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Electronic Supplementary Information

Fused Heterocycle-Based Energetic Salts: Alliance of Pyrazole and 1,2,3-Triazole

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Table of Contents

Table S1. Crystal data and structure refinement for **19** and **20**.

Compound	**19**	**20**
CCDC number	1439832	1439833
Empirical formula	$C_5H_9N_9O_3$	$C_5H_{10}N_{10}O_3$
Formula weight	243.21	258.23
Temperature/K	100	100
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	I2/a
a/Å	9.1162(6)	21.0998(14)
b/Å	7.8445(5)	3.8430(3)
c/Å	14.1930(9)	25.414(2)
α/°	90	90
β/°	104.811(2)	93.027(2)
γ/°	90	90
Volume/Å^3	981.25(11)	2057.9(3)
Z	4	8
ρ_{calc} g/cm^3	1.646	1.667
μ/mm-1	0.137	0.139
F(000)	504.0	1072.0
Crystal size/mm3	0.3 × 0.2 × 0.06	0.4 × 0.075 × 0.02
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.938 to 61.226	6.422 to 56.544
Index ranges	-13 ≤ h ≤ 13, -11 ≤ k ≤ 11, -20 ≤ l ≤ 20	-28 ≤ h ≤ 28, -5 ≤ k ≤ 5, -33 ≤ l ≤ 33
Reflections collected	38245	40862
Independent reflections	3012 [R_{int} = 0.0337, R_{sigma} = 0.0175]	2538 [R_{int} = 0.0512, R_{sigma} = 0.0216]
Data/restraints/parameters	3012/0/190	2538/0/203
Goodness-of-fit on F^2	1.052	1.111
Final R indexes [I>=2σ (I)]	R_1 = 0.0354, wR_2 = 0.0824	R_1 = 0.0391, wR_2 = 0.0820
Final R indexes [all data]	R_1 = 0.0479, wR_2 = 0.0882	R_1 = 0.0554, wR_2 = 0.0887
Largest diff. peak/hole / e Å^{-3}	0.56/-0.20	0.32/-0.24

Table S2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **19**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	3348.8(8)	10012.8(9)	5809.8(5)	14.56(16)
O2	-2716.3(9)	5718.7(10)	4596.5(6)	18.58(17)
O3	-2295.0(9)	4796.3(10)	3240.7(5)	18.10(17)
N1	-97.7(10)	8256.8(11)	5915.2(6)	13.07(17)
N2	1149.1(10)	9200.0(11)	6269.2(6)	13.18(17)
N3	2072.0(9)	9126.5(10)	5657.6(6)	11.46(17)
N4	1589.9(9)	7453.5(11)	4053.8(6)	12.07(17)
N5	377.8(9)	6475.2(11)	3644.5(6)	13.05(17)
N6	-1943.4(10)	5634.4(11)	3999.9(6)	13.54(17)
C1	-545.1(11)	6554.7(12)	4235.5(7)	12.21(19)
C2	62.9(11)	7576.1(12)	5067.9(7)	11.40(18)
C3	1420.5(11)	8103.5(12)	4906.8(7)	11.05(18)
C4	2911.0(12)	7503.3(15)	3655.5(8)	16.6(2)
N7	4438.4(11)	3430.4(13)	2713.9(7)	16.36(19)
N8	4081.3(10)	2021.1(12)	4063.0(6)	14.95(18)
N9	2066.7(10)	3340.2(11)	2997.7(7)	13.89(17)
C5	3515.5(11)	2934.8(12)	3258.5(7)	11.77(19)

Table S3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **19**. 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}
O1	11.0(3)	15.7(3)	16.8(4)	-2.4(3)	3.2(3)	-3.7(3)

O2	16.4(4)	20.7(4)	20.3(4)	-0.7(3)	7.7(3)	-2.0(3)
O3	18.0(4)	18.4(4)	16.0(4)	-4.5(3)	0.8(3)	-3.7(3)
N1	13.8(4)	12.8(4)	12.7(4)	0.3(3)	3.6(3)	-0.4(3)
N2	13.4(4)	14.1(4)	12.7(4)	-0.1(3)	4.6(3)	0.2(3)
N3	11.9(4)	11.4(4)	11.0(4)	0.1(3)	2.9(3)	-0.3(3)
N4	12.8(4)	12.8(4)	10.3(4)	-1.0(3)	2.4(3)	-2.2(3)
N5	13.5(4)	12.7(4)	11.9(4)	0.5(3)	1.2(3)	-1.3(3)
N6	13.1(4)	12.2(4)	14.0(4)	2.0(3)	1.1(3)	0.4(3)
C1	12.3(4)	11.7(4)	11.7(4)	1.1(3)	1.2(3)	-0.6(3)
C2	11.3(4)	10.7(4)	11.9(4)	2.0(3)	2.5(3)	0.3(3)
C3	12.2(4)	10.6(4)	10.0(4)	1.2(3)	2.2(3)	0.4(3)
C4	17.1(5)	20.9(5)	14.6(5)	-3.5(4)	8.9(4)	-5.2(4)
N7	11.4(4)	23.5(5)	14.5(4)	5.2(4)	3.8(3)	-0.1(3)
N8	13.6(4)	18.6(4)	13.7(4)	3.8(3)	5.4(3)	3.3(3)
N9	11.5(4)	15.6(4)	14.8(4)	2.9(3)	3.8(3)	0.4(3)
C5	12.4(4)	11.5(4)	11.6(4)	-2.1(3)	3.3(3)	-1.2(3)

Table S4 Bond Lengths for **19**.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
O1	N3	1.3252(11)	N4	C4	1.4559(13)
O2	N6	1.2340(11)	N5	C1	1.3328(13)
O3	N6	1.2327(11)	N6	C1	1.4283(13)
N1	N2	1.3416(12)	C1	C2	1.4178(14)
N1	C2	1.3575(13)	C2	C3	1.3784(13)
N2	N3	1.3558(12)	N7	C5	1.3376(13)
N3	C3	1.3449(12)	N8	C5	1.3350(13)
N4	N5	1.3488(12)	N9	C5	1.3162(13)
N4	C3	1.3584(12)			

Table S5 Bond Angles for **19**.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
N2	N1	C2	106.01(8)	N5	C1	N6	119.88(9)
N1	N2	N3	109.98(8)	N5	C1	C2	112.07(9)
O1	N3	N2	122.43(8)	C2	C1	N6	128.03(9)
O1	N3	C3	129.33(8)	N1	C2	C1	148.52(9)
C3	N3	N2	108.19(8)	N1	C2	C3	109.49(9)

N5	N4	C3	109.28(8)	C3	C2	C1	101.99(9)
N5	N4	C4	121.06(8)	N3	C3	N4	143.36(9)
C3	N4	C4	129.03(8)	N3	C3	C2	106.32(9)
C1	N5	N4	106.36(8)	N4	C3	C2	110.29(9)
O2	N6	C1	116.38(8)	N8	C5	N7	119.19(9)
O3	N6	O2	124.18(9)	N9	C5	N7	120.09(9)
O3	N6	C1	119.43(9)	N9	C5	N8	120.72(9)

Table S6 Hydrogen Bonds for **19**.

D	**H**	**A**	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
N7	H7A	O3[1]	0.843(17)	2.278(17)	3.0719(12)	157.0(15)
N7	H7B	O1[2]	0.867(16)	2.041(16)	2.8999(12)	170.9(14)
N8	H8A	O1[3]	0.880(16)	2.421(15)	3.1497(12)	140.4(12)
N8	H8B	O1[4]	0.893(16)	1.918(16)	2.8019(12)	170.0(15)
N9	H9A	N2[2]	0.866(16)	2.203(16)	3.0647(13)	173.1(14)
N9	H9B	N1[5]	0.885(17)	2.048(17)	2.9305(13)	175.0(14)

[1]1+X,+Y,+Z; [2]+X,3/2-Y,-1/2+Z; [3]+X,-1+Y,+Z; [4]1-X,1-Y,1-Z; [5]-X,1-Y,1-Z

Table S7 Torsion Angles for **19**.

A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
O1	N3	C3	N4	1.2(2)	N4	N5	C1	C2	-1.14(11)
O1	N3	C3	C2	-176.26(9)	N5	N4	C3	N3	-178.29(13)
O2	N6	C1	N5	177.56(9)	N5	N4	C3	C2	-0.91(11)
O2	N6	C1	C2	-0.83(15)	N5	C1	C2	N1	179.35(15)
O3	N6	C1	N5	-1.23(14)	N5	C1	C2	C3	0.59(11)
O3	N6	C1	C2	-179.63(9)	N6	C1	C2	N1	-2.1(2)
N1	N2	N3	O1	176.60(8)	N6	C1	C2	C3	179.09(9)
N1	N2	N3	C3	-0.85(11)	C1	C2	C3	N3	178.57(8)

N1	C2	C3	N3	-0.75(11)	C1	C2	C3	N4	0.20(10)
N1	C2	C3	N4	-179.11(8)	C2	N1	N2	N3	0.37(10)
N2	N1	C2	C1	-178.49(15)	C3	N4	N5	C1	1.24(10)
N2	N1	C2	C3	0.23(11)	C4	N4	N5	C1	172.97(9)
N2	N3	C3	N4	178.39(13)	C4	N4	C3	N3	10.8(2)
N2	N3	C3	C2	0.96(10)	C4	N4	C3	C2	-171.78(10)
N4	N5	C1	N6	-179.78(8)					

Table S8 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **19**.

Atom	***x***	***y***	***z***	**U(eq)**
H4A	2597(16)	7184(19)	2993(11)	22(3)
H4B	3658(18)	6710(20)	4026(11)	31(4)
H4C	3278(17)	8650(20)	3702(11)	25(4)
H7A	5380(20)	3550(20)	2960(12)	33(4)
H7B	4043(17)	3960(19)	2172(11)	24(4)
H8A	3491(17)	1821(19)	4454(11)	23(4)
H8B	4966(18)	1480(20)	4138(11)	28(4)
H9A	1733(17)	4050(20)	2522(11)	24(4)
H9B	1432(18)	2850(20)	3292(11)	30(4)

Table S9 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **20**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
O1	3058.2(4)	8313(3)	4481.3(4)	16.3(2)
O3	4098.0(5)	280(3)	2276.1(4)	18.5(2)
O2	4776.5(5)	-60(3)	2951.0(4)	19.3(2)
N6	4270.0(5)	902(3)	2735.5(4)	13.3(2)
N5	2990.3(5)	5334(3)	3266.8(4)	12.4(2)
N1'	3502.7(5)	11285(3)	5423.3(5)	14.6(3)
N1	3469.5(5)	6654(3)	4195.1(4)	12.4(2)
N4	3275.7(5)	3683(3)	2871.5(4)	12.4(2)
N3	4374.6(5)	4128(3)	4020.5(4)	15.1(3)

N2	4059.5(5)	5803(3)	4386.7(4)	15.2(3)
N2'	3023.0(6)	13105(4)	5676.5(5)	17.6(3)
N4'	4485.7(6)	8768(4)	5454.6(5)	19.1(3)
N3'	4121.9(6)	11401(4)	6197.2(5)	20.1(3)
C3	3855.7(6)	2829(4)	3059.9(5)	11.8(3)
C2	3968.6(6)	3926(4)	3587.6(5)	11.9(3)
C1	3404.4(6)	5500(4)	3696.1(5)	11.6(3)
C1'	4039.2(6)	10480(4)	5694.1(5)	13.9(3)
C4	2354.1(6)	6782(4)	3184.2(6)	14.4(3)

Table S10 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **20**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	$\mathbf{U_{11}}$	$\mathbf{U_{22}}$	$\mathbf{U_{33}}$	$\mathbf{U_{23}}$	$\mathbf{U_{13}}$	$\mathbf{U_{12}}$
O1	13.0(5)	20.0(6)	15.9(5)	-6.7(4)	0.1(4)	2.9(4)
O3	18.1(5)	25.4(6)	11.7(5)	-3.4(4)	0.0(4)	-1.0(4)
O2	14.3(5)	24.9(6)	18.4(5)	1.6(4)	-1.1(4)	4.9(4)
N6	13.1(5)	13.6(6)	13.1(5)	1.4(4)	0.8(4)	-2.2(5)
N5	12.2(5)	14.3(6)	10.6(5)	-0.5(4)	-2.0(4)	-0.4(5)
N1'	12.1(5)	19.2(7)	12.4(6)	-3.7(5)	-0.3(4)	2.3(5)
N1	11.4(5)	13.3(6)	12.2(5)	-0.6(5)	-1.8(4)	-0.5(5)
N4	12.7(5)	12.8(6)	11.9(5)	0.6(4)	0.9(4)	-1.7(5)
N3	13.5(6)	18.6(6)	13.0(5)	-1.2(5)	-2.0(4)	0.4(5)
N2	12.2(5)	18.0(6)	14.9(6)	-1.0(5)	-2.4(4)	1.3(5)
N2'	13.2(6)	17.6(7)	21.8(6)	-5.1(5)	-0.2(5)	1.9(5)

N4'	13.4(6)	28.4(7)	15.1(6)	-4.4(5)	-4.0(5)	5.6(5)
N3'	16.5(6)	29.4(8)	13.8(6)	-5.3(5)	-3.8(5)	3.8(6)
C3	11.9(6)	11.6(7)	11.7(6)	2.0(5)	-0.4(5)	-2.1(5)
C2	11.7(6)	10.1(7)	13.7(6)	1.6(5)	-1.0(5)	-1.0(5)
C1	12.4(6)	9.8(7)	12.3(6)	1.3(5)	-1.7(5)	-2.8(5)
C1'	13.7(6)	13.5(7)	14.4(6)	0.6(5)	-0.4(5)	-2.9(5)
C4	11.3(6)	17.3(7)	14.4(7)	-0.4(6)	-2.1(5)	2.7(6)

Table S11 Bond Lengths for **20**.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
O1	N1	1.3249(15)	N1	N2	1.3526(15)
O3	N6	1.2277(15)	N1	C1	1.3437(17)
O2	N6	1.2315(14)	N4	C3	1.3316(17)
N6	C3	1.4381(18)	N3	N2	1.3369(17)
N5	N4	1.3558(16)	N3	C2	1.3604(17)
N5	C1	1.3627(16)	N4'	C1'	1.3234(19)
N5	C4	1.4580(17)	N3'	C1'	1.3293(18)
N1'	N2'	1.4131(17)	C3	C2	1.4141(18)
N1'	C1'	1.3298(17)	C2	C1	1.3762(19)

Table S12 Bond Angles for **20**.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O3	N6	O2	124.79(12)	N4	C3	N6	119.73(11)
O3	N6	C3	119.16(11)	N4	C3	C2	111.90(12)
O2	N6	C3	116.04(11)	C2	C3	N6	128.33(12)
N4	N5	C1	108.91(11)	N3	C2	C3	148.36(13)
N4	N5	C4	120.89(11)	N3	C2	C1	109.11(12)
C1	N5	C4	130.08(12)	C1	C2	C3	102.53(11)
C1'	N1'	N2'	119.34(12)	N5	C1	C2	110.11(12)
O1	N1	N2	122.40(10)	N1	C1	N5	143.17(13)
O1	N1	C1	129.76(11)	N1	C1	C2	106.72(11)
C1	N1	N2	107.83(11)	N4'	C1'	N1'	119.00(13)
C3	N4	N5	106.54(10)	N4'	C1'	N3'	120.94(13)
N2	N3	C2	105.98(11)	N3'	C1'	N1'	120.06(13)
N3	N2	N1	110.36(10)				

Table S13 Hydrogen Bonds for **20**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N3'	H3'A	O2[1]	0.866(19)	2.305(19)	3.1341(16)	160.3(16)
N2'	H2'A	O1[2]	0.92(2)	2.03(2)	2.9429(17)	170.0(17)
N4'	H4'A	N3[1]	0.87(2)	2.05(2)	2.9090(17)	173.5(18)
N4'	H4'B	N2	0.910(19)	2.134(19)	3.0359(17)	171.3(17)
N2'	H2'B	O1[3]	0.91(2)	2.46(2)	3.0455(16)	122.8(15)
N1'	H1'	O1	0.876(19)	1.917(19)	2.7709(15)	164.4(17)

[1]1-X,1-Y,1-Z; [2]1/2-X,+Y,1-Z; [3]1/2-X,1+Y,1-Z

Table S14 Torsion Angles for **20**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	N1	N2	N3	179.53(12)	N3	C2	C1	N1	-0.02(16)
O1	N1	C1	N5	0.7(3)	N2	N1	C1	N5	-179.87(18)
O1	N1	C1	C2	-179.44(13)	N2	N1	C1	C2	-0.02(15)
O3	N6	C3	N4	4.97(19)	N2	N3	C2	C3	179.4(2)
O3	N6	C3	C2	-177.50(13)	N2	N3	C2	C1	0.06(16)
O2	N6	C3	N4	-173.82(12)	N2'	N1'	C1'	N4'	179.86(14)
O2	N6	C3	C2	3.7(2)	N2'	N1'	C1'	N3'	-0.3(2)
N6	C3	C2	N3	3.0(3)	C3	C2	C1	N5	0.21(15)
N6	C3	C2	C1	-177.59(13)	C3	C2	C1	N1	-179.69(11)
N5	N4	C3	N6	177.54(12)	C2	N3	N2	N1	-0.07(15)
N5	N4	C3	C2	-0.37(15)	C1	N5	N4	C3	0.50(15)
N4	N5	C1	N1	179.39(18)	C1	N1	N2	N3	0.06(15)
N4	N5	C1	C2	-0.45(16)	C4	N5	N4	C3	176.95(12)
N4	C3	C2	N3	-179.3(2)	C4	N5	C1	N1	3.4(3)
N4	C3	C2	C1	0.10(15)	C4	N5	C1	C2	-176.48(14)
N3	C2	C1	N5	179.88(11)					

Table S15 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **20**.

Atom	***x***	***y***	***z***	**U(eq)**
H3'A	4480(9)	10930(50)	6364(7)	23(5)
H4A	2091(9)	5070(50)	2991(7)	27(5)
H4B	2189(8)	7230(50)	3512(7)	22(4)
H2'A	2667(9)	11700(50)	5665(7)	31(5)
H4'A	4825(9)	8050(50)	5627(7)	30(5)
H4C	2379(8)	8970(50)	2990(7)	22(4)
H4'B	4390(8)	8030(50)	5120(7)	28(5)
H3'B	3832(9)	12680(50)	6329(7)	27(5)
H2'B	2928(9)	14970(60)	5466(8)	33(5)
H1'	3435(9)	10410(50)	5107(8)	26(5)