Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Insensitive 5-Nitroaminotetrazolate Ionic Liquids as Potential Liquid Energetic Materials

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Figure S1 Molecular Structure of **1.**

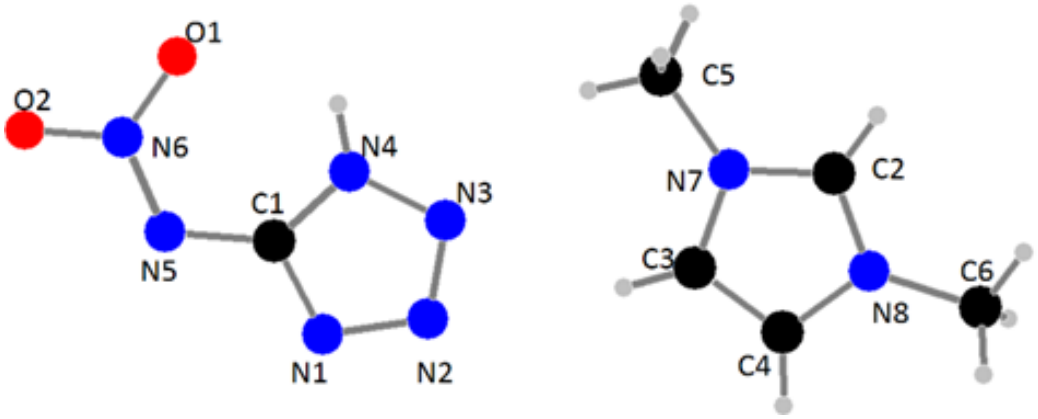


Figure S2. Packing Diagram of **1** Viewed down the *a*-axis.

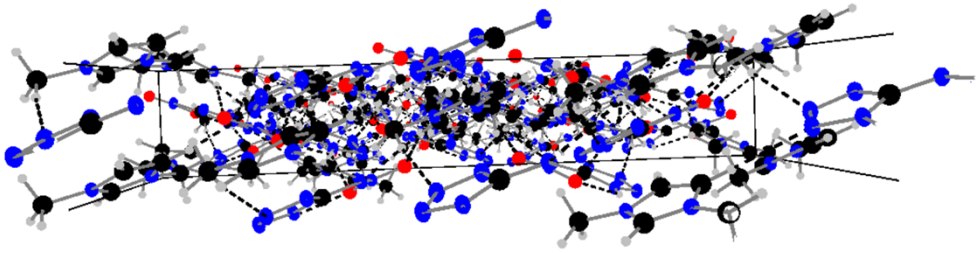


Figure S3. Packing Diagram of **1** Viewed down the *b*-axis.

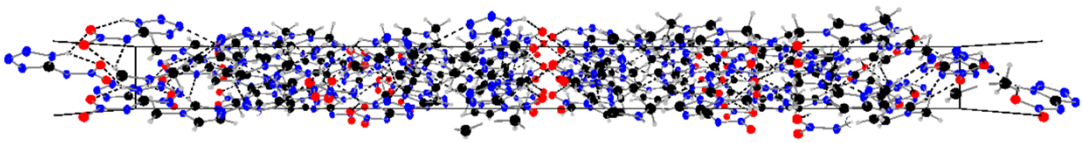


Figure S4. Packing Diagram of **1** Viewed down the *c*-axis.

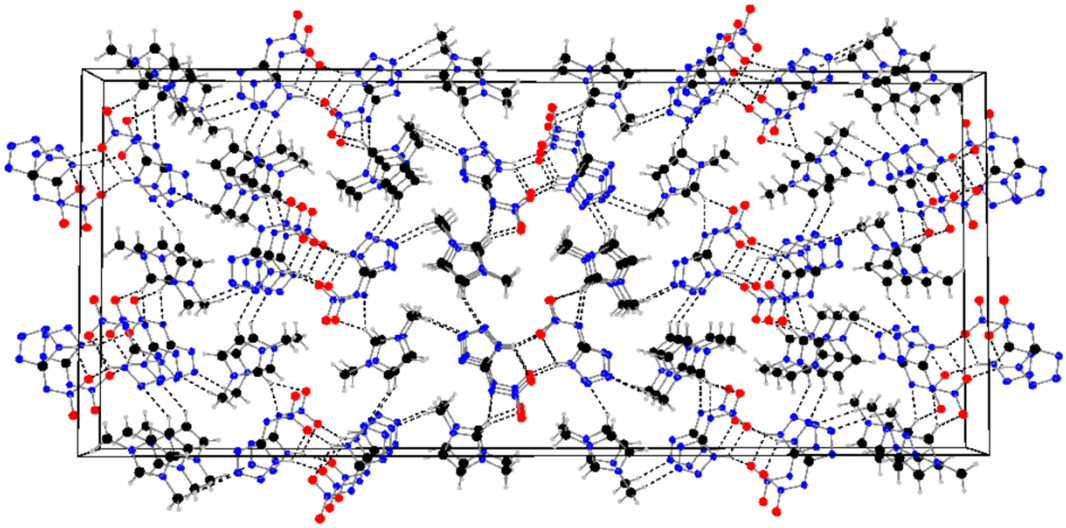


Table S1 Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for 1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
N8	4070.8(3)	5506.8(6)	131(4)	19.1(3)
N7	4395.0(3)	4824.8(6)	760(4)	19.0(3)
C2	4333.3(3)	5407.9(8)	-381(5)	20.3(3)
C4	3959.8(3)	4965.0(8)	1667(5)	23.1(4)
C3	4163.1(3)	4540.4(8)	2057(5)	22.3(4)
C6	3924.3(4)	6094.5(8)	-779(5)	25.8(4)
C5	4666.0(3)	4536.6(9)	690(6)	32.6(4)
O1	4940.6(2)	1908.5(5)	8062(3)	23.7(3)
O2	4832.4(3)	981.0(5)	10368(4)	29.7(3)
N1	4171.8(3)	2441.6(6)	8569(4)	23.4(3)
N2	4159.9(3)	3044.2(7)	7224(5)	25.7(3)
N3	4396.7(3)	3237.0(6)	6167(4)	24.9(3)
N4	4569.1(3)	2749.6(6)	6831(4)	20.2(3)
N5	4505.4(3)	1662.4(6)	9452(4)	20.0(3)
N6	4765.5(3)	1524.9(6)	9275(4)	19.2(3)
C1	4429.8(3)	2262.9(7)	8299(4)	17.6(3)

Table S2 Anisotropic Displacement Parameters (Å²×10³) for 1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N8	19.8(7)	15.9(6)	21.5(7)	1.3(6)	-0.1(6)	-0.8(5)
N7	15.6(7)	20.7(6)	20.7(7)	-1.0(6)	-0.8(6)	-0.6(5)
C2	19.4(8)	21.2(8)	20.3(8)	-0.6(6)	-1.2(6)	-4.6(6)
C4	18.1(8)	20.0(8)	31.3(9)	1.8(7)	4.6(7)	-3.5(6)
C3	21.7(9)	18.5(8)	26.6(9)	4.0(7)	2.4(7)	-1.3(6)
C6	28.0(9)	18.6(8)	30.7(10)	3.8(7)	-3.6(7)	3.0(7)
C5	16.7(9)	35.9(10)	45.1(11)	-2.1(10)	-1.1(8)	5.5(7)
O1	15.1(6)	22.9(6)	33.2(7)	4.4(5)	1.1(5)	-3.4(4)
O2	26.2(7)	21.5(6)	41.4(8)	10.7(6)	3.4(6)	5.7(5)
N1	17.4(7)	21.9(7)	30.9(8)	2.1(7)	0.4(6)	0.7(5)
N2	21.4(7)	22.1(7)	33.6(8)	1.0(7)	-2.2(6)	3.8(6)
N3	21.4(7)	20.2(7)	33.2(9)	2.8(7)	-1.4(6)	2.5(5)
N4	15.2(6)	18.3(6)	27.3(7)	2.7(6)	-0.7(5)	0.0(5)
N5	14.9(7)	17.8(6)	27.4(7)	1.7(6)	1.6(6)	0.0(5)
N6	18.8(7)	18.0(6)	20.7(7)	1.0(6)	0.7(5)	-1.1(5)
C1	16.1(8)	17.4(7)	19.2(7)	-1.6(7)	-2.0(6)	-2.0(6)

Table S3 Bond Lengths for 1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N8	C2	1.325(2)	O2	N6	1.2512(17)
N8	C4	1.381(2)	N1	C1	1.330(2)
N8	C6	1.465(2)	N1	N2	1.3558(19)
N7	C2	1.326(2)	N2	N3	1.296(2)
N7	C3	1.376(2)	N3	N4	1.3500(18)
N7	C5	1.466(2)	N4	C1	1.343(2)
C4	C3	1.347(2)	N5	N6	1.3165(18)
O1	N6	1.2615(17)	N5	C1	1.378(2)

Table S4 Bond Angles for 1.

Atom	Atom	Atom	Angle/	Atom	Atom	Atom	Angle/
C2	N8	C4	108.58(13)	N3	N2	N1	111.13(13)
C2	N8	C6	125.48(14)	N2	N3	N4	106.17(13)
C4	N8	C6	125.94(14)	C1	N4	N3	108.83(13)
C2	N7	C3	108.50(13)	N6	N5	C1	116.59(12)
C2	N7	C5	125.56(14)	O2	N6	O1	120.78(13)
C3	N7	C5	125.93(14)	O2	N6	N5	116.09(13)
N8	C2	N7	108.81(14)	O1	N6	N5	123.13(13)
C3	C4	N8	106.82(14)	N1	C1	N4	107.91(14)
C4	C3	N7	107.28(14)	N1	C1	N5	119.46(14)
C1	N1	N2	105.95(13)	N4	C1	N5	132.63(14)

Table S5 Torsion Angles for 1.

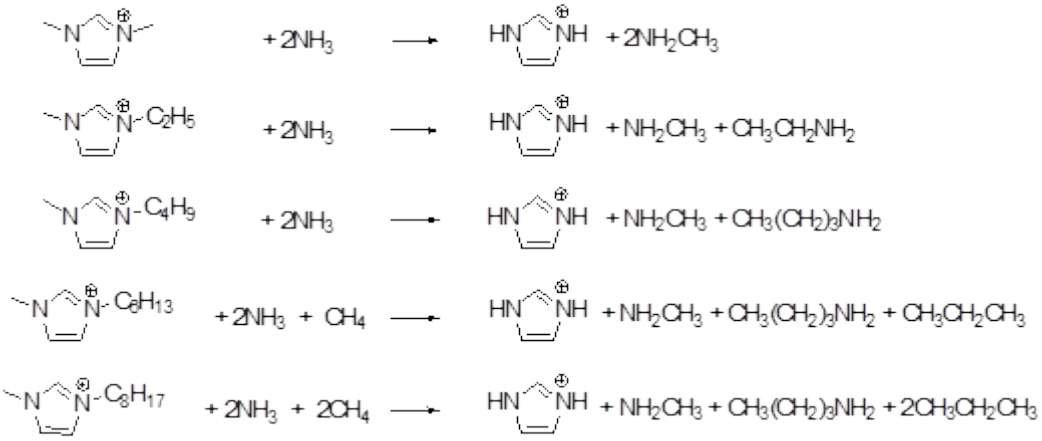
A	B	C	D	Angle/	A	B	C	D	Angle/
C4	N8	C2	N7	0.04(19)	N1	N2	N3	N4	0.00(19)
C6	N8	C2	N7	179.93(15)	N2	N3	N4	C1	0.09(18)
C3	N7	C2	N8	-0.07(19)	C1	N5	N6	O2	179.21(14)
C5	N7	C2	N8	-179.36(16)	C1	N5	N6	O1	-1.3(2)
C2	N8	C4	C3	0.02(19)	N2	N1	C1	N4	0.14(18)
C6	N8	C4	C3	-179.88(17)	N2	N1	C1	N5	-179.68(15)
N8	C4	C3	N7	-0.1(2)	N3	N4	C1	N1	-0.15(18)
C2	N7	C3	C4	0.1(2)	N3	N4	C1	N5	179.64(17)
C5	N7	C3	C4	179.36(17)	N6	N5	C1	N1	-176.84(15)

C1 N1 N2 N3	-0.09(19)	N6 N5 C1 N4	3.4(3)

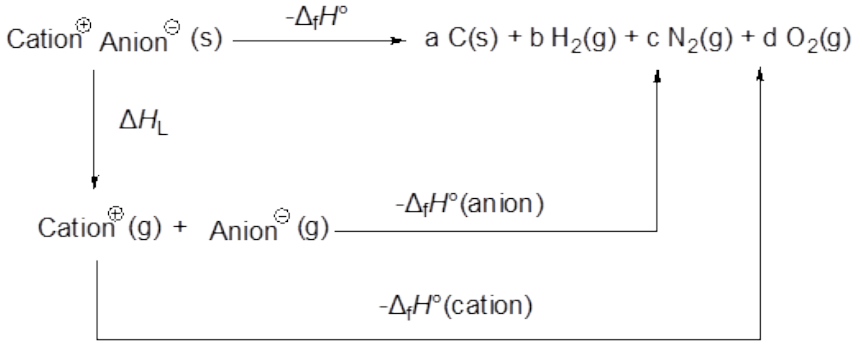
Table S6 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for 1.

Atom	*x*	*y*	*z*	U(eq)
H2	4457	5706	-1400	24
H4	3775	4903	2322	28
H3	4149	4122	3044	27
H6A	3870	6314	1449	39
H6B	3762	5988	-2189	39
H6C	4042	6375	-2204	39
H5A	4724	4482	-1822	49
H5B	4661	4119	1890	49
H5C	4794	4817	1956	49
H4A	4744	2751	6375	24

Scheme S1 The isodesmic reactions of the 1,3-dialkylimidazolium cations.



Scheme S2 Born-Haber cycle for the formation of ionic liquids.



where a, b, c, d are the numbers of moles of the respective products

Scheme S3 Combustion equations and thermochemical equations of Hess's Law for the ionic liquids **1**–**5**.

1: $C_6H_{10}N_8O_2(s) + 15/2O_2(g) \rightarrow 6CO_2(g) + 5H_2O(l) + 4N_2(g)$ [I]

$\Delta_fH^o_{298}$ (**1**, s) = $6\Delta_fH^o_{298}$ (CO_2, g) + $5\Delta_fH^o_{298}$ (H_2O, l) – $\Delta_cH^o_{298}$ (**1**, s) (4)

2: $C_7H_{12}N_8O_2(l) + 9O_2(g) \rightarrow 7CO_2(g) + 6H_2O(l) + 4N_2(g)$ [II]

$\Delta_fH^o_{298}$ (**2**, l) = $7\Delta_fH^o_{298}$ (CO_2, g) + $6\Delta_fH^o_{298}$ (H_2O, l) – $\Delta_cH^o_{298}$ (**2**,l) (5)

3: $C_9H_{16}N_8O_2(l) + 12O_2(g) \rightarrow 9CO_2(g) + 8H_2O(l) + 4N_2(g)$ [III]

$\Delta_fH^o_{298}$ (**3**, l) = $9\Delta_fH^o_{298}$ (CO_2, g) + $8\Delta_fH^o_{298}$ (H_2O, l) – $\Delta_cH^o_{298}$ (**3**, l) (6)

4: $C_{11}H_{20}N_8O_2(l) + 15O_2(g) \rightarrow 11CO_2(g) + 10H_2O(l) + 4N_2(g)$ [IV]

$\Delta_fH^o_{298}$ (**4**, l) = $11\Delta_fH^o_{298}$ (CO_2, g) + $10\Delta_fH^o_{298}$ (H_2O, l) – $\Delta_cH^o_{298}$ (**4**, l) (7)

5: $C_{13}H_{24}N_8O_2(l) + 18O_2(g) \rightarrow 13CO_2(g) + 12H_2O(l) + 4N_2(g)$ [V]

$\Delta_fH^o_{298}$ (**5**, l) = $13\Delta_fH^o_{298}$ (CO_2, g) + $12\Delta_fH^o_{298}$ (H_2O, l) – $\Delta_cH^o_{298}$ (**5**, l) (8)