N(14A)-C(18A)-N(17A)	0.36(19)
N(19A)-N(14A)-C(18A)-N(17A)	178.23(18)
C(18B)-N(14B)-C(15B)-N(16B)	-0.5(2)
N(19B)-N(14B)-C(15B)-N(16B)	-178.33(16)
N(14B)-C(15B)-N(16B)-N(17B)	0.8(2)
C(15B)-N(16B)-N(17B)-C(18B)	-0.85(19)
N(16B)-N(17B)-C(18B)-N(14B)	0.58(19)
C(15B)-N(14B)-C(18B)-N(17B)	-0.08(18)
N(19B)-N(14B)-C(18B)-N(17B)	177.99(15)

Table 6. Torsion angles [°] for compound 9.

Table 7. Hydrogen bonds for compound 9 [Å and °].

D-HA	d(D-H)	d(HA)	d(DA)	<(DHA)	
N(17A)-H(17A)	O(9)#1 0.86	1.71	2.5370(19)	161.4	
N(19A)-H(19A)	O(8)#20.94(2)	2.34(3)	3.230(3)	156(2)	
N(19A)-H(19B).	N(16B)#30.93(2)	2.44(2)	3.176(3)	136.1(19)	
N(17B)-H(17B).	N(4)#3 0.86	1.98	2.7988(19)	158.1	
N(19B)-H(19C).	O(13)#40.85(2)	2.19(2)	3.028(2)	172(2)	
N(19B)-H(19D).	O(9)#50.83(2)	2.43(2)	2.935(2)	120.2(18)	

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,y-1/2,-z+1/2 #2 x-1/2,-y+3/2,z+1/2

#3 -x,-y+2,-z+1 #4 -x-1/2,y+1/2,-z+1/2 #5 x-1,y,z

Identification code	SHRV77	
Empirical formula	$C_3H_4N_4O_2$	
Formula weight	128.10	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 12.4884(7) Å	α= 90°.
	b = 5.0947(3) Å	β= 99.941(1)°.
	c = 17.4942(10) Å	$\gamma = 90^{\circ}$.
Volume	$1096.35(11)^{3}$ Å ³	•
Ζ	8	
Density (calculated)	1.552 Mg/m^3	
Absorption coefficient	0.132 mm^{-1}	
F(000)	528	
Crystal size	$0.32 \ge 0.15 \ge 0.02 \text{ mm}^3$	
Theta range for data collection	1.66 to 26.37°.	
Index ranges	-15<=h<=15, -6<=k<=5, -	21<=l<=21
Reflections collected	8688	
Independent reflections	$2252 [R_{int} = 0.0200]$	
Completeness to theta = 26.37°	99.9 %	
Absorption correction	Semi-empirical from equi	valents
Max. and min. transmission	0.7454 and 0.6774	
Refinement method	Full-matrix least-squares of	on F^2
Data / restraints / parameters	2252 / 0 / 163	
Goodness-of-fit on F^2	1.032	
Final R indices [I>2sigma(I)]	$R_1 = 0.0332, wR_2 = 0.083$	5
R indices (all data)	$R_1 = 0.0416$, $wR_2 = 0.089$	1
Largest diff. peak and hole	0.153 and -0.204 e.Å ⁻³	

Table 1. Crystal data and structure refinement for compound 15.

	Х	у	Z	U(eq)	
N(1A)	-7330(1)	1783(3)	950(1)	55(1)	
N(2A)	-6788(1)	900(3)	402(1)	46(1)	
N(3A)	-5859(1)	2061(3)	441(1)	43(1)	
N(4A)	-5792(1)	3753(2)	1029(1)	30(1)	
C(5A)	-6685(1)	3539(4)	1335(1)	47(1)	
C(6A)	-4810(1)	5260(3)	1289(1)	34(1)	
C(7A)	-4044(1)	3748(3)	1899(1)	33(1)	
O(8A)	-3162(1)	5110(2)	2133(1)	47(1)	
O(9A)	-4246(1)	1613(2)	2125(1)	52(1)	
N(1B)	-1559(1)	2377(3)	3000(1)	40(1)	
N(2B)	-1232(1)	172(3)	2669(1)	46(1)	
N(3B)	-263(1)	-451(3)	2994(1)	42(1)	
N(4B)	49(1)	1358(2)	3550(1)	31(1)	
C(5B)	-753(1)	3068(3)	3543(1)	33(1)	
C(6B)	1151(1)	1357(3)	3989(1)	37(1)	
C(7B)	1425(1)	-1206(3)	4411(1)	35(1)	
O(8B)	2489(1)	-1533(2)	4556(1)	52(1)	
O(9B)	772(1)	-2696(2)	4597(1)	47(1)	

Table 2. Atomic coordinates $(x \ 10^4)$ and equivalent isotropic displacement parameters (Å²x 10³) for compound **15**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

N(1A)-C(5A)	1.3096(19)	N(1A)-N(2A)	1.3444(19)
N(2A)-N(3A)	1.2931(17)	N(3A)-N(4A)	1.3335(16)
N(4A)-C(5A)	1.3222(17)	N(4A)-C(6A)	1.4530(16)
C(5A)-H(5AA)	0.9300	C(6A)-C(7A)	1.5136(17)
C(6A)-H(6AA)	0.9700	C(6A)-H(6AB)	0.9700
C(7A)-O(9A)	1.1993(17)	C(7A)-O(8A)	1.3068(16)
O(8A)-H(8AA)	0.8200	N(1B)-C(5B)	1.3082(17)
N(1B)-N(2B)	1.3587(18)	N(2B)-N(3B)	1.2844(17)
N(3B)-N(4B)	1.3487(16)	N(4B)-C(5B)	1.3255(17)
N(4B)-C(6B)	1.4552(16)	C(5B)-H(5BA)	0.9300
C(6B)-C(7B)	1.5096(19)	C(6B)-H(6BA)	0.9700
C(6B)-H(6BB)	0.9700	C(7B)-O(9B)	1.1990(17)
C(7B)-O(8B)	1.3195(16)	O(8B)-H(8BA)	0.8200
C(5A)-N(1A)-N(2A)	104.71(12)	N(3A)-N(2A)-N(1A)	111.56(12)
N(2A)-N(3A)-N(4A)	105.79(11)	C(5A)-N(4A)-N(3A)	108.34(11)
C(5A)-N(4A)-C(6A)	129.97(12)	N(3A)-N(4A)-C(6A)	121.35(11)
N(1A)-C(5A)-N(4A)	109.58(13)	N(1A)-C(5A)-H(5AA)	125.2
N(4A)-C(5A)-H(5AA)	125.2	N(4A)-C(6A)-C(7A)	110.39(11)
N(4A)-C(6A)-H(6AA)	109.6	C(7A)-C(6A)-H(6AA)	109.6
N(4A)-C(6A)-H(6AB)	109.6	C(7A)-C(6A)-H(6AB)	109.6
H(6AA)-C(6A)-H(6AB)	108.1	O(9A)-C(7A)-O(8A)	126.27(12)
O(9A)-C(7A)-C(6A)	123.46(12)	O(8A)-C(7A)-C(6A)	110.27(12)
C(7A)-O(8A)-H(8AA)	109.5	C(5B)-N(1B)-N(2B)	106.32(11)
N(3B)-N(2B)-N(1B)	110.24(11)	N(2B)-N(3B)-N(4B)	106.46(11)
C(5B)-N(4B)-N(3B)	108.55(11)	C(5B)-N(4B)-C(6B)	130.48(12)
N(3B)-N(4B)-C(6B)	120.67(11)	N(1B)-C(5B)-N(4B)	108.43(12)
N(1B)-C(5B)-H(5BA)	125.8	N(4B)-C(5B)-H(5BA)	125.8
N(4B)-C(6B)-C(7B)	111.86(11)	N(4B)-C(6B)-H(6BA)	109.2
C(7B)-C(6B)-H(6BA)	109.2	N(4B)-C(6B)-H(6BB)	109.2
C(7B)-C(6B)-H(6BB)	109.2	H(6BA)-C(6B)-H(6BB)	107.9
O(9B)-C(7B)-O(8B)	125.26(13)	O(9B)-C(7B)-C(6B)	124.93(12)
O(8B)-C(7B)-C(6B)	109.80(12)	C(7B)-O(8B)-H(8BA)	109.5

Table 3.Bond lengths [Å] and angles [°] for compound 15.

	U^{11}	U^{22}	U ³³	U^{23}	U^{13}	U^{12}
$\overline{N(1A)}$	43(1)	71(1)	51(1)	-11(1)	7(1)	-22(1)
N(2A)	46(1)	43(1)	46(1)	-9(1)	-4(1)	-10(1)
N(3A)	41(1)	46(1)	39(1)	-13(1)	2(1)	-4(1)
N(4A)	28(1)	32(1)	28(1)	-2(1)	-2(1)	-2(1)
C(5A)	35(1)	64(1)	44(1)	-16(1)	9(1)	-11(1)
C(6A)	31(1)	36(1)	33(1)	4(1)	-1(1)	-7(1)
C(7A)	28(1)	38(1)	31(1)	0(1)	2(1)	-1(1)
O(8A)	32(1)	51(1)	51(1)	6(1)	-11(1)	-6(1)
O(9A)	44(1)	46(1)	59(1)	19(1)	-8(1)	-5(1)
N(1B)	28(1)	47(1)	44(1)	-1(1)	0(1)	1(1)
N(2B)	41(1)	47(1)	46(1)	-8(1)	-4(1)	-5(1)
N(3B)	43(1)	36(1)	45(1)	-9(1)	1(1)	1(1)
N(4B)	28(1)	28(1)	34(1)	0(1)	0(1)	1(1)
C(5B)	29(1)	34(1)	36(1)	0(1)	2(1)	2(1)
C(6B)	28(1)	30(1)	50(1)	5(1)	-4(1)	1(1)
C(7B)	36(1)	29(1)	36(1)	-1(1)	-3(1)	2(1)
O(8B)	35(1)	42(1)	72(1)	20(1)	-5(1)	6(1)
O(9B)	45(1)	38(1)	57(1)	12(1)	2(1)	-4(1)

Table 4. Anisotropic displacement parameters ($Å^2 x \ 10^3$) for compound **15**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2}U^{11} + ... + 2h k a^* b^* U^{12}]$

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å²x 10^3) for compound **15**.

	Х	у	Z	U(eq)	
H(5AA)	-6833	4489	1759	56	
H(6AA)	-4997	6919	1505	41	
H(6AB)	-4452	5633	851	41	
H(8AA)	-2753	4273	2462	70	
H(5BA)	-743	4513	3868	40	
H(6BA)	1227	2780	4363	45	
H(6BB)	1660	1662	3638	45	
H(8BA)	2634	-2928	4784	77	

C(5A)-N(1A)-N(2A)-N(3A)	-0.46(19)
N(1A)-N(2A)-N(3A)-N(4A)	-0.16(17)
N(2A)-N(3A)-N(4A)-C(5A)	0.72(16)
N(2A)-N(3A)-N(4A)-C(6A)	174.64(12)
N(2A)-N(1A)-C(5A)-N(4A)	0.90(19)
N(3A)-N(4A)-C(5A)-N(1A)	-1.04(18)
C(6A)-N(4A)-C(5A)-N(1A)	-174.26(13)
C(5A)-N(4A)-C(6A)-C(7A)	83.85(18)
N(3A)-N(4A)-C(6A)-C(7A)	-88.61(15)
N(4A)-C(6A)-C(7A)-O(9A)	-0.32(19)
N(4A)-C(6A)-C(7A)-O(8A)	-179.89(11)
C(5B)-N(1B)-N(2B)-N(3B)	-0.29(16)
N(1B)-N(2B)-N(3B)-N(4B)	0.40(16)
N(2B)-N(3B)-N(4B)-C(5B)	-0.36(15)
N(2B)-N(3B)-N(4B)-C(6B)	-174.73(12)
N(2B)-N(1B)-C(5B)-N(4B)	0.05(15)
N(3B)-N(4B)-C(5B)-N(1B)	0.19(15)
C(6B)-N(4B)-C(5B)-N(1B)	173.82(13)
C(5B)-N(4B)-C(6B)-C(7B)	128.40(15)
N(3B)-N(4B)-C(6B)-C(7B)	-58.63(17)
N(4B)-C(6B)-C(7B)-O(9B)	-24.1(2)
N(4B)-C(6B)-C(7B)-O(8B)	157.02(12)

Table 6.	Torsion angles	[°]	for compound	1	5	•
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Tuble 7. Trydrogen bonds for compound 15 /11 und	and °].	ind 15 [compound	bonds fo	Hydrogen	Table 7.
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D-HA	d(D-H)	d(HA)	d(DA)	<(DHA)	
O(8A)-H(8AA)N(1H	3) 0.82	1.89	2.6822(15)	163.6	
O(8B)-H(8BA)N(2A	A)#10.82	1.93	2.7382(16)	169.8	

Symmetry transformations used to generate equivalent atoms: #1 x+1,-y-1/2,z+1/2

Computation information

The remaining task is to determine the heats of formation of the 5-nitroiminotetrazolate salts; these values of 4-(carboxylatomethyl)-5-nitroiminotetrazolate anion were computed by using the method of isodesmic reactions. Calculations were carried out by using the Gaussian 03 (Revision D.01) suite of programs. The geometric optimization of the structures and frequency analyses were carried out by using the B3LYP functional with the 6-31+G** basis set, and single-point energies were calculated at the MP2/6-311++G** level.



Scheme S1. Isodesmic reations

Calculated (B3LYP/6-31+G**//MP2/6-311++G**) Total Energy (E₀), Zero Point Energy (ZPE), Values of Thermal correction (H_T), and Heats of Formation (HoF) [kJ/mol] of the compounds.



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+	E ₀	ZPE	H_{T}	HoF
NH ₄	-56.755055	0.04963	0.00381	9 626.4
H ₃ N−NH ₂	E ₀	ZPE	H_{T}	HoF
	-111.97353	0.06803	0.00430	9 770.0
+				U.D.
NH ₂ 	E ₀	ZPE	H_{T}	HoF
H ₂ N NH ₂	-204.8735031	0.075945	0.005496	26.0
H ₂ N、+ NH	E ₀	ZPE	H_{T}	HoF
H ₂ N NH ₂	-260.5457263	0.114876	0.006227	566.7
+ NH2	Fo	7 PF	$\mathbf{H}_{\mathbf{r}}$	HoF
H_2N N H_2 NH_2 H_1 H_2 H_2 H_2 H_1 H_2 H_2 H_2 H_2 H_1 H_2	-315.7583524	0.13361	0.007123	769.0176204
H ₂ N、+ NH	E ₀	ZPE	H_{T}	HoF
$H_2N_N_N_N^{H_2}$	-370.9707208	0.152308 (0.008131 8	71.4723014