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Electronic Supplementary Information

Asymmetric N,N'-Ethylene-Bridged Azole-Based Compounds: Two Way Control of the Energetic Properties of Compounds

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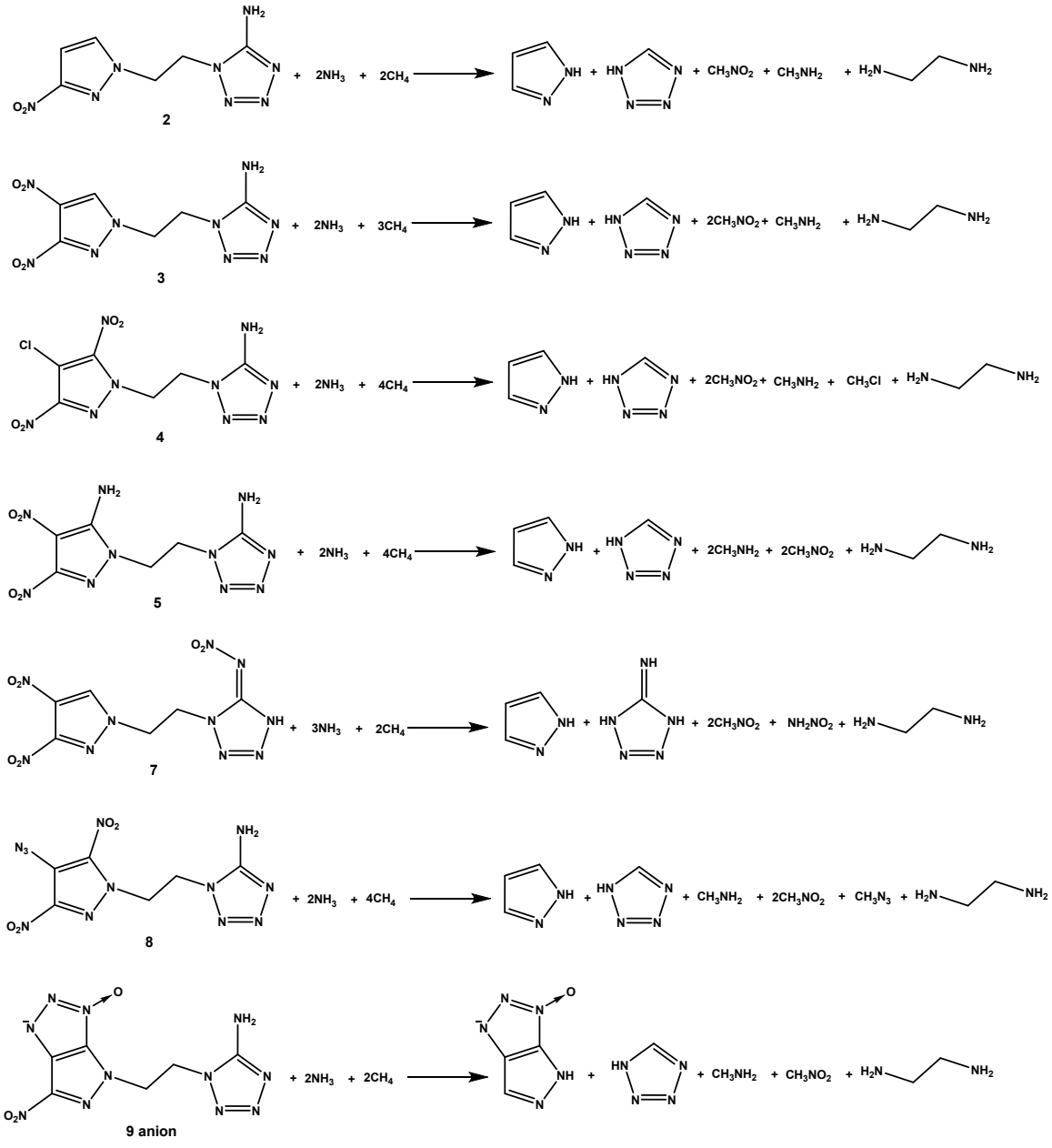
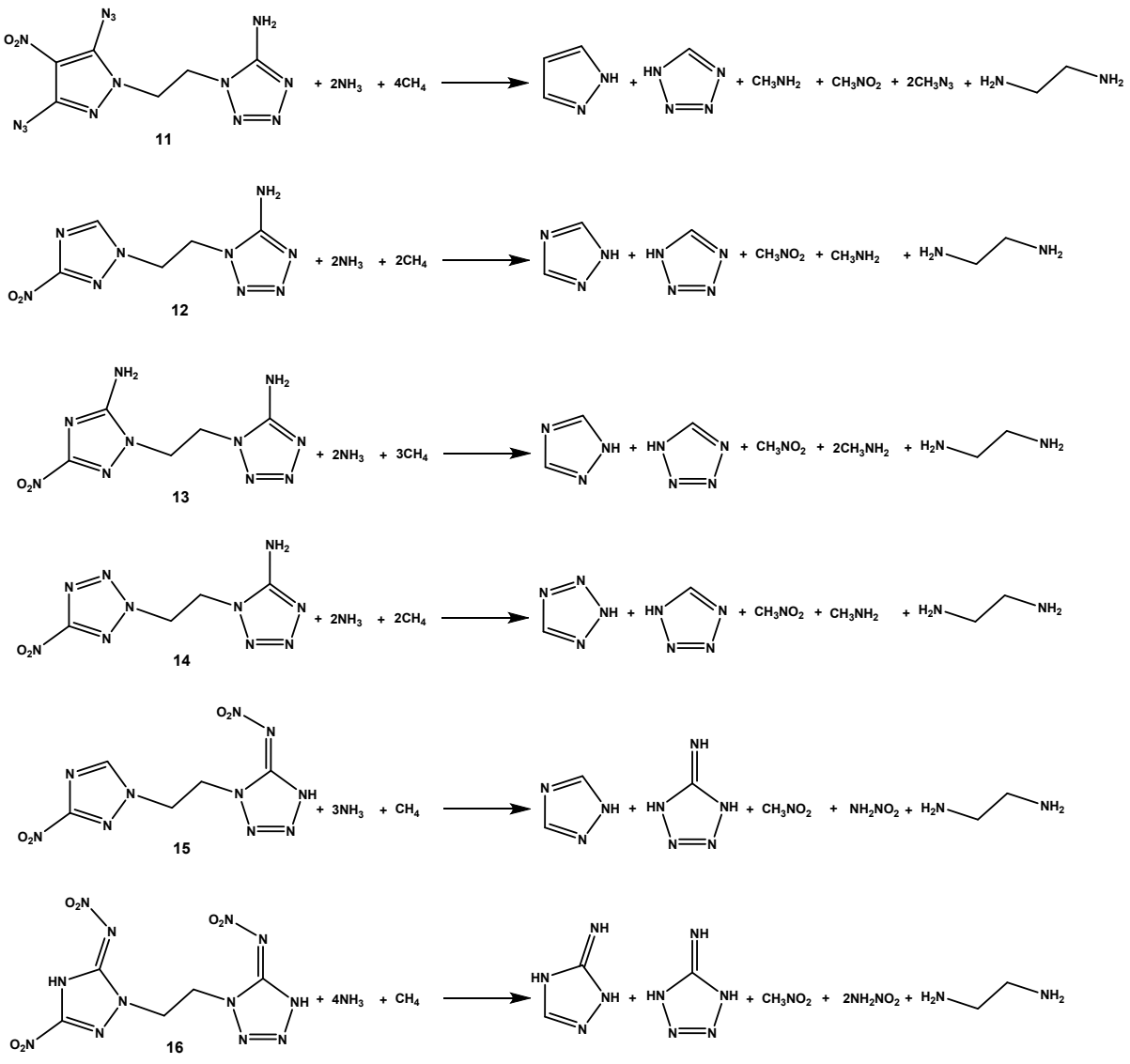
1. Isodesmic Reactions



Scheme S1: Isodesmic reactions for the compounds **2 - 9**



Scheme S2: Isodesmic reactions for the compounds **11 - 16**

3. Crystal Structure Data

Table S1. Crystal data and structure refinement for compound **4**.

Identification code	shrv364	
Empirical formula	$C_6H_6ClN_9O_4$	
Formula weight	303.65	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 18.302(7) Å	α= 90°
	b = 5.631(2) Å	β= 97.094(10)°
	c = 11.142(4) Å	γ = 90°
Volume	1139.5(7) $Å^3$	
Z	4	
Density (-123 °C)	1.770 Mg/m^3	
Density (20 °C)	1.713 Mg/m^3	
Absorption coefficient	0.371 mm^{-1}	
F(000)	616	
Crystal size	0.213 x 0.041 x 0.005 mm^3	
Theta range for data collection	1.842 to 27.377°.	
Index ranges	-23<=h<=23, -6<=k<=7, -14<=l<=14	
Reflections collected	7893	
Independent reflections	2537 [$R_{(int)}$ = 0.0630]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.5751	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2537 / 0 / 188	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R_1 = 0.0751, wR_2 = 0.2088	
R indices (all data)	R_1 = 0.1000, wR_2 = 0.2396	
Largest diff. peak and hole	0.664 and -0.499 $e.Å^{-3}$	
CCDC	1474898	

Table S2. Bond lengths [Å] and angles [°] for compound **4**.

N(1)-C(2)	1.344(7)	N(1)-H(1A)	0.86(9)
N(1)-H(1B)	0.80(9)	C(2)-N(3)	1.319(6)
C(2)-N(6)	1.349(7)	N(3)-N(4)	1.357(7)
N(4)-N(5)	1.292(7)	N(5)-N(6)	1.368(6)
N(6)-C(7)	1.457(7)	C(7)-C(8)	1.525(8)
C(7)-H(7A)	0.9900	C(7)-H(7B)	0.9900

C(8)-N(9)	1.466(7)	C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900	N(9)-N(10)	1.332(6)
N(9)-C(17)	1.354(7)	N(10)-C(11)	1.334(7)
C(11)-C(15)	1.396(8)	C(11)-N(12)	1.441(7)
N(12)-O(14)	1.224(7)	N(12)-O(13)	1.225(7)
C(15)-C(17)	1.381(8)	C(15)-Cl(16)	1.685(6)
C(17)-N(18)	1.447(7)	N(18)-O(19)	1.209(7)
N(18)-O(20)	1.226(7)		

C(2)-N(1)-H(1A)	113(5)	C(2)-N(1)-H(1B)	122(6)
H(1A)-N(1)-H(1B)	114(8)	N(3)-C(2)-N(1)	126.6(6)
N(3)-C(2)-N(6)	108.2(5)	N(1)-C(2)-N(6)	125.2(5)
C(2)-N(3)-N(4)	106.4(5)	N(5)-N(4)-N(3)	111.3(4)
N(4)-N(5)-N(6)	105.9(5)	C(2)-N(6)-N(5)	108.2(4)
C(2)-N(6)-C(7)	130.9(5)	N(5)-N(6)-C(7)	120.8(5)
N(6)-C(7)-C(8)	112.7(5)	N(6)-C(7)-H(7A)	109.0
C(8)-C(7)-H(7A)	109.0	N(6)-C(7)-H(7B)	109.0
C(8)-C(7)-H(7B)	109.0	H(7A)-C(7)-H(7B)	107.8
N(9)-C(8)-C(7)	112.3(4)	N(9)-C(8)-H(8A)	109.2
C(7)-C(8)-H(8A)	109.2	N(9)-C(8)-H(8B)	109.2
C(7)-C(8)-H(8B)	109.2	H(8A)-C(8)-H(8B)	107.9
N(10)-N(9)-C(17)	111.4(4)	N(10)-N(9)-C(8)	116.8(4)
C(17)-N(9)-C(8)	131.7(5)	N(9)-N(10)-C(11)	104.5(4)
N(10)-C(11)-C(15)	113.4(5)	N(10)-C(11)-N(12)	117.4(5)
C(15)-C(11)-N(12)	129.2(5)	O(14)-N(12)-O(13)	125.0(5)
O(14)-N(12)-C(11)	117.5(5)	O(13)-N(12)-C(11)	117.4(5)
C(17)-C(15)-C(11)	102.1(5)	C(17)-C(15)-Cl(16)	129.4(5)
C(11)-C(15)-Cl(16)	128.5(4)	N(9)-C(17)-C(15)	108.6(5)
N(9)-C(17)-N(18)	122.9(5)	C(15)-C(17)-N(18)	128.4(5)
O(19)-N(18)-O(20)	125.8(5)	O(19)-N(18)-C(17)	117.1(5)
O(20)-N(18)-C(17)	117.1(5)		

Table S3. Hydrogen bonds for compound **4** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...N(3)#1	0.86(9)	2.22(9)	3.053(8)	162(7)
N(1)-H(1B)...N(4)#2	0.80(9)	2.17(9)	2.937(7)	163(8)
C(7)-H(7A)...O(20)	0.99	2.58	3.141(7)	116.0
C(8)-H(8A)...N(4)#2	0.99	2.63	3.394(7)	134.1
C(8)-H(8A)...O(20)#3	0.99	2.59	3.354(7)	134.0
C(8)-H(8B)...O(13)#2	0.99	2.45	3.128(7)	125.0

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

Table S4. Crystal data and structure refinement for compound **11**.

Identification code	shrv395	
Empirical formula	$C_6H_6N_{14}O_2$	
Formula weight	306.25	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 14.8551(19) Å	α= 90°
	b = 5.9407(7) Å	β= 105.001(9)°
	c = 28.617(3) Å	γ = 90°
Volume	2439.4(5) $Å^3$	
Z	8	
Density (-123 °C)	1.668 Mg/m^3	
Density (20 °C)	1.624 Mg/m^3	
Absorption coefficient	0.135 mm^{-1}	
F(000)	1248	
Crystal size	0.280 x 0.087 x 0.025 mm^3	
Theta range for data collection	2.839 to 30.627°.	
Index ranges	-18<=h<=20, -8<=k<=8, -38<=l<=39	
Reflections collected	13809	
Independent reflections	3524 [$R_{(int)}$ = 0.0782]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6580	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3524 / 0 / 205	
Goodness-of-fit on F^2	1.020	
Final R indices [I>2sigma(I)]	R_1 = 0.0631, wR_2 = 0.1467	
R indices (all data)	R_1 = 0.1369, wR_2 = 0.1752	
Largest diff. peak and hole	0.594 and -0.328 e.$Å^{-3}$	
CCDC	1474901	

Table S5. Bond lengths [Å] and angles [°] for compound **11**.

N(1)-C(2)	1.343(3)	N(1)-H(1A)	0.85(3)
N(1)-H(1B)	0.81(3)	C(2)-N(3)	1.332(3)
C(2)-N(6)	1.344(3)	N(3)-N(4)	1.361(3)
N(4)-N(5)	1.283(3)	N(5)-N(6)	1.368(3)
N(6)-C(7)	1.459(3)	C(7)-C(8)	1.523(3)
C(7)-H(7A)	0.9900	C(7)-H(7B)	0.9900

C(8)-N(9)	1.456(3)	C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900	N(9)-C(19)	1.341(3)
N(9)-N(10)	1.376(3)	N(10)-C(11)	1.327(3)
C(11)-N(12)	1.400(3)	C(11)-C(15)	1.411(4)
N(12)-N(13)	1.263(3)	N(13)-N(14)	1.123(3)
C(15)-N(16)	1.413(3)	C(15)-C(19)	1.417(4)
N(16)-O(17)	1.229(3)	N(16)-O(18)	1.247(3)
C(19)-N(20)	1.363(3)	N(20)-N(21)	1.257(3)
N(21)-N(22)	1.120(3)		
C(2)-N(1)-H(1A)	116(2)	C(2)-N(1)-H(1B)	117(2)
H(1A)-N(1)-H(1B)	120(3)	N(3)-C(2)-N(1)	125.8(2)
N(3)-C(2)-N(6)	108.5(2)	N(1)-C(2)-N(6)	125.6(2)
C(2)-N(3)-N(4)	105.2(2)	N(5)-N(4)-N(3)	112.26(19)
N(4)-N(5)-N(6)	105.81(19)	C(2)-N(6)-N(5)	108.23(19)
C(2)-N(6)-C(7)	132.2(2)	N(5)-N(6)-C(7)	119.39(19)
N(6)-C(7)-C(8)	112.38(19)	N(6)-C(7)-H(7A)	109.1
C(8)-C(7)-H(7A)	109.1	N(6)-C(7)-H(7B)	109.1
C(8)-C(7)-H(7B)	109.1	H(7A)-C(7)-H(7B)	107.9
N(9)-C(8)-C(7)	112.26(19)	N(9)-C(8)-H(8A)	109.2
C(7)-C(8)-H(8A)	109.2	N(9)-C(8)-H(8B)	109.2
C(7)-C(8)-H(8B)	109.2	H(8A)-C(8)-H(8B)	107.9
C(19)-N(9)-N(10)	113.0(2)	C(19)-N(9)-C(8)	128.8(2)
N(10)-N(9)-C(8)	118.14(19)	C(11)-N(10)-N(9)	105.2(2)
N(10)-C(11)-N(12)	121.3(2)	N(10)-C(11)-C(15)	111.1(2)
N(12)-C(11)-C(15)	127.5(2)	N(13)-N(12)-C(11)	111.1(2)
N(14)-N(13)-N(12)	173.1(3)	C(11)-C(15)-N(16)	128.0(2)
C(11)-C(15)-C(19)	105.2(2)	N(16)-C(15)-C(19)	126.8(2)
O(17)-N(16)-O(18)	123.8(2)	O(17)-N(16)-C(15)	118.9(2)
O(18)-N(16)-C(15)	117.3(2)	N(9)-C(19)-N(20)	116.4(2)
N(9)-C(19)-C(15)	105.5(2)	N(20)-C(19)-C(15)	137.8(2)
N(21)-N(20)-C(19)	119.7(2)	N(22)-N(21)-N(20)	168.2(3)

Table S6. Hydrogen bonds for compound **11** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(8)-H(8B)...O(17)#1	0.99	2.57	3.526(3)	161.5
N(1)-H(1A)...N(3)#2	0.85(3)	2.17(3)	3.010(3)	175(3)
N(1)-H(1B)...N(4)#3	0.81(3)	2.16(3)	2.954(3)	166(3)

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

Table S7. Crystal data and structure refinement for compound **14**.

Identification code	shrv388	
Empirical formula	$C_4 H_6 N_{10} O_2$	
Formula weight	226.19	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P 2_1/c$	
Unit cell dimensions	a = 10.042(8) Å	α= 90°.
	b = 6.453(5) Å	β= 99.147(11)°.
	c = 27.04(2) Å	γ = 90°.
Volume	1730(2) $Å^3$	
Z	8	
Density (-123°C)	1.737 Mg/m^3	
Density (20°C)	1.704 Mg/m^3	
Absorption coefficient	0.144 mm^{-1}	
F(000)	928	
Crystal size	0.400 x 0.104 x 0.024 mm^3	
Theta range for data collection	5.416 to 25.341°.	
Index ranges	-12<=h<=11, -7<=k<=7, -32<=l<=32	
Reflections collected	10025	
Independent reflections	3183 [R_{int} = 0.0871]	
Completeness to theta = 25.242°	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.5848	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3183 / 0 / 290	
Goodness-of-fit on F^2	1.143	
Final R indices [I>2sigma(I)]	R_1 = 0.0933, wR_2 = 0.2689	
R indices (all data)	R_1 = 0.1221, wR_2 = 0.2974	
Largest diff. peak and hole	0.498 and -0.518 $e.Å^{-3}$	
CCDC	1474900	

Table S8. Bond lengths [Å] and angles [°] for compound **14**.

O(1A)-N(3A)	1.224(9)	O(2A)-N(3A)	1.222(9)
N(3A)-C(4A)	1.430(10)	C(4A)-N(5A)	1.324(10)
C(4A)-N(8A)	1.332(10)	N(5A)-N(6A)	1.322(10)
N(6A)-N(7A)	1.328(9)	N(7A)-N(8A)	1.313(9)
N(7A)-C(9A)	1.461(10)	C(9A)-C(10A)	1.495(10)
C(9A)-H(8A)	0.9900	C(9A)-H(9A)	0.9900
C(10A)-N(11A)	1.467(10)	C(10A)-H(11A)	0.9900
C(10A)-H(10A)	0.9900	N(11A)-C(15A)	1.318(10)
N(11A)-N(12A)	1.341(9)	N(12A)-N(13A)	1.306(10)
N(13A)-N(14A)	1.352(10)	N(14A)-C(15A)	1.300(10)
C(15A)-N(16A)	1.365(10)	N(16A)-H(16A)	0.8800
N(16A)-H(17A)	0.8800	O(1B)-N(3B)	1.219(9)
O(2B)-N(3B)	1.228(9)	N(3B)-C(4B)	1.436(10)
C(4B)-N(8B)	1.316(10)	C(4B)-N(5B)	1.321(10)
N(5B)-N(6B)	1.315(10)	N(6B)-N(7B)	1.324(9)
N(7B)-N(8B)	1.331(8)	N(7B)-C(9B)	1.445(9)
C(9B)-C(10C)	1.502(11)	C(9B)-H(8B)	0.9900
C(9B)-H(9B)	0.9900	C(10C)-N(11B)	1.486(10)
C(10C)-H(11B)	0.9900	C(10C)-H(10B)	0.9900
N(11B)-C(15B)	1.304(10)	N(11B)-N(12B)	1.366(9)
N(12B)-N(13B)	1.286(9)	N(13B)-N(14B)	1.349(9)
N(14B)-C(15B)	1.317(10)	C(15B)-N(16B)	1.352(9)
N(16B)-H(16B)	0.8800	N(16B)-H(17B)	0.8800

O(2A)-N(3A)-O(1A)	125.1(7)	O(2A)-N(3A)-C(4A)	117.6(6)
O(1A)-N(3A)-C(4A)	117.3(7)	N(5A)-C(4A)-N(8A)	115.6(7)
N(5A)-C(4A)-N(3A)	122.9(7)	N(8A)-C(4A)-N(3A)	121.5(7)
N(6A)-N(5A)-C(4A)	104.5(6)	N(5A)-N(6A)-N(7A)	105.5(6)
N(8A)-N(7A)-N(6A)	115.4(6)	N(8A)-N(7A)-C(9A)	121.3(6)
N(6A)-N(7A)-C(9A)	123.3(6)	N(7A)-N(8A)-C(4A)	98.9(6)
N(7A)-C(9A)-C(10A)	112.5(6)	N(7A)-C(9A)-H(8A)	109.1
C(10A)-C(9A)-H(8A)	109.1	N(7A)-C(9A)-H(9A)	109.1
C(10A)-C(9A)-H(9A)	109.1	H(8A)-C(9A)-H(9A)	107.8
N(11A)-C(10A)-C(9A)	113.3(6)	N(11A)-C(10A)-H(11A)	108.9
C(9A)-C(10A)-H(11A)	108.9	N(11A)-C(10A)-H(10A)	108.9
C(9A)-C(10A)-H(10A)	108.9	H(11A)-C(10A)-H(10A)	107.7
C(15A)-N(11A)-N(12A)	108.6(6)	C(15A)-N(11A)-C(10A)	130.5(7)
N(12A)-N(11A)-C(10A)	119.4(7)	N(13A)-N(12A)-N(11A)	105.6(7)
N(12A)-N(13A)-N(14A)	110.5(7)	C(15A)-N(14A)-N(13A)	105.7(6)
N(14A)-C(15A)-N(11A)	109.6(6)	N(14A)-C(15A)-N(16A)	126.1(7)
N(11A)-C(15A)-N(16A)	124.3(7)	C(15A)-N(16A)-H(16A)	120.0

C(15A)-N(16A)-H(17A)	120.0	H(16A)-N(16A)-H(17A)	120.0
O(1B)-N(3B)-O(2B)	125.3(7)	O(1B)-N(3B)-C(4B)	117.8(6)
O(2B)-N(3B)-C(4B)	116.8(7)	N(8B)-C(4B)-N(5B)	115.7(7)
N(8B)-C(4B)-N(3B)	121.5(7)	N(5B)-C(4B)-N(3B)	122.7(7)
N(6B)-N(5B)-C(4B)	104.6(6)	N(5B)-N(6B)-N(7B)	106.4(6)
N(6B)-N(7B)-N(8B)	113.8(6)	N(6B)-N(7B)-C(9B)	124.2(6)
N(8B)-N(7B)-C(9B)	121.7(6)	C(4B)-N(8B)-N(7B)	99.5(6)
N(7B)-C(9B)-C(10C)	114.1(6)	N(7B)-C(9B)-H(8B)	108.7
C(10C)-C(9B)-H(8B)	108.7	N(7B)-C(9B)-H(9B)	108.7
C(10C)-C(9B)-H(9B)	108.7	H(8B)-C(9B)-H(9B)	107.6
N(11B)-C(10C)-C(9B)	112.3(6)	N(11B)-C(10C)-H(11B)	109.2
C(9B)-C(10C)-H(11B)	109.2	N(11B)-C(10C)-H(10B)	109.2
C(9B)-C(10C)-H(10B)	109.2	H(11B)-C(10C)-H(10B)	107.9
C(15B)-N(11B)-N(12B)	109.4(6)	C(15B)-N(11B)-C(10C)	128.7(6)
N(12B)-N(11B)-C(10C)	121.8(6)	N(13B)-N(12B)-N(11B)	104.3(6)
N(12B)-N(13B)-N(14B)	112.1(6)	C(15B)-N(14B)-N(13B)	105.1(6)
N(11B)-C(15B)-N(14B)	108.9(6)	N(11B)-C(15B)-N(16B)	125.6(7)
N(14B)-C(15B)-N(16B)	125.2(7)	C(15B)-N(16B)-H(16B)	120.0
C(15B)-N(16B)-H(17B)	120.0	H(16B)-N(16B)-H(17B)	120.0

Table S9. Hydrogen bonds for compound **14** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(16A)-H(16A)...N(14B)#1	0.88	2.14	2.994(9)	164.0
N(16A)-H(17A)...N(13B)	0.88	2.06	2.913(9)	163.1
N(16B)-H(16B)...N(13A)#2	0.88	2.13	2.926(10)	150.6
N(16B)-H(17B)...N(14A)#1	0.88	2.26	3.094(10)	159.2

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

Table S10. Crystal data and structure refinement for compound **15**.

Identification code	shrv389	
Empirical formula	$C_5H_6N_{10}O_4$	
Formula weight	270.20	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 7.9667(5) Å	α= 90°
	b = 12.8656(9) Å	β= 108.131(2)°
	c = 10.6222(7) Å	γ = 90°
Volume	1034.68(12) $Å^3$	
Z	4	
Density (-123 °C)	1.735 Mg/m^3	
Density (20 °C)	1.693 Mg/m^3	
Absorption coefficient	0.150 mm^{-1}	
F(000)	552	
Crystal size	0.200 x 0.168 x 0.034 mm^3	
Theta range for data collection	2.565 to 30.560°.	
Index ranges	-9<=h<=11, -17<=k<=18, -14<=l<=15	
Reflections collected	12230	
Independent reflections	2995 [$R_{(int)}$ = 0.0325]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6842	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2995 / 0 / 175	
Goodness-of-fit on F^2	1.018	
Final R indices [I>2sigma(I)]	R_1 = 0.0370, wR_2 = 0.0812	
R indices (all data)	R_1 = 0.0595, wR_2 = 0.0903	
Largest diff. peak and hole	0.323 and -0.247 $e.Å^{-3}$	
CCDC	1474899	

Table S11. Bond lengths [Å] and angles [°] for compound **15**.

O(1)-N(3)	1.2432(14)	O(2)-N(3)	1.2384(14)
N(3)-N(4)	1.3565(15)	N(4)-C(5)	1.3336(16)
C(5)-N(6)	1.3438(16)	C(5)-N(9)	1.3566(16)
N(6)-N(7)	1.3639(16)	N(6)-H(6)	0.861(18)
N(7)-N(8)	1.2750(16)	N(8)-N(9)	1.3615(15)
N(9)-C(10)	1.4620(16)	C(10)-C(11)	1.5230(17)

C(10)-H(10A)	0.9900	C(10)-H(10B)	0.9900
C(11)-N(12)	1.4596(16)	C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900	N(12)-C(16)	1.3376(16)
N(12)-N(13)	1.3539(14)	N(13)-C(14)	1.3096(16)
C(14)-N(15)	1.3403(16)	C(14)-N(17)	1.4473(16)
N(15)-C(16)	1.3261(16)	C(16)-H(16)	0.9500
N(17)-O(18)	1.2256(14)	N(17)-O(19)	1.2260(14)
O(2)-N(3)-O(1)	122.43(11)	O(2)-N(3)-N(4)	115.66(11)
O(1)-N(3)-N(4)	121.90(11)	C(5)-N(4)-N(3)	115.34(10)
N(4)-C(5)-N(6)	136.95(12)	N(4)-C(5)-N(9)	119.56(11)
N(6)-C(5)-N(9)	103.47(11)	C(5)-N(6)-N(7)	110.29(11)
C(5)-N(6)-H(6)	129.0(11)	N(7)-N(6)-H(6)	120.6(11)
N(8)-N(7)-N(6)	108.16(11)	N(7)-N(8)-N(9)	107.98(11)
C(5)-N(9)-N(8)	110.09(10)	C(5)-N(9)-C(10)	129.26(11)
N(8)-N(9)-C(10)	120.03(10)	N(9)-C(10)-C(11)	113.26(10)
N(9)-C(10)-H(10A)	108.9	C(11)-C(10)-H(10A)	108.9
N(9)-C(10)-H(10B)	108.9	C(11)-C(10)-H(10B)	108.9
H(10A)-C(10)-H(10B)	107.7	N(12)-C(11)-C(10)	111.16(10)
N(12)-C(11)-H(11A)	109.4	C(10)-C(11)-H(11A)	109.4
N(12)-C(11)-H(11B)	109.4	C(10)-C(11)-H(11B)	109.4
H(11A)-C(11)-H(11B)	108.0	C(16)-N(12)-N(13)	110.67(10)
C(16)-N(12)-C(11)	129.20(11)	N(13)-N(12)-C(11)	119.89(10)
C(14)-N(13)-N(12)	100.32(10)	N(13)-C(14)-N(15)	117.78(11)
N(13)-C(14)-N(17)	120.71(11)	N(15)-C(14)-N(17)	121.48(11)
C(16)-N(15)-C(14)	101.24(10)	N(15)-C(16)-N(12)	109.98(11)
N(15)-C(16)-H(16)	125.0	N(12)-C(16)-H(16)	125.0
O(18)-N(17)-O(19)	125.14(11)	O(18)-N(17)-C(14)	117.63(11)
O(19)-N(17)-C(14)	117.22(11)		

Table S12. Hydrogen bonds for compound **15** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(10)-H(10A)...O(1)#1	0.99	2.57	3.4866(16)	153.7
C(10)-H(10B)...O(1)#2	0.99	2.43	3.2289(16)	137.0
C(11)-H(11A)...O(19)#3	0.99	2.43	2.9544(16)	112.6
C(16)-H(16)...N(13)#4	0.95	2.62	3.4664(16)	149.4
N(6)-H(6)...N(15)#5	0.861(18)	1.978(18)	2.8142(16)	163.2(15)

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