Electronic Supplementary Information

Highly Energetic Furazan-triazole Hybrid with Dinitromethyl and Nitramino Groups: Decreasing Sensitivity via Formation of a Planar Anion

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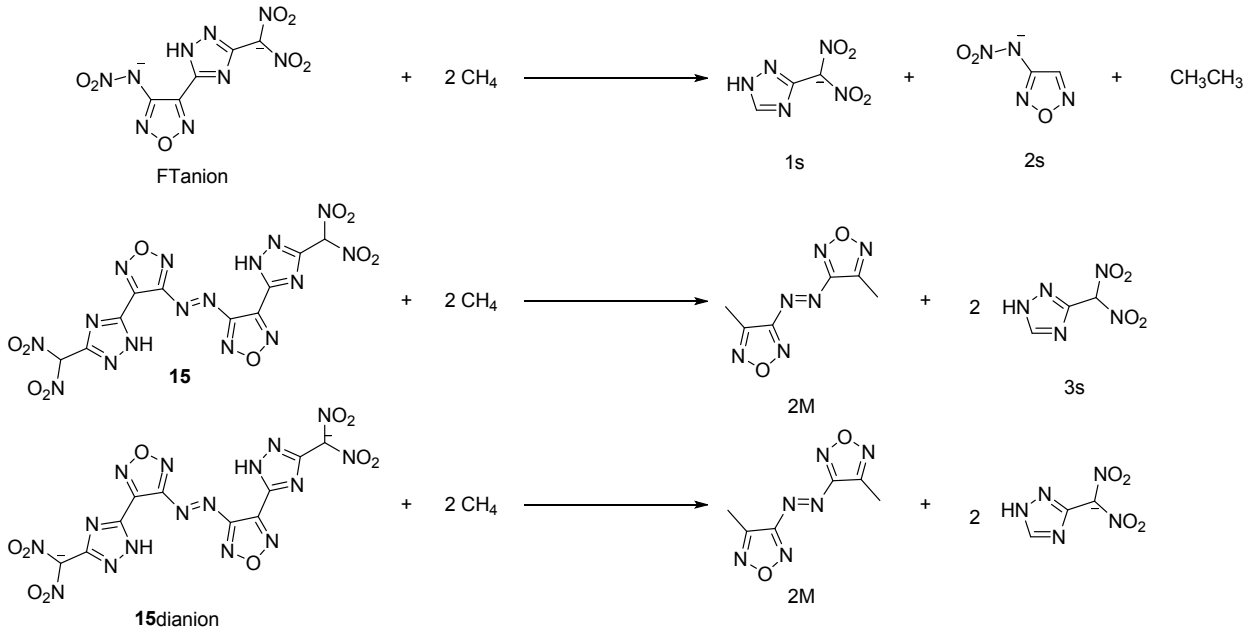
Computational Methods: The gas phase enthalpies of formation were calculated based on isodesmic reactions (Scheme S1). The enthalpy of reaction is obtained by combining the MP2/6–311++G** energy difference for the reactions, the scaled zero point energies (ZPE), values of thermal correction (HT), and other thermal factors. The solid state heats of formation were calculated with Trouton's rule according to equation 1 (*T* represents either the melting point or the decomposition temperature when no melting occurs prior to decomposition).[1]

$$\Delta H_{sub} = 188 / Jmol^{-1}K^{-1} \times T \quad (1)$$

For energetic salts, the solid-phase enthalpy of formation is obtained using a Born−Haber energy cycle.[2] For the compound which is a hydrate (**14·2H$_2$O**), the solid-phase enthalpy of formation is obtained by adding the gas phase heat of formation of anhydrous compound to that of water (-241.8 kJ mol^{-1}).[3]



Scheme S1. Isodesmic reaction for FTanion, **15** and **15**dianion

Crystal Structure Analysis

Table S1. Crystal data and structure refinement for **5**

Identification code	**5**
CCDC number	1891124
Empirical formula	$C_5H_9N_{11}O_{8.19}$
Formula weight	354.27
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1

Unit cell dimensions	a = 4.4903(5) Å	α = 78.415(3)°.
	b = 9.9764(10) Å	β = 82.415(3)°.
	c = 14.3321(14) Å	γ = 87.929(3)°.
Volume	623.42(11) Å^3	
Z	2	
Density (-123°C)	1.887 Mg/m^3	
Density (20°C)	1.863 Mg/m^3	
Absorption coefficient	0.175 mm^{-1}	
F(000)	363	
Crystal size	0.170 × 0.077 × 0.010 mm^3	
Theta range for data collection	2.773 to 25.431°.	
Index ranges	-5<=h<=5, -12<=k<=12, -17<=l<=17	
Reflections collected	5428	
Independent reflections	2271 [R_{int} = 0.0480]	
Completeness to theta = 25.242°	98.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7452 and 0.6485	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2271 / 12 / 257	
Goodness-of-fit on F^2	1.026	
Final R indices [I>2sigma(I)]	R_1 = 0.0559, wR_2 = 0.1219	
R indices (all data)	R_1 = 0.1128, wR_2 = 0.1414	
Largest diff. peak and hole	0.437 and -0.569 e.Å^{-3}	

Table S2. Bond lengths [Å] and angles [°] for **5**

O(1)-N(3)	1.247(3)	O(2)-N(3)	1.272(4)
N(3)-N(4)	1.309(4)	N(4)-C(5)	1.382(4)
C(5)-N(6)	1.314(4)	C(5)-C(9)	1.432(5)
N(6)-O(7)	1.391(4)	O(7)-N(8)	1.372(3)
N(8)-C(9)	1.305(4)	C(9)-C(10)	1.465(4)
C(10)-N(11)	1.323(4)	C(10)-N(14)	1.363(4)
N(11)-N(12)	1.349(3)	N(12)-C(13)	1.348(4)
N(12)-H(12)	0.8800	C(13)-N(14)	1.337(4)
C(13)-C(15)	1.455(4)	C(15)-N(16)	1.375(4)
C(15)-N(19)	1.410(4)	N(16)-O(18)	1.235(3)
N(16)-O(17)	1.269(3)	N(19)-O(21B)	1.19(3)
N(19)-O(21A)	1.235(5)	N(19)-O(20A)	1.246(5)
N(19)-O(20B)	1.25(3)	N(22A)-O(23)	1.54(2)
N(22A)-H(22E)	0.9100	N(22A)-H(22F)	0.9100
N(22A)-H(22G)	0.9100	O(23)-H(23)	0.821(9)
N(22B)-H(22A)	0.9099(11)	N(22B)-H(22B)	0.9099(11)
N(22B)-H(22C)	0.9100(11)	N(22B)-H(22D)	0.9100(11)
O(24)-N(25)	1.351(5)	O(24)-H(24)	0.821(9)
N(25)-H(25A)	0.9100	N(25)-H(25B)	0.9100
N(25)-H(25C)	0.9100		
O(1)-N(3)-O(2)	119.6(3)	O(1)-N(3)-N(4)	124.9(3)
O(2)-N(3)-N(4)	115.4(2)	N(3)-N(4)-C(5)	116.7(3)
N(6)-C(5)-N(4)	130.9(3)	N(6)-C(5)-C(9)	109.1(3)
N(4)-C(5)-C(9)	120.0(3)	C(5)-N(6)-O(7)	104.9(2)
N(8)-O(7)-N(6)	111.1(2)	C(9)-N(8)-O(7)	106.2(3)
N(8)-C(9)-C(5)	108.6(3)	N(8)-C(9)-C(10)	120.7(3)
C(5)-C(9)-C(10)	130.7(3)	N(11)-C(10)-N(14)	115.0(3)
N(11)-C(10)-C(9)	123.1(3)	N(14)-C(10)-C(9)	121.9(3)
C(10)-N(11)-N(12)	102.2(3)	C(13)-N(12)-N(11)	110.9(2)
C(13)-N(12)-H(12)	124.5	N(11)-N(12)-H(12)	124.5
N(14)-C(13)-N(12)	109.0(3)	N(14)-C(13)-C(15)	127.0(3)
N(12)-C(13)-C(15)	124.1(3)	C(13)-N(14)-C(10)	102.9(3)
N(16)-C(15)-N(19)	118.2(3)	N(16)-C(15)-C(13)	121.5(3)
N(19)-C(15)-C(13)	120.3(3)	O(18)-N(16)-O(17)	119.8(3)
O(18)-N(16)-C(15)	122.7(3)	O(17)-N(16)-C(15)	117.6(2)
O(21A)-N(19)-O(20A)	120.1(3)	O(21B)-N(19)-O(20B)	123(2)
O(21B)-N(19)-C(15)	115.4(16)	O(21A)-N(19)-C(15)	118.9(3)
O(20A)-N(19)-C(15)	121.0(3)	O(20B)-N(19)-C(15)	121.4(13)
O(23)-N(22A)-H(22E)	109.5	O(23)-N(22A)-H(22F)	109.5
H(22E)-N(22A)-H(22F)	109.5	O(23)-N(22A)-H(22G)	109.5
H(22E)-N(22A)-H(22G)	109.5	H(22F)-N(22A)-H(22G)	109.5
N(22A)-O(23)-H(23)	95.7(15)	H(22A)-N(22B)-H(22B)	109.49(18)
H(22A)-N(22B)-H(22C)	109.48(18)	H(22B)-N(22B)-H(22C)	128(2)
H(22A)-N(22B)-H(22D)	109.48(18)	H(22B)-N(22B)-H(22D)	89(3)
H(22C)-N(22B)-H(22D)	109.48(18)	N(25)-O(24)-H(24)	111.5(8)
O(24)-N(25)-H(25A)	109.5	O(24)-N(25)-H(25B)	109.5
H(25A)-N(25)-H(25B)	109.5	O(24)-N(25)-H(25C)	109.5
H(25A)-N(25)-H(25C)	109.5	H(25B)-N(25)-H(25C)	109.5

Table S3. Torsion angles [°] for **5**

O(1)-N(3)-N(4)-C(5)	-0.6(6)
O(2)-N(3)-N(4)-C(5)	178.0(3)
N(3)-N(4)-C(5)-N(6)	1.5(6)
N(3)-N(4)-C(5)-C(9)	-177.8(4)
N(4)-C(5)-N(6)-O(7)	-178.7(4)
C(9)-C(5)-N(6)-O(7)	0.7(4)
C(5)-N(6)-O(7)-N(8)	-0.2(4)
N(6)-O(7)-N(8)-C(9)	-0.4(4)
O(7)-N(8)-C(9)-C(5)	0.9(4)
O(7)-N(8)-C(9)-C(10)	-178.2(3)
N(6)-C(5)-C(9)-N(8)	-1.1(5)
N(4)-C(5)-C(9)-N(8)	178.4(3)
N(6)-C(5)-C(9)-C(10)	177.8(4)
N(4)-C(5)-C(9)-C(10)	-2.7(7)
N(8)-C(9)-C(10)-N(11)	-179.4(4)
C(5)-C(9)-C(10)-N(11)	1.8(6)
N(8)-C(9)-C(10)-N(14)	1.4(6)
C(5)-C(9)-C(10)-N(14)	-177.4(4)
N(14)-C(10)-N(11)-N(12)	0.3(4)
C(9)-C(10)-N(11)-N(12)	-179.0(3)
C(10)-N(11)-N(12)-C(13)	-0.4(4)
N(11)-N(12)-C(13)-N(14)	0.3(4)
N(11)-N(12)-C(13)-C(15)	-177.9(3)
N(12)-C(13)-N(14)-C(10)	-0.2(4)
C(15)-C(13)-N(14)-C(10)	178.0(4)
N(11)-C(10)-N(14)-C(13)	-0.1(4)
C(9)-C(10)-N(14)-C(13)	179.2(3)
N(14)-C(13)-C(15)-N(16)	179.6(3)
N(12)-C(13)-C(15)-N(16)	-2.5(6)
N(14)-C(13)-C(15)-N(19)	-1.7(6)
N(12)-C(13)-C(15)-N(19)	176.2(3)
N(19)-C(15)-N(16)-O(18)	-0.7(5)
C(13)-C(15)-N(16)-O(18)	178.0(4)
N(19)-C(15)-N(16)-O(17)	179.3(3)
C(13)-C(15)-N(16)-O(17)	-2.0(5)
N(16)-C(15)-N(19)-O(21B)	-152(2)
C(13)-C(15)-N(19)-O(21B)	29(2)
N(16)-C(15)-N(19)-O(21A)	176.1(6)
C(13)-C(15)-N(19)-O(21A)	-2.6(7)
N(16)-C(15)-N(19)-O(20A)	-3.3(8)
C(13)-C(15)-N(19)-O(20A)	178.0(7)
N(16)-C(15)-N(19)-O(20B)	36(3)
C(13)-C(15)-N(19)-O(20B)	-143(3)

Table S4. Hydrogen bonds for **5** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(12)-H(12)...O(17)	0.88	1.98	2.550(3)	120.8
N(12)-H(12)...O(17)#1	0.88	2.23	3.073(3)	159.0
N(22A)-H(22E)...N(11)#2	0.91	2.24	2.956(10)	135.0
N(22A)-H(22F)...O(20A)#3	0.91	2.23	2.956(13)	135.9
N(22A)-H(22G)...O(18)#4	0.91	1.98	2.706(7)	135.9
N(22B)-H(22A)...O(2)#2	0.9099(11)	2.051(13)	2.853(5)	146.3(18)
N(22B)-H(22B)...O(18)#4	0.9099(11)	2.000(10)	2.877(5)	161(2)
N(22B)-H(22C)...O(18)#5	0.9100(11)	2.388(17)	3.088(5)	133.8(17)
N(22B)-H(22D)...N(11)#2	0.9100(11)	2.191(11)	3.038(5)	155(2)
O(24)-H(24)...O(2)#6	0.821(9)	2.430(14)	3.034(6)	131.2(9)
N(25)-H(25A)...N(14)	0.91	2.05	2.943(4)	167.8
N(25)-H(25A)...O(21A)	0.91	2.28	2.800(5)	115.6
N(25)-H(25A)...O(21B)	0.91	2.23	2.73(3)	114.1
N(25)-H(25B)...O(1)#7	0.91	2.34	2.877(4)	117.5
N(25)-H(25B)...N(6)#7	0.91	2.16	3.030(4)	158.8
N(25)-H(25C)...O(1)#8	0.91	2.17	2.876(4)	133.5
N(25)-H(25C)...O(2)#6	0.91	2.39	3.046(4)	128.8

Symmetry transformations used to generate equivalent atoms:
#1 -x-1,-y+1,-z+1 #2 x+1,y,z #3 x+1,y-1,z
#4 -x,-y+1,-z+1 #5 -x+1,-y+1,-z+1 #6 x+1,y+1,z
#7 -x+1,-y+1,-z #8 x,y+1,z

Table S5. Crystal data and structure refinement for **15**

Identification code	**15**	
CCDC number	1891126	
Empirical formula	$C_{10}H_4N_{16}O_{10}$, 0.25 CH_3CN	
Formula weight	518.56	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 21.7441(5) Å	α = 90°.
	b = 9.4048(2) Å	β = 104.7490(10)°.
	c = 39.3917(9) Å	γ = 90°.
Volume	7790.1(3) $Å^3$	
Z	16	
Density (-123°C)	1.769 Mg/m^3	
Density (20°C)	1.731 Mg/m^3	
Absorption coefficient	0.158 mm^{-1}	
F(000)	4184	
Crystal size	0.340 × 0.212 × 0.106 mm^3	
Theta range for data collection	0.980 to 29.998°.	
Index ranges	-28<=h<=29, -12<=k<=12, -55<=l<=55	

Reflections collected	90206
Independent reflections	22003 [R_{int} = 0.0477]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7460 and 0.6936
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	22003 / 49 / 1390
Goodness-of-fit on F^2	1.016
Final R indices [I>2sigma(I)]	R_1 = 0.0552, wR_2 = 0.1341
R indices (all data)	R_1 = 0.1029, wR_2 = 0.1582
Largest diff. peak and hole	0.720 and -0.596 e.Å^{-3}

Table S6. Bond lengths [Å] and angles [°] for **15**

O(1)-N(3)	1.195(3)	O(2)-N(3)	1.215(3)
N(3)-C(4)	1.516(3)	C(4)-C(8)	1.481(3)
C(4)-N(5)	1.512(3)	C(4)-H(4)	1.0000
N(5)-O(6)	1.184(3)	N(5)-O(7)	1.202(3)
N(5)-O(6B)	1.455(12)	C(8)-N(9)	1.323(2)
C(8)-N(12)	1.352(2)	N(9)-N(10)	1.349(2)
N(10)-C(11)	1.333(2)	N(10)-H(10)	0.8800
C(11)-N(12)	1.334(2)	C(11)-C(13)	1.457(3)
C(13)-N(14)	1.308(2)	C(13)-C(17)	1.430(3)
N(14)-O(15)	1.375(2)	O(15)-N(16)	1.357(2)
N(16)-C(17)	1.315(3)	C(17)-N(18)	1.409(3)
N(18)-N(19)	1.258(2)	N(19)-C(20)	1.422(2)
C(20)-N(21)	1.307(3)	C(20)-C(24)	1.426(3)
N(21)-O(22)	1.367(2)	O(22)-N(23)	1.379(2)
N(23)-C(24)	1.301(3)	C(24)-C(25)	1.456(3)
C(25)-N(29)	1.327(2)	C(25)-N(26)	1.336(2)
N(26)-N(27)	1.348(2)	N(26)-H(26)	0.8800
N(27)-C(28)	1.318(2)	C(28)-N(29)	1.359(2)
C(28)-C(30)	1.485(3)	C(30)-N(31)	1.495(3)
C(30)-N(34)	1.514(4)	C(30)-N(34B)	1.53(2)
C(30)-N(31B)	1.56(2)	C(30)-H(30)	1.0000
N(31)-O(32)	1.207(4)	N(31)-O(33)	1.221(4)
N(34)-O(35)	1.203(4)	N(34)-O(36)	1.206(4)
N(31B)-O(32B)	1.195(17)	N(31B)-O(33B)	1.201(16)
N(34B)-O(35B)	1.179(17)	N(34B)-O(36B)	1.190(17)
O(37)-N(39)	1.214(2)	O(38)-N(39)	1.205(3)
N(39)-C(40)	1.514(3)	C(40)-C(44)	1.483(3)
C(40)-N(41)	1.501(3)	C(40)-H(40)	1.0000
N(41)-O(43)	1.203(3)	N(41)-O(42)	1.217(3)
C(44)-N(45)	1.325(2)	C(44)-N(48)	1.353(2)
N(45)-N(46)	1.349(2)	N(46)-C(47)	1.334(2)
N(46)-H(46)	0.8800	C(47)-N(48)	1.333(2)
C(47)-C(49)	1.455(3)	C(49)-N(50)	1.304(2)
C(49)-C(53)	1.435(3)	N(50)-O(51)	1.380(2)
O(51)-N(52)	1.361(2)	N(52)-C(53)	1.308(3)
C(53)-N(54)	1.405(2)	N(54)-N(55)	1.257(2)
N(55)-C(56)	1.422(2)	C(56)-N(57)	1.307(2)
C(56)-C(60)	1.428(3)	N(57)-O(58)	1.369(2)
O(58)-N(59)	1.385(2)	N(59)-C(60)	1.310(2)
C(60)-C(61)	1.450(3)	C(61)-N(65)	1.327(2)
C(61)-N(62)	1.338(2)	N(62)-N(63)	1.345(2)
N(62)-H(62)	0.8800	N(63)-C(64)	1.322(2)
C(64)-N(65)	1.354(2)	C(64)-C(66)	1.494(3)
C(66)-N(67)	1.508(3)	C(66)-N(70)	1.515(3)
C(66)-H(66)	1.0000	N(67)-O(69)	1.205(3)
N(67)-O(68)	1.222(3)	N(70)-O(71)	1.201(3)
N(70)-O(72)	1.218(2)	O(73)-N(75)	1.200(3)
O(74)-N(75)	1.208(3)	N(75)-C(76)	1.509(3)
C(76)-C(80)	1.486(3)	C(76)-N(77)	1.504(3)
C(76)-H(76)	1.0000	N(77)-O(79)	1.204(3)

N(77)-O(78)	1.220(3)	C(80)-N(81)	1.323(2)
C(80)-N(84)	1.356(3)	N(81)-N(82)	1.344(2)
N(82)-C(83)	1.338(2)	N(82)-H(82)	0.8800
C(83)-N(84)	1.328(2)	C(83)-C(85)	1.453(3)
C(85)-N(86)	1.310(2)	C(85)-C(89)	1.419(3)
N(86)-O(87)	1.385(2)	O(87)-N(88)	1.370(2)
N(88)-C(89)	1.310(3)	C(89)-N(90)	1.421(2)
N(90)-N(91)	1.254(2)	N(91)-C(92)	1.410(2)
C(92)-N(93)	1.311(2)	C(92)-C(96)	1.433(3)
N(93)-O(94)	1.360(2)	O(94)-N(95)	1.375(2)
N(95)-C(96)	1.309(2)	C(96)-C(97)	1.459(3)
C(97)-N(101)	1.329(2)	C(97)-N(98)	1.334(2)
N(98)-N(99)	1.349(2)	N(98)-H(98)	0.8800
N(99)-C(100)	1.323(2)	C(100)-N(101)	1.352(2)
C(100)-C(102)	1.488(3)	C(102)-N(103)	1.513(3)
C(102)-N(106)	1.516(3)	C(102)-H(102)	1.0000
N(103)-O(104)	1.211(3)	N(103)-O(105)	1.218(3)
N(106)-O(108)	1.202(3)	N(106)-O(107)	1.221(2)
O(109)-N(111)	1.218(2)	O(110)-N(111)	1.217(2)
N(111)-C(112)	1.507(3)	C(112)-C(116)	1.483(3)
C(112)-N(113)	1.520(3)	C(112)-H(112)	1.0000
N(113)-O(114)	1.208(3)	N(113)-O(115)	1.210(2)
C(116)-N(117)	1.322(2)	C(116)-N(120)	1.363(2)
N(117)-N(118)	1.353(2)	N(118)-C(119)	1.338(2)
N(118)-H(118)	0.8800	C(119)-N(120)	1.333(2)
C(119)-C(121)	1.457(3)	C(121)-N(122)	1.304(2)
C(121)-C(125)	1.424(3)	N(122)-O(123)	1.380(2)
O(123)-N(124)	1.363(2)	N(124)-C(125)	1.306(3)
C(125)-N(126)	1.421(2)	N(126)-N(127)	1.260(2)
N(127)-C(128)	1.407(2)	C(128)-N(129)	1.310(2)
C(128)-C(132)	1.432(3)	N(129)-O(130)	1.360(2)
O(130)-N(131)	1.378(2)	N(131)-C(132)	1.302(2)
C(132)-C(133)	1.456(3)	C(133)-N(134)	1.335(2)
C(133)-N(137)	1.337(2)	N(134)-N(135)	1.343(2)
N(134)-H(134)	0.8800	N(135)-C(136)	1.321(2)
C(136)-N(137)	1.350(2)	C(136)-C(138)	1.488(3)
C(138)-N(139)	1.513(3)	C(138)-N(142)	1.518(3)
C(138)-H(138)	1.0000	N(139)-O(141)	1.206(2)
N(139)-O(140)	1.213(2)	N(142)-O(143)	1.209(2)
N(142)-O(144)	1.208(2)	C(145)-C(146)	1.451(4)
C(145)-H(14A)	0.9800	C(145)-H(14B)	0.9800
C(145)-H(14C)	0.9800	C(146)-N(147)	1.144(4)

O(1)-N(3)-O(2)	125.9(2)	O(1)-N(3)-C(4)	117.6(2)
O(2)-N(3)-C(4)	115.9(2)	C(8)-C(4)-N(5)	114.58(17)
C(8)-C(4)-N(3)	112.07(17)	N(5)-C(4)-N(3)	105.31(18)
C(8)-C(4)-H(4)	108.2	N(5)-C(4)-H(4)	108.2
N(3)-C(4)-H(4)	108.2	O(6)-N(5)-O(7)	121.6(3)
O(7)-N(5)-O(6B)	125.3(4)	O(6)-N(5)-C(4)	121.2(2)
O(7)-N(5)-C(4)	116.4(2)	O(6B)-N(5)-C(4)	101.8(5)
N(9)-C(8)-N(12)	115.45(18)	N(9)-C(8)-C(4)	124.30(18)

N(12)-C(8)-C(4)	120.18(17)	C(8)-N(9)-N(10)	101.93(15)
C(11)-N(10)-N(9)	110.45(16)	C(11)-N(10)-H(10)	124.8
N(9)-N(10)-H(10)	124.8	N(10)-C(11)-N(12)	110.01(17)
N(10)-C(11)-C(13)	127.76(18)	N(12)-C(11)-C(13)	122.20(17)
C(11)-N(12)-C(8)	102.15(15)	N(14)-C(13)-C(17)	107.97(17)
N(14)-C(13)-C(11)	117.02(18)	C(17)-C(13)-C(11)	134.91(17)
C(13)-N(14)-O(15)	106.00(16)	N(16)-O(15)-N(14)	111.57(14)
C(17)-N(16)-O(15)	105.54(17)	N(16)-C(17)-N(18)	115.24(18)
N(16)-C(17)-C(13)	108.91(17)	N(18)-C(17)-C(13)	135.84(18)
N(19)-N(18)-C(17)	112.87(16)	N(18)-N(19)-C(20)	111.60(16)
N(21)-C(20)-N(19)	123.69(17)	N(21)-C(20)-C(24)	109.56(17)
N(19)-C(20)-C(24)	126.74(17)	C(20)-N(21)-O(22)	104.70(16)
N(21)-O(22)-N(23)	111.91(15)	C(24)-N(23)-O(22)	105.34(16)
N(23)-C(24)-C(20)	108.47(17)	N(23)-C(24)-C(25)	121.49(18)
C(20)-C(24)-C(25)	130.03(17)	N(29)-C(25)-N(26)	110.34(17)
N(29)-C(25)-C(24)	125.09(17)	N(26)-C(25)-C(24)	124.57(17)
C(25)-N(26)-N(27)	110.10(15)	C(25)-N(26)-H(26)	124.9
N(27)-N(26)-H(26)	124.9	C(28)-N(27)-N(26)	102.29(15)
N(27)-C(28)-N(29)	115.24(17)	N(27)-C(28)-C(30)	122.48(18)
N(29)-C(28)-C(30)	122.28(17)	C(25)-N(29)-C(28)	102.03(16)
C(28)-C(30)-N(31)	110.70(18)	C(28)-C(30)-N(34)	111.9(2)
N(31)-C(30)-N(34)	107.8(2)	C(28)-C(30)-N(34B)	109.7(8)
C(28)-C(30)-N(31B)	112.2(7)	N(34B)-C(30)-N(31B)	102.0(11)
C(28)-C(30)-H(30)	108.8	N(31)-C(30)-H(30)	108.8
N(34)-C(30)-H(30)	108.8	O(32)-N(31)-O(33)	126.0(3)
O(32)-N(31)-C(30)	118.7(3)	O(33)-N(31)-C(30)	115.2(3)
O(35)-N(34)-O(36)	125.8(3)	O(35)-N(34)-C(30)	118.2(3)
O(36)-N(34)-C(30)	115.8(3)	O(32B)-N(31B)-O(33B)	124(2)
O(32B)-N(31B)-C(30)	121.2(18)	O(33B)-N(31B)-C(30)	115.0(15)
O(35B)-N(34B)-O(36B)	129(3)	O(35B)-N(34B)-C(30)	110.7(19)
O(36B)-N(34B)-C(30)	120(2)	O(38)-N(39)-O(37)	126.6(2)
O(38)-N(39)-C(40)	115.58(19)	O(37)-N(39)-C(40)	117.78(19)
C(44)-C(40)-N(41)	113.26(17)	C(44)-C(40)-N(39)	112.82(17)
N(41)-C(40)-N(39)	106.75(17)	C(44)-C(40)-H(40)	107.9
N(41)-C(40)-H(40)	107.9	N(39)-C(40)-H(40)	107.9
O(43)-N(41)-O(42)	126.8(3)	O(43)-N(41)-C(40)	117.9(2)
O(42)-N(41)-C(40)	115.3(2)	N(45)-C(44)-N(48)	115.41(17)
N(45)-C(44)-C(40)	123.79(17)	N(48)-C(44)-C(40)	120.80(17)
C(44)-N(45)-N(46)	102.17(15)	C(47)-N(46)-N(45)	110.02(15)
C(47)-N(46)-H(46)	125.0	N(45)-N(46)-H(46)	125.0
N(48)-C(47)-N(46)	110.55(16)	N(48)-C(47)-C(49)	121.57(16)
N(46)-C(47)-C(49)	127.85(17)	C(47)-N(48)-C(44)	101.85(15)
N(50)-C(49)-C(53)	107.89(17)	N(50)-C(49)-C(47)	116.49(17)
C(53)-C(49)-C(47)	135.62(17)	C(49)-N(50)-O(51)	106.20(16)
N(52)-O(51)-N(50)	111.07(14)	C(53)-N(52)-O(51)	105.89(16)
N(52)-C(53)-N(54)	114.86(17)	N(52)-C(53)-C(49)	108.93(17)
N(54)-C(53)-C(49)	136.20(18)	N(55)-N(54)-C(53)	113.25(16)
N(54)-N(55)-C(56)	111.75(16)	N(57)-C(56)-N(55)	125.13(18)
N(57)-C(56)-C(60)	109.55(17)	N(55)-C(56)-C(60)	125.31(17)
C(56)-N(57)-O(58)	105.17(16)	N(57)-O(58)-N(59)	111.59(14)
C(60)-N(59)-O(58)	105.29(16)	N(59)-C(60)-C(56)	108.39(17)

N(59)-C(60)-C(61)	121.65(17)	C(56)-C(60)-C(61)	129.92(17)
N(65)-C(61)-N(62)	110.67(17)	N(65)-C(61)-C(60)	125.01(17)
N(62)-C(61)-C(60)	124.19(16)	C(61)-N(62)-N(63)	109.93(15)
C(61)-N(62)-H(62)	125.0	N(63)-N(62)-H(62)	125.0
C(64)-N(63)-N(62)	102.13(16)	N(63)-C(64)-N(65)	115.62(17)
N(63)-C(64)-C(66)	121.99(17)	N(65)-C(64)-C(66)	122.36(16)
C(61)-N(65)-C(64)	101.65(15)	C(64)-C(66)-N(67)	109.40(16)
C(64)-C(66)-N(70)	113.45(17)	N(67)-C(66)-N(70)	105.97(16)
C(64)-C(66)-H(66)	109.3	N(67)-C(66)-H(66)	109.3
N(70)-C(66)-H(66)	109.3	O(69)-N(67)-O(68)	126.0(2)
O(69)-N(67)-C(66)	115.8(2)	O(68)-N(67)-C(66)	118.1(2)
O(71)-N(70)-O(72)	126.2(2)	O(71)-N(70)-C(66)	118.51(18)
O(72)-N(70)-C(66)	115.3(2)	O(73)-N(75)-O(74)	125.0(2)
O(73)-N(75)-C(76)	119.6(2)	O(74)-N(75)-C(76)	115.4(2)
C(80)-C(76)-N(77)	112.05(17)	C(80)-C(76)-N(75)	112.25(18)
N(77)-C(76)-N(75)	106.75(17)	C(80)-C(76)-H(76)	108.6
N(77)-C(76)-H(76)	108.6	N(75)-C(76)-H(76)	108.6
O(79)-N(77)-O(78)	127.7(2)	O(79)-N(77)-C(76)	114.3(2)
O(78)-N(77)-C(76)	118.0(2)	N(81)-C(80)-N(84)	115.60(17)
N(81)-C(80)-C(76)	122.99(18)	N(84)-C(80)-C(76)	121.36(17)
C(80)-N(81)-N(82)	102.05(16)	C(83)-N(82)-N(81)	110.11(15)
C(83)-N(82)-H(82)	124.9	N(81)-N(82)-H(82)	124.9
N(84)-C(83)-N(82)	110.59(17)	N(84)-C(83)-C(85)	125.33(17)
N(82)-C(83)-C(85)	124.03(17)	C(83)-N(84)-C(80)	101.63(16)
N(86)-C(85)-C(89)	108.76(18)	N(86)-C(85)-C(83)	121.71(18)
C(89)-C(85)-C(83)	129.52(17)	C(85)-N(86)-O(87)	105.10(16)
N(88)-O(87)-N(86)	111.59(15)	C(89)-N(88)-O(87)	105.02(16)
N(88)-C(89)-C(85)	109.53(17)	N(88)-C(89)-N(90)	125.07(18)
C(85)-C(89)-N(90)	125.39(17)	N(91)-N(90)-C(89)	112.14(16)
N(90)-N(91)-C(92)	113.22(16)	N(93)-C(92)-N(91)	114.66(17)
N(93)-C(92)-C(96)	109.04(17)	N(91)-C(92)-C(96)	136.22(18)
C(92)-N(93)-O(94)	105.61(16)	N(93)-O(94)-N(95)	111.51(14)
C(96)-N(95)-O(94)	106.02(15)	N(95)-C(96)-C(92)	107.80(17)
N(95)-C(96)-C(97)	116.24(17)	C(92)-C(96)-C(97)	135.91(17)
N(101)-C(97)-N(98)	110.61(16)	N(101)-C(97)-C(96)	121.27(16)
N(98)-C(97)-C(96)	128.11(17)	C(97)-N(98)-N(99)	109.78(15)
C(97)-N(98)-H(98)	125.1	N(99)-N(98)-H(98)	125.1
C(100)-N(99)-N(98)	102.34(15)	N(99)-C(100)-N(101)	115.24(17)
N(99)-C(100)-C(102)	122.48(17)	N(101)-C(100)-C(102)	122.28(16)
C(97)-N(101)-C(100)	102.01(15)	C(100)-C(102)-N(103)	108.88(16)
C(100)-C(102)-N(106)	112.76(17)	N(103)-C(102)-N(106)	106.82(16)
C(100)-C(102)-H(102)	109.4	N(103)-C(102)-H(102)	109.4
N(106)-C(102)-H(102)	109.4	O(104)-N(103)-O(105)	126.7(2)
O(104)-N(103)-C(102)	115.64(19)	O(105)-N(103)-C(102)	117.6(2)
O(108)-N(106)-O(107)	126.5(2)	O(108)-N(106)-C(102)	118.52(18)
O(107)-N(106)-C(102)	114.9(2)	O(110)-N(111)-O(109)	126.34(19)
O(110)-N(111)-C(112)	115.55(18)	O(109)-N(111)-C(112)	118.11(18)
C(116)-C(112)-N(111)	114.40(16)	C(116)-C(112)-N(113)	113.19(16)
N(111)-C(112)-N(113)	106.59(16)	C(116)-C(112)-H(112)	107.4
N(111)-C(112)-H(112)	107.4	N(113)-C(112)-H(112)	107.4
O(114)-N(113)-O(115)	127.0(2)	O(114)-N(113)-C(112)	114.59(19)

O(115)-N(113)-C(112)	118.24(18)	N(117)-C(116)-N(120)	115.31(17)
N(117)-C(116)-C(112)	123.89(17)	N(120)-C(116)-C(112)	120.80(16)
C(116)-N(117)-N(118)	102.11(15)	C(119)-N(118)-N(117)	110.36(15)
C(119)-N(118)-H(118)	124.8	N(117)-N(118)-H(118)	124.8
N(120)-C(119)-N(118)	110.18(16)	N(120)-C(119)-C(121)	125.12(16)
N(118)-C(119)-C(121)	124.70(17)	C(119)-N(120)-C(116)	102.05(15)
N(122)-C(121)-C(125)	108.59(17)	N(122)-C(121)-C(119)	121.51(17)
C(125)-C(121)-C(119)	129.90(17)	C(121)-N(122)-O(123)	105.13(16)
N(124)-O(123)-N(122)	111.89(14)	C(125)-N(124)-O(123)	105.01(16)
N(124)-C(125)-N(126)	123.65(17)	N(124)-C(125)-C(121)	109.37(17)
N(126)-C(125)-C(121)	126.94(17)	N(127)-N(126)-C(125)	111.41(15)
N(126)-N(127)-C(128)	112.86(16)	N(129)-C(128)-N(127)	115.54(17)
N(129)-C(128)-C(132)	108.72(17)	N(127)-C(128)-C(132)	135.58(17)
C(128)-N(129)-O(130)	105.67(16)	N(129)-O(130)-N(131)	111.47(14)
C(132)-N(131)-O(130)	105.79(16)	N(131)-C(132)-C(128)	108.32(17)
N(131)-C(132)-C(133)	116.87(17)	C(128)-C(132)-C(133)	134.47(17)
N(134)-C(133)-N(137)	110.35(16)	N(134)-C(133)-C(132)	127.43(17)
N(137)-C(133)-C(132)	122.13(16)	C(133)-N(134)-N(135)	110.05(15)
C(133)-N(134)-H(134)	125.0	N(135)-N(134)-H(134)	125.0
C(136)-N(135)-N(134)	102.31(15)	N(135)-C(136)-N(137)	115.64(17)
N(135)-C(136)-C(138)	120.62(17)	N(137)-C(136)-C(138)	123.56(17)
C(133)-N(137)-C(136)	101.64(15)	C(136)-C(138)-N(139)	108.82(16)
C(136)-C(138)-N(142)	111.29(16)	N(139)-C(138)-N(142)	106.85(16)
C(136)-C(138)-H(138)	109.9	N(139)-C(138)-H(138)	109.9
N(142)-C(138)-H(138)	109.9	O(141)-N(139)-O(140)	126.1(2)
O(141)-N(139)-C(138)	118.51(19)	O(140)-N(139)-C(138)	115.26(18)
O(143)-N(142)-O(144)	125.9(2)	O(143)-N(142)-C(138)	117.51(18)
O(144)-N(142)-C(138)	116.56(18)	C(146)-C(145)-H(14A)	109.5
C(146)-C(145)-H(14B)	109.5	H(14A)-C(145)-H(14B)	109.5
C(146)-C(145)-H(14C)	109.5	H(14A)-C(145)-H(14C)	109.5
H(14B)-C(145)-H(14C)	109.5	N(147)-C(146)-C(145)	178.7(4)

Table S7. Torsion angles [°] for **15**

O(1)-N(3)-C(4)-C(8)	0.6(4)	O(2)-N(3)-C(4)-C(8)	-170.8(2)
O(1)-N(3)-C(4)-N(5)	-124.6(3)	O(2)-N(3)-C(4)-N(5)	64.0(3)
C(8)-C(4)-N(5)-O(6)	-25.9(5)	N(3)-C(4)-N(5)-O(6)	97.7(5)
C(8)-C(4)-N(5)-O(7)	144.6(2)	N(3)-C(4)-N(5)-O(7)	-91.8(3)
C(8)-C(4)-N(5)-O(6B)	-75.7(6)	N(3)-C(4)-N(5)-O(6B)	47.9(6)
N(5)-C(4)-C(8)-N(9)	44.9(3)	N(3)-C(4)-C(8)-N(9)	-75.0(3)
N(5)-C(4)-C(8)-N(12)	-138.1(2)	N(3)-C(4)-C(8)-N(12)	101.9(2)
N(12)-C(8)-N(9)-N(10)	0.8(2)	C(4)-C(8)-N(9)-N(10)	177.86(18)
C(8)-N(9)-N(10)-C(11)	-1.0(2)	N(9)-N(10)-C(11)-N(12)	0.9(2)
N(9)-N(10)-C(11)-C(13)	-176.98(18)	N(10)-C(11)-N(12)-C(8)	-0.4(2)
C(13)-C(11)-N(12)-C(8)	177.64(18)	N(9)-C(8)-N(12)-C(11)	-0.3(2)
C(4)-C(8)-N(12)-C(11)	-177.49(18)	N(10)-C(11)-C(13)-N(14)	-175.21(19)
N(12)-C(11)-C(13)-N(14)	7.2(3)	N(10)-C(11)-C(13)-C(17)	9.0(4)
N(12)-C(11)-C(13)-C(17)	-168.6(2)	C(17)-C(13)-N(14)-O(15)	0.9(2)
C(11)-C(13)-N(14)-O(15)	-175.98(16)	C(13)-N(14)-O(15)-N(16)	-0.1(2)
N(14)-O(15)-N(16)-C(17)	-0.8(2)	O(15)-N(16)-C(17)-N(18)	-177.99(17)
O(15)-N(16)-C(17)-C(13)	1.3(2)	N(14)-C(13)-C(17)-N(16)	-1.4(2)
C(11)-C(13)-C(17)-N(16)	174.6(2)	N(14)-C(13)-C(17)-N(18)	177.7(2)
C(11)-C(13)-C(17)-N(18)	-6.3(4)	N(16)-C(17)-N(18)-N(19)	170.93(19)
C(13)-C(17)-N(18)-N(19)	-8.1(3)	C(17)-N(18)-N(19)-C(20)	-177.63(17)
N(18)-N(19)-C(20)-N(21)	7.7(3)	N(18)-N(19)-C(20)-C(24)	-173.52(19)
N(19)-C(20)-N(21)-O(22)	179.41(18)	C(24)-C(20)-N(21)-O(22)	0.5(2)
C(20)-N(21)-O(22)-N(23)	-0.1(2)	N(21)-O(22)-N(23)-C(24)	-0.3(2)
O(22)-N(23)-C(24)-C(20)	0.6(2)	O(22)-N(23)-C(24)-C(25)	179.86(18)
N(21)-C(20)-C(24)-N(23)	-0.7(2)	N(19)-C(20)-C(24)-N(23)	-179.59(19)
N(21)-C(20)-C(24)-C(25)	-179.9(2)	N(19)-C(20)-C(24)-C(25)	1.2(3)
N(23)-C(24)-C(25)-N(29)	-179.5(2)	C(20)-C(24)-C(25)-N(29)	-0.4(3)
N(23)-C(24)-C(25)-N(26)	0.1(3)	C(20)-C(24)-C(25)-N(26)	179.2(2)
N(29)-C(25)-N(26)-N(27)	0.6(2)	C(24)-C(25)-N(26)-N(27)	-179.01(18)
C(25)-N(26)-N(27)-C(28)	-0.4(2)	N(26)-N(27)-C(28)-N(29)	0.0(2)
N(26)-N(27)-C(28)-C(30)	179.03(18)	N(26)-C(25)-N(29)-C(28)	-0.6(2)
C(24)-C(25)-N(29)-C(28)	179.04(19)	N(27)-C(28)-N(29)-C(25)	0.4(2)
C(30)-C(28)-N(29)-C(25)	-178.66(19)	N(27)-C(28)-C(30)-N(31)	29.2(3)
N(29)-C(28)-C(30)-N(31)	-151.8(2)	N(27)-C(28)-C(30)-N(34)	-91.1(3)
N(29)-C(28)-C(30)-N(34)	87.9(3)	N(27)-C(28)-C(30)-N(34B)	-49.6(9)
N(29)-C(28)-C(30)-N(34B)	129.4(9)	N(27)-C(28)-C(30)-N(31B)	62.9(10)
N(29)-C(28)-C(30)-N(31B)	-118.1(9)	C(28)-C(30)-N(31)-O(32)	-84.2(3)
N(34)-C(30)-N(31)-O(32)	38.5(3)	C(28)-C(30)-N(31)-O(33)	92.2(3)
N(34)-C(30)-N(31)-O(33)	-145.1(3)	C(28)-C(30)-N(34)-O(35)	-8.1(4)
N(31)-C(30)-N(34)-O(35)	-130.1(3)	C(28)-C(30)-N(34)-O(36)	175.7(3)
N(31)-C(30)-N(34)-O(36)	53.7(4)	C(28)-C(30)-N(31B)-O(32B)	-37(3)
N(34B)-C(30)-N(31B)-O(32B)	80(3)	C(28)-C(30)-N(31B)-O(33B)	147.1(17)
N(34B)-C(30)-N(31B)-O(33B)	-96(2)	C(28)-C(30)-N(34B)-O(35B)	-69(2)
N(31B)-C(30)-N(34B)-O(35B)	171.9(19)	C(28)-C(30)-N(34B)-O(36B)	105(3)
N(31B)-C(30)-N(34B)-O(36B)	-14(3)	O(38)-N(39)-C(40)-C(44)	-38.1(3)
O(37)-N(39)-C(40)-C(44)	144.82(19)	O(38)-N(39)-C(40)-N(41)	-163.2(2)
O(37)-N(39)-C(40)-N(41)	19.8(3)	C(44)-C(40)-N(41)-O(43)	-52.6(3)
N(39)-C(40)-N(41)-O(43)	72.1(2)	C(44)-C(40)-N(41)-O(42)	126.4(2)

N(39)-C(40)-N(41)-O(42)	-108.8(2)	N(41)-C(40)-C(44)-N(45)	64.5(3)
N(39)-C(40)-C(44)-N(45)	-56.9(3)	N(41)-C(40)-C(44)-N(48)	-115.2(2)
N(39)-C(40)-C(44)-N(48)	123.4(2)	N(48)-C(44)-N(45)-N(46)	-0.3(2)
C(40)-C(44)-N(45)-N(46)	179.96(18)	C(44)-N(45)-N(46)-C(47)	0.0(2)
N(45)-N(46)-C(47)-N(48)	0.4(2)	N(45)-N(46)-C(47)-C(49)	-177.82(18)
N(46)-C(47)-N(48)-C(44)	-0.5(2)	C(49)-C(47)-N(48)-C(44)	177.81(17)
N(45)-C(44)-N(48)-C(47)	0.5(2)	C(40)-C(44)-N(48)-C(47)	-179.74(18)
N(48)-C(47)-C(49)-N(50)	-4.1(3)	N(46)-C(47)-C(49)-N(50)	173.97(19)
N(48)-C(47)-C(49)-C(53)	175.8(2)	N(46)-C(47)-C(49)-C(53)	-6.2(4)
C(53)-C(49)-N(50)-O(51)	-0.4(2)	C(47)-C(49)-N(50)-O(51)	179.52(16)
C(49)-N(50)-O(51)-N(52)	-0.2(2)	N(50)-O(51)-N(52)-C(53)	0.8(2)
O(51)-N(52)-C(53)-N(54)	179.57(16)	O(51)-N(52)-C(53)-C(49)	-1.0(2)
N(50)-C(49)-C(53)-N(52)	0.9(2)	C(47)-C(49)-C(53)-N(52)	-179.0(2)
N(50)-C(49)-C(53)-N(54)	-179.9(2)	C(47)-C(49)-C(53)-N(54)	0.3(4)
N(52)-C(53)-N(54)-N(55)	-175.79(18)	C(49)-C(53)-N(54)-N(55)	5.0(3)
C(53)-N(54)-N(55)-C(56)	-177.27(16)	N(54)-N(55)-C(56)-N(57)	0.5(3)
N(54)-N(55)-C(56)-C(60)	178.96(18)	N(55)-C(56)-N(57)-O(58)	179.01(18)
C(60)-C(56)-N(57)-O(58)	0.3(2)	C(56)-N(57)-O(58)-N(59)	-0.7(2)
N(57)-O(58)-N(59)-C(60)	0.8(2)	O(58)-N(59)-C(60)-C(56)	-0.5(2)
O(58)-N(59)-C(60)-C(61)	-178.59(17)	N(57)-C(56)-C(60)-N(59)	0.1(2)
N(55)-C(56)-C(60)-N(59)	-178.55(18)	N(57)-C(56)-C(60)-C(61)	177.98(19)
N(55)-C(56)-C(60)-C(61)	-0.7(3)	N(59)-C(60)-C(61)-N(65)	162.40(19)
C(56)-C(60)-C(61)-N(65)	-15.2(3)	N(59)-C(60)-C(61)-N(62)	-13.1(3)
C(56)-C(60)-C(61)-N(62)	169.23(19)	N(65)-C(61)-N(62)-N(63)	-0.4(2)
C(60)-C(61)-N(62)-N(63)	175.66(17)	C(61)-N(62)-N(63)-C(64)	0.1(2)
N(62)-N(63)-C(64)-N(65)	0.3(2)	N(62)-N(63)-C(64)-C(66)	-177.41(17)
N(62)-C(61)-N(65)-C(64)	0.6(2)	C(60)-C(61)-N(65)-C(64)	-175.48(18)
N(63)-C(64)-N(65)-C(61)	-0.6(2)	C(66)-C(64)-N(65)-C(61)	177.15(18)
N(63)-C(64)-C(66)-N(67)	26.5(3)	N(65)-C(64)-C(66)-N(67)	-151.10(19)
N(63)-C(64)-C(66)-N(70)	-91.6(2)	N(65)-C(64)-C(66)-N(70)	90.8(2)
C(64)-C(66)-N(67)-O(69)	82.3(2)	N(70)-C(66)-N(67)-O(69)	-155.00(19)
C(64)-C(66)-N(67)-O(68)	-95.0(2)	N(70)-C(66)-N(67)-O(68)	27.6(3)
C(64)-C(66)-N(70)-O(71)	5.5(3)	N(67)-C(66)-N(70)-O(71)	-114.6(2)
C(64)-C(66)-N(70)-O(72)	-173.53(18)	N(67)-C(66)-N(70)-O(72)	66.4(2)
O(73)-N(75)-C(76)-C(80)	-33.1(3)	O(74)-N(75)-C(76)-C(80)	146.7(2)
O(73)-N(75)-C(76)-N(77)	90.0(3)	O(74)-N(75)-C(76)-N(77)	-90.1(2)
C(80)-C(76)-N(77)-O(79)	-64.7(3)	N(75)-C(76)-N(77)-O(79)	172.0(2)
C(80)-C(76)-N(77)-O(78)	116.1(2)	N(75)-C(76)-N(77)-O(78)	-7.1(3)
N(77)-C(76)-C(80)-N(81)	-40.0(3)	N(75)-C(76)-C(80)-N(81)	80.1(2)
N(77)-C(76)-C(80)-N(84)	142.87(19)	N(75)-C(76)-C(80)-N(84)	-97.0(2)
N(84)-C(80)-N(81)-N(82)	0.5(2)	C(76)-C(80)-N(81)-N(82)	-176.80(18)
C(80)-N(81)-N(82)-C(83)	0.6(2)	N(81)-N(82)-C(83)-N(84)	-1.4(2)
N(81)-N(82)-C(83)-C(85)	176.29(17)	N(82)-C(83)-N(84)-C(80)	1.6(2)
C(85)-C(83)-N(84)-C(80)	-176.11(18)	N(81)-C(80)-N(84)-C(83)	-1.3(2)
C(76)-C(80)-N(84)-C(83)	176.04(18)	N(84)-C(83)-C(85)-N(86)	158.2(2)
N(82)-C(83)-C(85)-N(86)	-19.2(3)	N(84)-C(83)-C(85)-C(89)	-21.0(3)
N(82)-C(83)-C(85)-C(89)	161.6(2)	C(89)-C(85)-N(86)-O(87)	-0.4(2)
C(83)-C(85)-N(86)-O(87)	-179.71(17)	C(85)-N(86)-O(87)-N(88)	0.7(2)
N(86)-O(87)-N(88)-C(89)	-0.7(2)	O(87)-N(88)-C(89)-C(85)	0.4(2)
O(87)-N(88)-C(89)-N(90)	-178.41(18)	N(86)-C(85)-C(89)-N(88)	0.0(2)
C(83)-C(85)-C(89)-N(88)	179.22(19)	N(86)-C(85)-C(89)-N(90)	178.81(18)

C(83)-C(85)-C(89)-N(90)	-1.9(3)	N(88)-C(89)-N(90)-N(91)	6.2(3)
C(85)-C(89)-N(90)-N(91)	-172.45(18)	C(89)-N(90)-N(91)-C(92)	177.64(16)
N(90)-N(91)-C(92)-N(93)	-174.77(17)	N(90)-N(91)-C(92)-C(96)	1.6(3)
N(91)-C(92)-N(93)-O(94)	176.86(16)	C(96)-C(92)-N(93)-O(94)	-0.5(2)
C(92)-N(93)-O(94)-N(95)	-0.1(2)	N(93)-O(94)-N(95)-C(96)	0.7(2)
O(94)-N(95)-C(96)-C(92)	-0.9(2)	O(94)-N(95)-C(96)-C(97)	177.20(16)
N(93)-C(92)-C(96)-N(95)	0.9(2)	N(91)-C(92)-C(96)-N(95)	-175.6(2)
N(93)-C(92)-C(96)-C(97)	-176.7(2)	N(91)-C(92)-C(96)-C(97)	6.9(4)
N(95)-C(96)-C(97)-N(101)	-7.5(3)	C(92)-C(96)-C(97)-N(101)	169.9(2)
N(95)-C(96)-C(97)-N(98)	171.77(19)	C(92)-C(96)-C(97)-N(98)	-10.8(4)
N(101)-C(97)-N(98)-N(99)	0.9(2)	C(96)-C(97)-N(98)-N(99)	-178.42(18)
C(97)-N(98)-N(99)-C(100)	-0.6(2)	N(98)-N(99)-C(100)-N(101)	0.2(2)
N(98)-N(99)-C(100)-C(102)	-179.59(17)	N(98)-C(97)-N(101)-C(100)	-0.7(2)
C(96)-C(97)-N(101)-C(100)	178.67(17)	N(99)-C(100)-N(101)-C(97)	0.3(2)
C(102)-C(100)-N(101)-C(97)	-179.90(18)	N(99)-C(100)-C(102)-N(103)	20.6(3)
N(101)-C(100)-C(102)-N(103)	-159.14(18)	N(99)-C(100)-C(102)-N(106)	-97.7(2)
N(101)-C(100)-C(102)-N(106)	82.5(2)	C(100)-C(102)-N(103)-O(104)	87.0(2)
N(106)-C(102)-N(103)-O(104)	-150.96(19)	C(100)-C(102)-N(103)-O(105)	-90.4(2)
N(106)-C(102)-N(103)-O(105)	31.7(2)	C(100)-C(102)-N(106)-O(108)	8.7(3)
N(103)-C(102)-N(106)-O(108)	-110.8(2)	C(100)-C(102)-N(106)-O(107)	-170.01
N(103)-C(102)-N(106)-O(107)	70.4(2)	O(110)-N(111)-C(112)-C(116)	131.4(2)
O(109)-N(111)-C(112)-C(116)	-48.9(3)	O(110)-N(111)-C(112)-N(113)	-102.7(2)
O(109)-N(111)-C(112)-N(113)	77.0(2)	C(116)-C(112)-N(113)-O(114)	-41.9(3)
N(111)-C(112)-N(113)-O(114)	-168.5(2)	C(116)-C(112)-N(113)-O(115)	143.07(19)
N(111)-C(112)-N(113)-O(115)	16.4(2)	N(111)-C(112)-C(116)-N(117)	61.7(3)
N(113)-C(112)-C(116)-N(117)	-60.7(2)	N(111)-C(112)-C(116)-N(120)	-118.5(2)
N(113)-C(112)-C(116)-N(120)	119.1(2)	N(120)-C(116)-N(117)-N(118)	-0.2(2)
C(112)-C(116)-N(117)-N(118)	179.59(17)	C(116)-N(117)-N(118)-C(119)	0.3(2)
N(117)-N(118)-C(119)-N(120)	-0.2(2)	N(117)-N(118)-C(119)-C(121)	-179.87
N(118)-C(119)-N(120)-C(116)	0.1(2)	C(121)-C(119)-N(120)-C(116)	179.73(18)
N(117)-C(116)-N(120)-C(119)	0.1(2)	C(112)-C(116)-N(120)-C(119)	-179.72
N(120)-C(119)-C(121)-N(122)	169.80(19)	N(118)-C(119)-C(121)-N(122)	-10.6(3)
N(120)-C(119)-C(121)-C(125)	-11.1(3)	N(118)-C(119)-C(121)-C(125)	168.5(2)
C(125)-C(121)-N(122)-O(123)	1.0(2)	C(119)-C(121)-N(122)-O(123)	-179.71
C(121)-N(122)-O(123)-N(124)	-0.2(2)	N(122)-O(123)-N(124)-C(125)	-0.7(2)
O(123)-N(124)-C(125)-N(126)	179.10(17)	O(123)-N(124)-C(125)-C(121)	1.3(2)
N(122)-C(121)-C(125)-N(124)	-1.5(2)	C(119)-C(121)-C(125)-N(124)	179.3(2)
N(122)-C(121)-C(125)-N(126)	-179.24(19)	C(119)-C(121)-C(125)-N(126)	1.6(3)
N(124)-C(125)-N(126)-N(127)	16.7(3)	C(121)-C(125)-N(126)-N(127)	-165.82
C(125)-N(126)-N(127)-C(128)	-174.89(16)	N(126)-N(127)-C(128)-N(129)	165.68(18)
N(126)-N(127)-C(128)-C(132)	-9.3(3)	N(127)-C(128)-N(129)-O(130)	-174.82
C(132)-C(128)-N(129)-O(130)	1.5(2)	C(128)-N(129)-O(130)-N(131)	-1.3(2)
N(129)-O(130)-N(131)-C(132)	0.6(2)	O(130)-N(131)-C(132)-C(128)	0.3(2)
O(130)-N(131)-C(132)-C(133)	-173.99(16)	N(129)-C(128)-C(132)-N(131)	-1.1(2)
N(127)-C(128)-C(132)-N(131)	174.1(2)	N(129)-C(128)-C(132)-C(133)	171.7(2)
N(127)-C(128)-C(132)-C(133)	-13.1(4)	N(131)-C(132)-C(133)-N(134)	-172.44
C(128)-C(132)-C(133)-N(134)	15.2(3)	N(131)-C(132)-C(133)-N(137)	11.1(3)
C(128)-C(132)-C(133)-N(137)	-161.2(2)	N(137)-C(133)-N(134)-N(135)	0.9(2)
C(132)-C(133)-N(134)-N(135)	-175.92(18)	C(133)-N(134)-N(135)-C(136)	-0.6(2)
N(134)-N(135)-C(136)-N(137)	0.2(2)	N(134)-N(135)-C(136)-C(138)	175.50(16)
N(134)-C(133)-N(137)-C(136)	-0.7(2)	C(132)-C(133)-N(137)-C(136)	176.30(17)

N(135)-C(136)-N(137)-C(133)	0.3(2)	C(138)-C(136)-N(137)-C(133)	-174.86
N(135)-C(136)-C(138)-N(139)	35.5(2)	N(137)-C(136)-C(138)-N(139)	-149.55
N(135)-C(136)-C(138)-N(142)	-82.0(2)	N(137)-C(136)-C(138)-N(142)	93.0(2)
C(136)-C(138)-N(139)-O(141)	-91.5(2)	N(142)-C(138)-N(139)-O(141)	28.8(2)
C(136)-C(138)-N(139)-O(140)	84.6(2)	N(142)-C(138)-N(139)-O(140)	-155.17
C(136)-C(138)-N(142)-O(143)	-5.1(3)	N(139)-C(138)-N(142)-O(143)	-123.8(2)
C(136)-C(138)-N(142)-O(144)	177.9(2)	N(139)-C(138)-N(142)-O(144)	59.2(3)

Table S8. Hydrogen bonds for **15** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(10)-H(10)...N(19)	0.88	2.18	2.878(2)	135.5
N(10)-H(10)...N(29)	0.88	2.19	2.860(2)	132.7
N(26)-H(26)...N(48)	0.88	2.36	2.967(2)	126.1
N(46)-H(46)...N(55)	0.88	2.22	2.910(2)	135.2
N(46)-H(46)...N(65)	0.88	2.17	2.839(2)	132.9
N(62)-H(62)...N(12)#1	0.88	2.06	2.918(2)	163.9
N N(82)-H(82)...N(137)#2	0.88	2.14	2.954(2)	153.3
N(98)-H(98)...N(84)	0.88	2.20	2.891(2)	135.6
N(98)-H(98)...N(90)	0.88	2.26	2.941(2)	134.2
N(118)-H(118)...N(101)	0.88	2.29	2.895(2)	126.3
N(134)-H(134)...N(120)	0.88	2.23	2.908(2)	133.8
N(134)-H(134)...N(126)	0.88	2.19	2.885(2)	135.0

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

References:

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