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Electronic Supplementary Information

Energetic fused triazoles – A promising *C-N* fused heterocyclic cation

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Table S1. Crystal data and structure refinement for **6**.

CCDC number	1052627	
Identification code	shrv279	
Empirical formula	$C_3H_{6.78}Br_{0.78}N_8$	
Formula weight	217.56	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 6.330(4) Å	α= 95.533(8)°.
	b = 6.711(4) Å	β= 90.022(7)°.
	c = 9.034(6) Å	γ = 90.076(8)°.
Volume	382.0(4) $Å^3$	
Z	2	
Density (-123 °C)	1.891 Mg/m^3	
Density (20 °C)	1.854 Mg/m^3	
Absorption coefficient	4.205 mm^{-1}	
F(000)	216	
Crystal size	0.178 x 0.170 x 0.028 mm^3	
Theta range for data collection	3.049 to 26.417°.	
Index ranges	-7<=h<=7, -7<=k<=8, -11<=l<=11	
Reflections collected	3383	
Independent reflections	1555 [$R_{(int)}$ = 0.0179]	
Completeness to theta = 25.242°	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.522 and 0.8910	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1555 / 0 / 116	
Goodness-of-fit on F^2	1.120	
Final R indices [I>2sigma(I)]	R_1 = 0.0204, wR_2 = 0.0552	
R indices (all data)	R_1 = 0.0210, wR_2 = 0.0556	
Largest diff. peak and hole	0.386 and -0.249 e.$Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 8. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	2500(1)	1204(1)	11534(1)	21(1)
N(1)	2500(2)	5928(2)	5260(2)	19(1)
N(2)	2499(3)	3960(2)	5657(2)	24(1)
C(3)	2501(3)	4288(2)	7132(2)	21(1)
N(4)	2499(2)	6302(2)	7654(2)	18(1)
C(5)	2500(2)	7330(2)	6430(2)	18(1)
N(6)	2500(2)	9160(2)	6068(2)	23(1)
N(7)	2499(2)	8826(2)	4513(2)	22(1)
C(8)	2501(3)	6884(3)	4009(2)	21(1)
N(9)	2499(3)	2866(2)	8057(2)	33(1)
N(10)	2498(3)	7053(2)	9153(2)	22(1)
N(11)	2500(3)	6041(3)	2626(2)	32(1)

Table S3. Bond lengths [Å] and angles [°] for 6.

N(1)-C(5)	1.345(2)
N(1)-C(8)	1.352(2)
N(1)-N(2)	1.402(2)
N(2)-C(3)	1.330(2)
C(3)-N(9)	1.327(2)
C(3)-N(4)	1.388(2)
N(4)-C(5)	1.359(2)
N(4)-N(10)	1.399(2)
C(5)-N(6)	1.301(2)
N(6)-N(7)	1.401(2)
N(7)-C(8)	1.338(2)
N(7)-H(7A)	0.8800
C(8)-N(11)	1.321(3)
N(9)-H(9A)	0.8800
N(9)-H(9B)	0.8800
N(10)-H(10B)	0.87(3)
N(10)-H(10C)	0.88(3)
N(11)-H(11A)	0.8800
N(11)-H(11B)	0.8800
C(5)-N(1)-C(8)	107.70(15)

C(5)-N(1)-N(2)	113.81(14)
C(8)-N(1)-N(2)	138.49(14)
C(3)-N(2)-N(1)	100.80(13)
N(9)-C(3)-N(2)	124.81(16)
N(9)-C(3)-N(4)	121.48(16)
N(2)-C(3)-N(4)	113.71(14)
C(5)-N(4)-C(3)	106.15(14)
C(5)-N(4)-N(10)	128.60(14)
C(3)-N(4)-N(10)	125.25(14)
N(6)-C(5)-N(1)	114.09(15)
N(6)-C(5)-N(4)	140.39(15)
N(1)-C(5)-N(4)	105.52(14)
C(5)-N(6)-N(7)	100.85(13)
C(8)-N(7)-N(6)	113.39(13)
C(8)-N(7)-H(7A)	123.3
N(6)-N(7)-H(7A)	123.3
N(11)-C(8)-N(7)	129.46(15)
N(11)-C(8)-N(1)	126.58(16)
N(7)-C(8)-N(1)	103.96(15)
C(3)-N(9)-H(9A)	120.0
C(3)-N(9)-H(9B)	120.0
H(9A)-N(9)-H(9B)	120.0
N(4)-N(10)-H(10B)	105.1(16)
N(4)-N(10)-H(10C)	105.2(16)
H(10B)-N(10)-H(10C)	109(2)
C(8)-N(11)-H(11A)	120.0
C(8)-N(11)-H(11B)	120.0
H(11A)-N(11)-H(11B)	120.0

Table S4. Anisotropic displacement parameters ($Å^2$x 10^3) for 6. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U11	U22	U33	U23
Br(1)	28(1)	18(1)	16(1)	3(1)
N(1)	28(1)	14(1)	16(1)	5(1)
N(2)	43(1)	12(1)	18(1)	4(1)
C(3)	29(1)	14(1)	21(1)	3(1)
N(4)	28(1)	13(1)	14(1)	2(1)
C(5)	21(1)	13(1)	21(1)	3(1)
N(6)	33(1)	14(1)	23(1)	6(1)

N(7)	27(1)	19(1)	23(1)	10(1)
C(8)	22(1)	21(1)	20(1)	9(1)
N(9)	68(1)	13(1)	20(1)	5(1)
N(10)	31(1)	20(1)	16(1)	-1(1)
N(11)	51(1)	28(1)	17(1)	8(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x $10^{3)}$ for 6.

	x	y	z	U(eq)
H(7A)	2498	9798	3924	27
H(9A)	2496	1598	7703	40
H(9B)	2500	3192	9024	40
H(11A)	2498	6792	1880	38
H(11B)	2501	4728	2451	38
H(10B)	3630(40)	7800(40)	9270(30)	38
H(10C)	1370(40)	7830(40)	9260(30)	38

Table S6. Torsion angles [°] for 6.

C(5)-N(1)-N(2)-C(3)	-0.03(18)
C(8)-N(1)-N(2)-C(3)	179.9(2)
N(1)-N(2)-C(3)-N(9)	179.93(18)
N(1)-N(2)-C(3)-N(4)	0.07(19)
N(9)-C(3)-N(4)-C(5)	-179.95(17)
N(2)-C(3)-N(4)-C(5)	-0.1(2)
N(9)-C(3)-N(4)-N(10)	0.1(3)
N(2)-C(3)-N(4)-N(10)	179.93(15)
C(8)-N(1)-C(5)-N(6)	0.05(19)
N(2)-N(1)-C(5)-N(6)	-179.98(14)
C(8)-N(1)-C(5)-N(4)	-179.99(14)

N(2)-N(1)-C(5)-N(4)	-0.01(17)
C(3)-N(4)-C(5)-N(6)	-180.0(2)
N(10)-N(4)-C(5)-N(6)	0.0(3)
C(3)-N(4)-C(5)-N(1)	0.05(16)
N(10)-N(4)-C(5)-N(1)	-179.96(16)
N(1)-C(5)-N(6)-N(7)	0.00(18)
N(4)-C(5)-N(6)-N(7)	-180.0(2)
C(5)-N(6)-N(7)-C(8)	-0.04(18)
N(6)-N(7)-C(8)-N(11)	179.96(17)
N(6)-N(7)-C(8)-N(1)	0.07(18)
C(5)-N(1)-C(8)-N(11)	-179.96(17)
N(2)-N(1)-C(8)-N(11)	0.1(3)
C(5)-N(1)-C(8)-N(7)	-0.07(17)
N(2)-N(1)-C(8)-N(7)	179.97(18)

Table S7. Hydrogen bonds for 6 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(7)-H(7A)...Br(1)#1	0.88	2.44	3.258(2)	155.1
N(9)-H(9A)...N(6)#2	0.88	2.10	2.925(3)	156.7
N(9)-H(9B)...Br(1)	0.88	2.74	3.434(2)	136.7
N(10)-H(10B)...Br(1)#3	0.87(3)	2.66(3)	3.451(3)	152(2)
N(10)-H(10C)...Br(1)#4	0.88(3)	2.65(3)	3.451(3)	151(2)
N(11)-H(11A)...Br(1)#1	0.88	3.01	3.693(3)	136.2
N(11)-H(11A)...N(10)#5	0.88	2.49	3.274(3)	149.3
N(11)-H(11B)...Br(1)#5	0.88	2.43	3.301(3)	170.5

Symmetry transformations used to generate equivalent atoms:
#1 x,y+1,z-1 #2 x,y-1,z #3 -x+1,-y+1,-z+2
#4 -x,-y+1,-z+2 #5 x,y,z-1

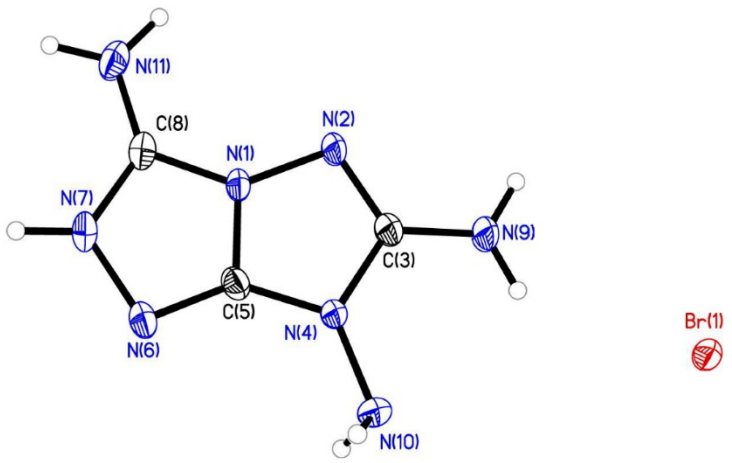

Figure S1. Single-crystal X-ray structure of 6

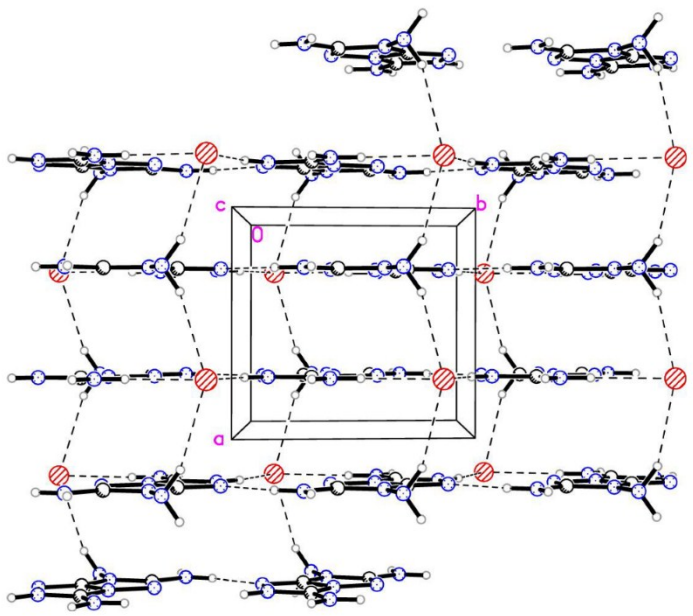

Figure S2. Ball and stick packing diagram of 6 viewed down the *c* axis.

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 8. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

N(1)	1109(2)	2203(2)	5642(1)	12(1)
N(2)	502(2)	2460(2)	4036(1)	13(1)
C(3)	2351(2)	2924(2)	2823(2)	12(1)
N(4)	3997(2)	3031(2)	3573(1)	13(1)
C(5)	3197(2)	2506(2)	5397(2)	12(1)
N(6)	3810(2)	2197(2)	6880(1)	14(1)
N(7)	1854(2)	1678(2)	8247(1)	14(1)
C(8)	269(2)	1715(2)	7466(2)	12(1)
N(9)	2688(2)	3308(2)	1036(1)	17(1)
N(10)	6058(2)	3548(2)	2570(1)	16(1)
N(11)	-1904(2)	1446(2)	8296(1)	15(1)

Table S9. Bond lengths [Å] and angles [°] for 8.

N(1)-C(5)	1.3484(15)	N(1)-C(8)	1.3687(14)
N(1)-N(2)	1.4036(13)	N(2)-C(3)	1.3258(15)
C(3)-N(9)	1.3368(15)	C(3)-N(4)	1.3882(15)
N(4)-C(5)	1.3706(15)	N(4)-N(10)	1.4009(13)
C(5)-N(6)	1.3035(15)	N(6)-N(7)	1.4361(14)
N(7)-C(8)	1.3267(15)	C(8)-N(11)	1.3565(15)
N(9)-H(9A)	0.876(17)	N(9)-H(9B)	0.896(17)
N(10)-H(10A)	0.893(18)	N(10)-H(10B)	0.872(18)
N(11)-H(11A)	0.866(18)	N(11)-H(11B)	0.869(17)
C(5)-N(1)-C(8)	105.43(10)	C(5)-N(1)-N(2)	113.89(10)
C(8)-N(1)-N(2)	140.67(10)	C(3)-N(2)-N(1)	101.18(9)
N(2)-C(3)-N(9)	126.07(11)	N(2)-C(3)-N(4)	113.59(10)
N(9)-C(3)-N(4)	120.33(11)	C(5)-N(4)-C(3)	106.31(10)
C(5)-N(4)-N(10)	129.55(10)	C(3)-N(4)-N(10)	124.13(10)
N(6)-C(5)-N(1)	114.00(11)	N(6)-C(5)-N(4)	141.04(11)
N(1)-C(5)-N(4)	104.95(10)	C(5)-N(6)-N(7)	103.26(9)
C(8)-N(7)-N(6)	108.76(10)	N(7)-C(8)-N(11)	127.12(11)
N(7)-C(8)-N(1)	108.52(10)	N(11)-C(8)-N(1)	124.27(11)
C(3)-N(9)-H(9A)	118.4(11)	C(3)-N(9)-H(9B)	120.2(10)
H(9A)-N(9)-H(9B)	119.3(15)	N(4)-N(10)-H(10A)	107.9(10)
N(4)-N(10)-H(10B)	109.3(11)	H(10A)-N(10)-H(10B)	104.9(15)
C(8)-N(11)-H(11A)	117.7(11)	C(8)-N(11)-H(11B)	117.2(11)

H(11A)-N(11)-H(11B)	117.0(15)

Table S10. Anisotropic displacement parameters ($Å^2 x 10^3$) for 8. 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}
N(1)	13(1)	18(1)	9(1)	0(1)	-4(1)	-9(1)
N(2)	15(1)	20(1)	8(1)	-1(1)	-5(1)	-9(1)
C(3)	14(1)	14(1)	12(1)	-2(1)	-5(1)	-7(1)
N(4)	14(1)	20(1)	10(1)	0(1)	-3(1)	-11(1)
C(5)	11(1)	14(1)	12(1)	-1(1)	-4(1)	-7(1)
N(6)	14(1)	19(1)	11(1)	0(1)	-4(1)	-9(1)
N(7)	14(1)	19(1)	11(1)	-1(1)	-4(1)	-9(1)
C(8)	14(1)	13(1)	9(1)	-2(1)	-3(1)	-5(1)
N(9)	21(1)	28(1)	9(1)	0(1)	-4(1)	-16(1)
N(10)	14(1)	20(1)	16(1)	-1(1)	-2(1)	-12(1)
N(11)	15(1)	25(1)	10(1)	0(1)	-4(1)	-12(1)

Table S11. Hydrogen coordinates ($x 10^4$) and isotropic displacement parameters ($Å^2 x 10^3$) for 8.

	x	y	z	U(eq)
H(9A)	4010(30)	3560(30)	350(20)	21
H(9B)	1830(30)	2970(30)	530(20)	21
H(10A)	5780(30)	4810(30)	2840(20)	19
H(10B)	7350(30)	2660(30)	2940(20)	19
H(11A)	-2680(30)	1350(30)	7620(20)	18
H(11B)	-2050(30)	730(30)	9360(20)	18

Table S12. Torsion angles [°] for 8.

C(5)-N(1)-N(2)-C(3)	0.24(13)
C(8)-N(1)-N(2)-C(3)	-179.34(15)
N(1)-N(2)-C(3)-N(9)	179.33(12)
N(1)-N(2)-C(3)-N(4)	-1.81(13)
N(2)-C(3)-N(4)-C(5)	2.73(14)
N(9)-C(3)-N(4)-C(5)	-178.33(11)
N(2)-C(3)-N(4)-N(10)	-178.34(10)
N(9)-C(3)-N(4)-N(10)	0.60(18)
C(8)-N(1)-C(5)-N(6)	1.95(14)
N(2)-N(1)-C(5)-N(6)	-177.78(10)
C(8)-N(1)-C(5)-N(4)	-178.92(9)
N(2)-N(1)-C(5)-N(4)	1.35(14)
C(3)-N(4)-C(5)-N(6)	176.42(16)
N(10)-N(4)-C(5)-N(6)	-2.4(3)
C(3)-N(4)-C(5)-N(1)	-2.31(13)
N(10)-N(4)-C(5)-N(1)	178.84(11)
N(1)-C(5)-N(6)-N(7)	-1.37(14)
N(4)-C(5)-N(6)-N(7)	179.97(15)
C(5)-N(6)-N(7)-C(8)	0.24(13)
N(6)-N(7)-C(8)-N(11)	-175.57(11)
N(6)-N(7)-C(8)-N(1)	0.91(13)
C(5)-N(1)-C(8)-N(7)	-1.67(13)
N(2)-N(1)-C(8)-N(7)	177.93(13)
C(5)-N(1)-C(8)-N(11)	174.93(11)
N(2)-N(1)-C(8)-N(11)	-5.5(2)

Table S13. Hydrogen bonds for 8 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(9)-H(9A)...N(11)#1	0.876(17)	2.523(17)	3.2014(16)	134.9(15)
N(9)-H(9B)...N(7)#2	0.896(17)	2.217(17)	3.0112(15)	147.5(14)
N(10)-H(10A)...N(6)#3	0.893(18)	2.293(18)	3.1619(16)	164.3(14)
N(10)-H(10B)...N(2)#4	0.872(18)	2.351(17)	3.0942(15)	143.2(14)
N(11)-H(11A)...N(6)#5	0.866(18)	2.254(17)	3.0413(15)	151.2(14)
N(11)-H(11B)...N(7)#6	0.869(17)	2.208(17)	3.0631(15)	167.8(15)

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

#4 x+1,y,z #5 x-1,y,z #6 -x,-y,-z+2

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 13. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	-4096(4)	3540(4)	4105(2)	27(1)
N(2)	-1976(4)	3009(4)	3831(2)	26(1)
C(3)	-1482(5)	3840(4)	2850(3)	20(1)
C(4)	-3261(5)	4904(4)	2449(2)	19(1)
C(5)	-4852(5)	4667(4)	3278(2)	21(1)
N(6)	638(4)	3501(4)	2296(2)	24(1)
O(7)	2067(4)	2552(3)	2780(2)	33(1)
O(8)	877(4)	4152(3)	1366(2)	31(1)
N(9)	-3410(4)	5966(4)	1417(2)	26(1)
O(10)	-2536(4)	7258(3)	1154(2)	32(1)
O(11)	-4410(4)	5503(4)	875(2)	40(1)
N(12)	-7090(4)	5460(4)	3334(2)	28(1)
O(13)	-7643(4)	6544(4)	2567(2)	34(1)
O(14)	-8285(4)	4979(3)	4139(2)	37(1)
N(15)	-1849(4)	-323(4)	2752(2)	18(1)
N(16)	-637(4)	625(4)	1882(2)	21(1)
C(17)	-2056(5)	1090(4)	1221(2)	20(1)
N(18)	-4058(4)	549(4)	1611(2)	20(1)
C(19)	-3902(5)	-368(4)	2596(2)	21(1)
N(20)	-5050(4)	-1211(4)	3397(2)	26(1)
N(21)	-3551(4)	-1696(4)	4118(2)	25(1)
C(22)	-1623(5)	-1153(4)	3736(2)	19(1)
N(23)	-1714(5)	1969(4)	231(2)	30(1)
N(24)	-5706(5)	745(5)	1008(2)	30(1)
N(25)	80(4)	-1307(4)	4211(2)	24(1)

Table S15. Bond lengths [Å] and angles [°] for 13.

N(1)-C(5)	1.344(4)	N(1)-N(2)	1.353(4)
N(2)-C(3)	1.338(4)	C(3)-C(4)	1.384(4)
C(3)-N(6)	1.442(4)	C(4)-C(5)	1.374(4)
C(4)-N(9)	1.448(4)	C(5)-N(12)	1.444(4)
N(6)-O(8)	1.231(3)	N(6)-O(7)	1.234(3)
N(9)-O(10)	1.225(4)	N(9)-O(11)	1.228(4)
N(12)-O(13)	1.228(4)	N(12)-O(14)	1.231(4)
N(15)-C(22)	1.347(4)	N(15)-C(19)	1.358(4)
N(15)-N(16)	1.413(3)	N(16)-C(17)	1.315(4)
C(17)-N(23)	1.346(4)	C(17)-N(18)	1.384(4)
N(18)-C(19)	1.359(4)	N(18)-N(24)	1.397(4)
C(19)-N(20)	1.300(4)	N(20)-N(21)	1.412(4)
N(21)-C(22)	1.342(4)	N(21)-H(21)	0.8800
C(22)-N(25)	1.319(4)	N(23)-H(23A)	0.98(4)
N(23)-H(23B)	0.81(4)	N(24)-H(24A)	0.88(4)
N(24)-H(24B)	0.79(4)	N(25)-H(25A)	0.89(4)
N(25)-H(25B)	0.78(4)		

C(5)-N(1)-N(2)	107.5(2)	C(3)-N(2)-N(1)	106.9(2)
N(2)-C(3)-C(4)	111.9(3)	N(2)-C(3)-N(6)	121.4(3)
C(4)-C(3)-N(6)	126.5(3)	C(5)-C(4)-C(3)	102.2(3)
C(5)-C(4)-N(9)	129.1(3)	C(3)-C(4)-N(9)	128.7(3)
N(1)-C(5)-C(4)	111.5(3)	N(1)-C(5)-N(12)	120.3(3)
C(4)-C(5)-N(12)	128.1(3)	O(8)-N(6)-O(7)	124.6(3)
O(8)-N(6)-C(3)	117.3(2)	O(7)-N(6)-C(3)	118.1(3)
O(10)-N(9)-O(11)	125.2(3)	O(10)-N(9)-C(4)	117.4(3)
O(11)-N(9)-C(4)	117.3(3)	O(13)-N(12)-O(14)	125.6(3)
O(13)-N(12)-C(5)	116.9(3)	O(14)-N(12)-C(5)	117.5(3)
C(22)-N(15)-C(19)	108.1(2)	C(22)-N(15)-N(16)	138.8(2)
C(19)-N(15)-N(16)	113.0(2)	C(17)-N(16)-N(15)	101.1(2)
N(16)-C(17)-N(23)	126.5(3)	N(16)-C(17)-N(18)	114.3(3)
N(23)-C(17)-N(18)	119.2(3)	C(19)-N(18)-C(17)	106.4(2)
C(19)-N(18)-N(24)	129.7(3)	C(17)-N(18)-N(24)	123.2(3)
N(20)-C(19)-N(15)	113.7(3)	N(20)-C(19)-N(18)	141.0(3)
N(15)-C(19)-N(18)	105.2(2)	C(19)-N(20)-N(21)	100.9(2)
C(22)-N(21)-N(20)	113.3(3)	C(22)-N(21)-H(21)	123.4
N(20)-N(21)-H(21)	123.4	N(25)-C(22)-N(21)	128.8(3)
N(25)-C(22)-N(15)	127.1(3)	N(21)-C(22)-N(15)	104.0(3)
C(17)-N(23)-H(23A)	117(2)	C(17)-N(23)-H(23B)	117(3)
H(23A)-N(23)-H(23B)	117(3)	N(18)-N(24)-H(24A)	106(3)

N(18)-N(24)-H(24B)	109(3)	H(24A)-N(24)-H(24B)	119(4)
C(22)-N(25)-H(25A)	120(2)	C(22)-N(25)-H(25B)	116(3)
H(25A)-N(25)-H(25B)	121(3)		

Table S16. Anisotropic displacement parameters ($Å^2$x 10^3) for 13. 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}
N(1)	24(2)	32(2)	23(2)	-2(1)	-4(1)	-5(1)
N(2)	21(2)	30(2)	24(2)	1(1)	-6(1)	-2(1)
C(3)	12(2)	22(2)	28(2)	-6(2)	-5(1)	-3(1)
C(4)	13(2)	21(2)	23(2)	-1(2)	-5(1)	-7(1)
C(5)	13(2)	25(2)	24(2)	-4(2)	0(1)	-7(1)
N(6)	13(1)	24(2)	38(2)	-8(2)	-7(1)	-3(1)
O(7)	18(1)	31(2)	54(2)	-12(1)	-14(1)	3(1)
O(8)	23(1)	37(2)	30(2)	-5(1)	4(1)	-9(1)
N(9)	20(2)	27(2)	28(2)	-4(2)	-4(1)	-2(1)
O(10)	34(2)	24(2)	33(2)	2(1)	-4(1)	-9(1)
O(11)	47(2)	50(2)	28(2)	-2(1)	-21(1)	-16(1)
N(12)	16(2)	35(2)	38(2)	-13(2)	-4(1)	-8(1)
O(13)	22(1)	38(2)	42(2)	-8(1)	-16(1)	3(1)
O(14)	23(1)	45(2)	42(2)	-13(1)	9(1)	-12(1)
N(15)	8(1)	24(2)	20(2)	1(1)	-3(1)	-4(1)
N(16)	16(1)	25(2)	19(2)	4(1)	-3(1)	-8(1)
C(17)	15(2)	22(2)	23(2)	-3(2)	-4(1)	-3(1)
N(18)	13(1)	28(2)	18(2)	-1(1)	-7(1)	-4(1)
C(19)	11(2)	24(2)	27(2)	-6(2)	-6(1)	-2(1)
N(20)	13(1)	39(2)	22(2)	4(1)	-6(1)	-8(1)
N(21)	14(1)	39(2)	20(2)	3(1)	-6(1)	-7(1)
C(22)	14(2)	19(2)	22(2)	-1(2)	-4(1)	-3(1)
N(23)	22(2)	36(2)	25(2)	6(2)	-3(1)	-9(1)
N(24)	14(2)	45(2)	30(2)	-10(2)	-12(1)	3(2)
N(25)	14(1)	35(2)	20(2)	0(1)	-5(1)	-7(1)

Table S17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 13.

	x	y	z	U(eq)
H(21)	-3851	-2295	4754	30
H(23A)	-2980(60)	2670(50)	-80(30)	36
H(23B)	-570(60)	2340(50)	40(30)	36
H(24A)	-5720(60)	-280(50)	930(30)	36
H(24B)	-6780(60)	1220(50)	1250(30)	36
H(25A)	80(50)	-1920(50)	4860(30)	28
H(25B)	1150(60)	-1070(50)	3860(30)	28

Table S18. Torsion angles [°] for 13.

C(5)-N(1)-N(2)-C(3)	0.8(4)	N(1)-N(2)-C(3)-C(4)	-1.2(4)
N(1)-N(2)-C(3)-N(6)	-176.5(3)	N(2)-C(3)-C(4)-C(5)	1.1(4)
N(6)-C(3)-C(4)-C(5)	176.1(3)	N(2)-C(3)-C(4)-N(9)	-177.8(3)
N(6)-C(3)-C(4)-N(9)	-2.9(6)	N(2)-N(1)-C(5)-C(4)	-0.1(4)
N(2)-N(1)-C(5)-N(12)	179.9(3)	C(3)-C(4)-C(5)-N(1)	-0.6(4)
N(9)-C(4)-C(5)-N(1)	178.4(3)	C(3)-C(4)-C(5)-N(12)	179.4(3)
N(9)-C(4)-C(5)-N(12)	-1.7(6)	N(2)-C(3)-N(6)-O(8)	170.9(3)
C(4)-C(3)-N(6)-O(8)	-3.7(5)	N(2)-C(3)-N(6)-O(7)	-7.5(5)
C(4)-C(3)-N(6)-O(7)	177.9(3)	C(5)-C(4)-N(9)-O(10)	108.1(4)
C(3)-C(4)-N(9)-O(10)	-73.2(5)	C(5)-C(4)-N(9)-O(11)	-71.5(5)
C(3)-C(4)-N(9)-O(11)	107.1(4)	N(1)-C(5)-N(12)-O(13)	176.2(3)
C(4)-C(5)-N(12)-O(13)	-3.8(5)	N(1)-C(5)-N(12)-O(14)	-4.7(5)
C(4)-C(5)-N(12)-O(14)	175.3(3)	C(22)-N(15)-N(16)-C(17)	-176.7(4)
C(19)-N(15)-N(16)-C(17)	-1.1(4)	N(15)-N(16)-C(17)-N(23)	-176.6(3)
N(15)-N(16)-C(17)-N(18)	1.5(4)	N(16)-C(17)-N(18)-C(19)	-1.3(4)
N(23)-C(17)-N(18)-C(19)	176.9(3)	N(16)-C(17)-N(18)-N(24)	-172.8(3)
N(23)-C(17)-N(18)-N(24)	5.4(5)	C(22)-N(15)-C(19)-N(20)	-1.9(4)
N(16)-N(15)-C(19)-N(20)	-178.8(3)	C(22)-N(15)-C(19)-N(18)	177.4(3)
N(16)-N(15)-C(19)-N(18)	0.4(4)	C(17)-N(18)-C(19)-N(20)	179.3(5)
N(24)-N(18)-C(19)-N(20)	-9.9(7)	C(17)-N(18)-C(19)-N(15)	0.5(4)
N(24)-N(18)-C(19)-N(15)	171.2(3)	N(15)-C(19)-N(20)-N(21)	1.3(4)
N(18)-C(19)-N(20)-N(21)	-177.5(5)	C(19)-N(20)-N(21)-C(22)	-0.3(4)
N(20)-N(21)-C(22)-N(25)	176.2(4)	N(20)-N(21)-C(22)-N(15)	-0.8(4)
C(19)-N(15)-C(22)-N(25)	-175.5(4)	N(16)-N(15)-C(22)-N(25)	0.2(7)
C(19)-N(15)-C(22)-N(21)	1.5(4)	N(16)-N(15)-C(22)-N(21)	177.2(4)

Table S19. Hydrogen bonds for 13 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(21)-H(21)...N(1)#1	0.88	2.01	2.816(4)	151.0
N(23)-H(23A)...O(11)#2	0.98(4)	2.23(4)	3.206(4)	173(3)
N(23)-H(23B)...O(10)#3	0.81(4)	2.34(4)	3.064(4)	150(4)
N(24)-H(24A)...O(10)#4	0.88(4)	2.58(4)	3.173(4)	125(3)
N(24)-H(24B)...O(7)#5	0.79(4)	2.58(4)	3.199(5)	137(4)
N(25)-H(25A)...N(2)#6	0.89(4)	2.21(4)	2.996(4)	147(3)
N(25)-H(25B)...N(20)#7	0.78(4)	2.36(4)	3.090(4)	156(4)

Symmetry transformations used to generate equivalent atoms:
#1 -x-1,-y,-z+1 #2 -x-1,-y+1,-z #3 -x,-y+1,-z
#4 x,y-1,z #5 x-1,y,z #6 -x,-y,-z+1 #7 x+1,y,z