Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Energetic π-conjugated vinyl bridged triazoles: a thermally stable and insensitive heterocyclic cation

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Table S1. Crystal data and structure refinement details for **4**, **5**, **6**, **7, 8, 9·3H$_2$O, 10, 11 and 14·2H$_2$O**

	4	**5**	**6**	**7**	**8**
Formula	$C_6H_{12}Cl_2N_{10}O_8$	$C_6H_{12}N_{10}O_4S$	$C_6H_{12}N_{12}O_6$	$C_{18}H_{16}N_{16}O_{14}$	$C_{18}H_{16}N_{16}O_{18}$
Molecular weight [g mol^{-1}]	423.16	320.32	348.28	680.47	744.47
T [K]	130	173	296	130	296
Crystal size [mm^3]	0.20×0.15×0.12	0.39×0.09×0.07	0.25×0.15×0.12	0.05×0.03×0.02	0.10×0.03×0.02
Crystal system	Tetragonal	Monoclinic	Orthorhombic	Monoclinic	Monoclinic
Space group	*I*4$_1$/*acd*	*P*2$_1$/*c*	*Pbcn*	*P*2$_1$/*n*	*P*2$_1$/*n*
a [Å]	12.2856(7)	6.4108(6)	15.095(3)	6.804(2)	11.2505(7)
b [Å]	12.2856(7)	13.4566(14)	6.7677(12)	8.943(3)	5.1854(3)
c [Å]	40.490(4)	14.2343(14)	13.289(2)	21.067(7)	23.7693(12)
α [˚]	90	90	90	90	90
β [˚]	90	98.654(3)	90	92.639(6)	101.493(5)
γ [˚]	90	90	90	90	90
V [Å^3]	6111.4(9)	1213.98(19)	1357.6(4)	1280.5(8)	838.24(19)
Z	16	4	4	2	2
λ [Å]	0.71073	0.71073	0.71073	0.71073	0.71073
ρ_{calc} [g cm^{-3}]	1.840	1.753	1.704	1.765	1.819
μ [mm^{-1}]	0.494	0.308	0.149	0.154	1.452
F (000)	3456	664	720	696	760
ϑ range [˚]	2.012-30.660	6.06-50.66	5.398-54.966	1.935-27.651	4.080-65.988
Reflections collected	28870 / 2368	6913 / 2187	9013 / 1547	9995 / 2957	5320 / 2292
Index ranges	-17≤*h*≤16 -17≤*k*≤11 -58≤*l*≤57	-6≤*h*≤7 -16≤*k*≤16 -16≤*l*≤17	-18≤*h*≤19 -8≤*k*≤8 -17≤*l*≤17	-8≤*h*≤8 -11≤*k*≤10 -27≤*l*≤22	-13≤*h*≤13 -5≤*k*≤6 -28≤*l*≤27
R_{int}	0.0542	0.0525	0.0620	0.1557	0.0454
Data / restraints / parameters	2368 / 2 / 142	2187 / 14 / 220	1547 / 6 / 110	2957 / 0 / 218	2292 / 30 / 263
Final R index [$I > 2\sigma(I)$]	R_1=0.0338, wR_2=0.0840	R_1=0.0380, wR_2=0.0841	R_1=0.0427, wR_2=0.1141	R_1=0.0747, wR_2=0.1570	R_1=0.0846, wR_2=0.2307
Final R index [all data]	R_1=0.0473, wR_2=0.0923	R_1=0.0703, wR_2=0.0952	R_1=0.0620, wR_2=0.1277	R_1=0.1935, wR_2=0.2130	R_1=0.1256, wR_2=0.2706
GOF on F^2	1.053	1.014	1.037	0.920	1.047
CCDC number	1524813	1524814	1526086	1524815	1524816

	9·3H$_2$O	**10**	**11**	**14·2H$_2$O**
Formula	$C_{12}H_{20}N_{18}O_{11}$	$C_{12}H_{12}N_{20}O_{12}$	$C_8H_{12}N_{14}O_3$	$C_8H_{16}N_{20}O_2$
Molecular weight [g	592.46	628.42	352.32	424.41

mol^{-1}]				
T [K]	130	173	130	130
Crystal size [mm^3]	0.25×0.20×0.15	0.22×0.19×0.15	0.10×0.08×0.02	0.12×0.05×0.03
Crystal system	Triclinic	Monoclinic	Monoclinic	Triclinic
Space group	*P*-1	*P*2/n	*C*2/*c*	*P*-1
a [Å]	6.413(2)	13.4466(13)	12.8678(14)	5.755(2)
b [Å]	10.1729(13)	5.9301(6)	6.4849(7)	8.863(4)
c [Å]	10.5386(13)	15.0419(16)	33.243(4)	9.154(4)
α [˚]	117.773(2)	90	90	77.761(7)
β [˚]	100.209(3)	97.917(4)	94.281(2)	80.303(7)
γ [˚]	97.012(3)	90	90	78.757(7)
V [$Å^3$]	581.9(2)	1188.0(2)	2766.3(5)	443.6(3)
Z	1	2	8	1
λ [Å]	0.71073	0.71073	0.71073	0.71073
ρ_{calc} [g cm^{-3}]	1.691	1.757	1.692	1.589
μ [mm^{-1}]	0.148	0.156	0.136	0.126
F (000)	306	640	1456	220
ϑ range [˚]	2.266-30.668	6.12-50.7	2.458-30.470	2.297-28.199
Reflections collected	5970 / 3566	6516 / 2150	13235 / 4191	3481 / 2092
Index ranges	-9≤*h*≤9	-16≤*h*≤16	-14≤*h*≤18	-7≤*h*≤7
	-14≤*k*≤10	-7≤*k*≤6	-9≤*k*≤9	-11≤*k*≤10
	-14≤*l*≤15	-18≤*l*≤18	-47≤*l*≤47	-11≤*l*≤10
R_{int}	0.0147	0.0590	0.0300	0.0262
Data / restraints / parameters	3566 / 2 / 237	2150 / 2 / 214	4191 / 0 / 274	2092 / 0 / 168
Final R index [$I > 2\sigma(I)$]	R_1=0.0388, wR_2=0.1012	R_1=0.0383, wR_2=0.0808	R_1=0.0531, wR_2=0.1312	R_1=0.0494, wR_2=0.1189
Final R index [all data]	R_1=0.0462, wR_2=0.1069	R_1=0.0805, wR_2=0.0935	R_1=0.0665, wR_2=0.1393	R_1=0.0807, wR_2=0.1373
GOF on F^2	1.053	1.051	1.053	0.962
CCDC number	1524817	1524818	1524819	1524820

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

	x	y	z	U(eq)
N(1)	-1282(1)	7082(1)	884(1)	13(1)
N(2)	-1861(1)	7646(1)	1123(1)	14(1)
N(3)	-2494(1)	7988(1)	623(1)	11(1)
N(4)	-3116(1)	8350(1)	355(1)	13(1)
N(5)	-1313(1)	6931(1)	293(1)	17(1)
C(1)	-1662(1)	7285(1)	581(1)	12(1)
C(2)	-2588(1)	8199(1)	959(1)	12(1)
C(3)	-3391(1)	8954(1)	1089(1)	14(1)
Cl(1)	944(1)	4668(1)	475(1)	15(1)
O(1)	116(1)	5389(1)	602(1)	25(1)
O(2)	1294(1)	5075(1)	160(1)	37(1)
O(3)	492(1)	3595(1)	435(1)	30(1)
O(4)	1846(1)	4630(1)	699(1)	34(1)

Table S3. Bond lengths [Å] and angles [°] for **4**.

N(1)-H(1)	0.80(2)
N(1)-N(2)	1.3864(16)
N(1)-C(1)	1.3359(18)
N(2)-C(2)	1.3047(18)
N(3)-N(4)	1.3998(16)
N(3)-C(1)	1.3491(18)
N(3)-C(2)	1.3892(17)
N(4)-H(4A)	0.89(2)
N(4)-H(4B)	0.88(2)
N(5)-H(5A)	0.83(2)
N(5)-H(5B)	0.81(2)
N(5)-C(1)	1.3184(18)
C(2)-C(3)	1.4536(19)
C(3)-C(3)#1	1.332(3)
C(3)-H(3)	0.95(2)
Cl(1)-O(1)	1.4441(12)
Cl(1)-O(2)	1.4350(13)
Cl(1)-O(3)	1.4402(12)
Cl(1)-O(4)	1.4329(13)

N(2)-N(1)-H(1)	119.5(16)
C(1)-N(1)-H(1)	128.6(16)
C(1)-N(1)-N(2)	111.61(12)
C(2)-N(2)-N(1)	104.79(12)
C(1)-N(3)-N(4)	121.38(11)
C(1)-N(3)-C(2)	107.72(11)
C(2)-N(3)-N(4)	130.86(12)
N(3)-N(4)-H(4A)	109.2(13)
N(3)-N(4)-H(4B)	108.3(14)
H(4A)-N(4)-H(4B)	112.8(18)
H(5A)-N(5)-H(5B)	122(2)
C(1)-N(5)-H(5A)	119.0(15)
C(1)-N(5)-H(5B)	118.6(17)
N(1)-C(1)-N(3)	105.65(12)
N(5)-C(1)-N(1)	129.73(14)
N(5)-C(1)-N(3)	124.59(13)
N(2)-C(2)-N(3)	110.23(12)
N(2)-C(2)-C(3)	127.74(13)
N(3)-C(2)-C(3)	122.02(12)
C(2)-C(3)-H(3)	117.0(12)

C(3)#1-C(3)-C(2)	122.86(17)
C(3)#1-C(3)-H(3)	120.1(12)
O(2)-Cl(1)-O(1)	108.34(9)
O(2)-Cl(1)-O(3)	109.62(9)
O(3)-Cl(1)-O(1)	109.27(8)
O(4)-Cl(1)-O(1)	109.77(8)
O(4)-Cl(1)-O(2)	110.00(9)
O(4)-Cl(1)-O(3)	109.82(8)

Symmetry transformations used to generate equivalent atoms:

#1 y-5/4,x+5/4,-z+1/4

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	13(1)	13(1)	12(1)	-2(1)	0(1)	4(1)
N(2)	15(1)	14(1)	12(1)	-2(1)	1(1)	2(1)
N(3)	11(1)	13(1)	10(1)	-1(1)	0(1)	2(1)
N(4)	12(1)	16(1)	12(1)	2(1)	-2(1)	1(1)
N(5)	19(1)	20(1)	13(1)	-2(1)	2(1)	7(1)
C(1)	11(1)	12(1)	13(1)	-1(1)	1(1)	0(1)
C(2)	13(1)	13(1)	11(1)	-2(1)	0(1)	0(1)
C(3)	14(1)	15(1)	13(1)	-1(1)	0(1)	3(1)
Cl(1)	13(1)	12(1)	21(1)	-3(1)	3(1)	0(1)
O(1)	29(1)	23(1)	23(1)	-2(1)	7(1)	14(1)
O(2)	42(1)	47(1)	23(1)	-4(1)	16(1)	-14(1)
O(3)	18(1)	12(1)	60(1)	-2(1)	-5(1)	-3(1)
O(4)	26(1)	24(1)	51(1)	-4(1)	-19(1)	2(1)

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

	x	y	z	U(eq)
H(1)	-824(18)	6654(18)	940(5)	28(6)
H(4A)	-2942(16)	9037(17)	310(5)	23(5)
H(4B)	-3812(19)	8268(17)	405(5)	28(6)
H(5A)	-1545(18)	7225(18)	121(5)	31(6)
H(5B)	-864(19)	6451(19)	289(6)	32(6)
H(3)	-3794(17)	9371(17)	932(5)	21(5)

Table S6. Torsion angles [°] for **4**.

N(1)-N(2)-C(2)-N(3)	0.83(15)
N(1)-N(2)-C(2)-C(3)	-178.10(14)
N(2)-N(1)-C(1)-N(3)	0.15(16)
N(2)-N(1)-C(1)-N(5)	177.96(15)
N(2)-C(2)-C(3)-C(3)#1	-6.08(19)
N(3)-C(2)-C(3)-C(3)#1	175.10(9)
N(4)-N(3)-C(1)-N(1)	-177.52(12)
N(4)-N(3)-C(1)-N(5)	4.5(2)
N(4)-N(3)-C(2)-N(2)	176.82(13)
N(4)-N(3)-C(2)-C(3)	-4.2(2)
C(1)-N(1)-N(2)-C(2)	-0.63(16)
C(1)-N(3)-C(2)-N(2)	-0.78(16)
C(1)-N(3)-C(2)-C(3)	178.23(13)
C(2)-N(3)-C(1)-N(1)	0.36(15)
C(2)-N(3)-C(1)-N(5)	-177.59(14)

Symmetry transformations used to generate equivalent atoms:

#1 y-5/4,x+5/4,-z+1/4

Table S7. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **5**. U(eq) is defined as 1 one third of of the trace of the orthogonalised U^{IJ} tensor.

Atom	x	y	z	U(eq)
C1	8640(4)	835.7(18)	1898.6(17)	14.2(6)
C2	9933(4)	958.8(18)	1256.4(17)	14.4(6)
C3	9369(4)	1156.2(18)	4420.3(17)	13.9(6)
C4	9420(4)	866.9(18)	2905.6(18)	12.5(6)

C5	9248(4)	1403.7(18)	-1253.6(18)	12.9(6)
C6	9163(4)	1048.0(17)	252.0(17)	12.2(6)
N1	11376(3)	825.7(16)	3299.9(14)	16.7(5)
N2	11336(4)	1008.3(16)	4251.1(15)	17.2(5)
N3	8116(3)	1062.4(15)	3578.9(14)	12.5(5)
N4	8753(4)	1368.7(19)	5242.1(16)	21.8(6)
N5	5932(3)	1247.1(17)	3478.9(16)	16.8(5)
N6	7224(3)	950.9(16)	-167.5(14)	15.4(5)
N7	7297(4)	1178.0(16)	-1114.7(15)	15.4(5)
N8	10475(3)	1317.9(15)	-400.9(14)	12.5(5)
N9	9881(4)	1670.1(17)	-2055.6(16)	19.2(5)
N10	12662(4)	1498.9(19)	-284.3(17)	19.2(5)
O1	4580(3)	4105.7(13)	793.7(12)	20.5(4)
O2	4108(3)	4062.3(13)	2444.4(12)	20.1(5)
O3	6127(3)	2778.3(13)	1813.2(13)	20.6(5)
O4	2355(3)	2861.5(13)	1344.9(13)	20.5(5)
S1	4302.7(10)	3449.4(5)	1596.0(5)	13.61(18)

Table S8. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **5**. 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}
C1	12.4(14)	15.5(14)	13.5(13)	-0.3(11)	-1.8(11)	-0.2(11)
C2	13.9(14)	16.0(14)	12.9(13)	-1.2(11)	0.3(11)	0.3(11)
C3	14.1(15)	16.0(13)	11.5(13)	1.9(11)	1.1(11)	-3.4(11)
C4	9.4(14)	14.8(13)	13.2(14)	0.4(10)	1.5(11)	0.9(11)
C5	12.1(14)	12.7(13)	13.4(13)	-0.4(10)	0.8(11)	1.2(11)
C6	13.5(15)	12.9(13)	10.7(13)	0.1(10)	3.0(11)	2.2(11)
N1	17.2(13)	23.6(13)	9.3(12)	-0.4(9)	2.1(10)	-0.7(10)
N2	11.4(13)	28.9(13)	10.0(12)	-1.4(10)	-2.9(9)	0.1(10)
N3	8.7(12)	17.4(12)	11.4(11)	0.4(9)	1.3(9)	-1.0(9)
N4	13.4(13)	38.3(15)	13.6(12)	-5.7(11)	2(1)	-4.5(12)
N5	8.6(13)	22.7(12)	18.4(12)	0.6(10)	0.4(10)	0.2(10)
N6	14.4(13)	21.4(12)	10.0(11)	1.7(9)	0.8(9)	0.6(10)
N7	12.5(13)	24.4(12)	8.4(11)	1.6(9)	-1.5(9)	0(1)
N8	10.5(12)	17.0(11)	10.2(11)	-1.2(9)	1.6(9)	-1.6(9)

N9	15.4(13)	30.3(13)	12.0(12)	3(1)	2.6(10)	-0.6(11)
N10	8.5(12)	30.3(14)	17.7(12)	-0.8(11)	-1.6(10)	-2.0(11)
O1	18.6(11)	28.0(11)	14.7(10)	4.4(8)	2.0(8)	-3.1(9)
O2	20.7(11)	26.7(11)	12(1)	-4.5(8)	-0.1(8)	6.8(9)
O3	17(1)	22.4(10)	21.5(11)	-1.6(8)	-0.3(8)	7.8(8)
O4	15.7(10)	25.1(11)	19.8(11)	0.5(8)	-0.3(8)	-4.8(8)
S1	12.4(3)	17.9(3)	10.1(3)	-0.4(3)	0.3(2)	0.8(3)

Table S9. Bond Lengths for **5**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.333(3)	C6	N6	1.302(3)
C1	C4	1.446(3)	C6	N8	1.392(3)
C2	C6	1.446(3)	N1	N2	1.380(3)
C3	N4	1.321(3)	N3	N5	1.408(3)
C3	N2	1.334(3)	N6	N7	1.390(3)
C3	N3	1.344(3)	N8	N10	1.408(3)
C4	N1	1.296(3)	O1	S1	1.4755(18)
C4	N3	1.388(3)	O2	S1	1.4831(18)
C5	N9	1.318(3)	O3	S1	1.4730(18)
C5	N7	1.330(3)	O4	S1	1.4760(19)
C5	N8	1.348(3)			

Table S10. Bond Angles for **5**.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C2	C1	C4	121.2(2)	C3	N2	N1	111.2(2)
C1	C2	C6	122.2(2)	C3	N3	C4	107.0(2)
N4	C3	N2	127.5(3)	C3	N3	N5	121.7(2)
N4	C3	N3	126.2(2)	C4	N3	N5	131.0(2)
N2	C3	N3	106.2(2)	C6	N6	N7	104.67(19)
N1	C4	N3	110.7(2)	C5	N7	N6	111.4(2)
N1	C4	C1	126.6(2)	C5	N8	C6	107.1(2)
N3	C4	C1	122.4(2)	C5	N8	N10	121.8(2)
N9	C5	N7	127.6(3)	C6	N8	N10	131.1(2)
N9	C5	N8	126.1(2)	O3	S1	O1	110.18(11)
N7	C5	N8	106.3(2)	O3	S1	O4	109.76(11)

N6	C6	N8	110.5(2)	O1	S1	O4	109.25(11)
N6	C6	C2	127.3(2)	O3	S1	O2	109.35(11)
N8	C6	C2	122.1(2)	O1	S1	O2	109.40(10)
C4	N1	N2	104.9(2)	O4	S1	O2	108.88(11)

Table S11. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **5**.

Atom	x	y	z	U(eq)
H1	7180	726	1691	17
H2	11410	989	1466	17
H2A	12460(30)	1000(20)	4680(16)	21
H4A	9680(40)	1590(20)	5697(16)	26
H4B	7450(30)	1360(20)	5280(20)	26
H5A	5230(40)	698(16)	3332(18)	20
H5B	5600(40)	1650(18)	2976(16)	20
H7A	6180(30)	1130(20)	-1567(15)	18
H9A	8930(40)	1810(20)	-2536(16)	23
H9B	11220(30)	1690(20)	-2090(20)	23
H10A	13320(40)	931(15)	-132(19)	23
H10B	12940(40)	1922(18)	199(16)	23

Table S12 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **6**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
N1	8450.3(11)	-7(3)	1635.2(12)	34.6(4)
O1	5393.9(11)	4127(3)	3426.4(10)	48.7(4)
O2	4986.0(9)	2698(2)	4803.5(11)	46.1(4)
O3	6358.7(9)	3517(2)	4587.9(9)	38.0(4)
N4	6881.2(9)	-92(2)	1633.6(10)	25.1(3)
N2	7510.4(10)	-643(2)	3047.0(11)	29.9(4)
N5	6804.6(11)	381(2)	609.4(10)	33.4(4)
N6	5562.6(10)	3454(2)	4270.0(11)	31.5(4)
C1	7678.1(12)	-226(2)	2086.0(13)	24.7(4)
C2	6241.5(12)	-462(2)	2358.7(13)	26.5(4)
C3	5304.5(12)	-480(3)	2142.9(14)	30.4(4)
N3	6615.3(11)	-785(2)	3231.6(11)	31.7(4)

Table S13 Anisotropic Displacement Parameters ($Å^2×10^3$) for **6**. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	18.5(9)	56.3(10)	29.1(8)	4.3(6)	-0.1(6)	-1.6(7)
O1	32.4(9)	88.9(12)	24.8(7)	9.4(7)	-4.0(6)	1.0(7)
O2	33.7(9)	65.4(10)	39.4(8)	3.4(7)	6.6(6)	-15.0(7)
O3	22.1(8)	64.0(9)	27.8(7)	2.0(6)	-4.2(5)	-1.4(6)
N4	18.6(8)	35.9(8)	20.9(7)	0.5(5)	-0.9(6)	0.4(6)
N2	18.3(8)	47.2(9)	24.4(7)	2.4(6)	-3.2(6)	0.0(6)
N5	28.2(10)	50.6(10)	21.5(7)	2.4(6)	-2.8(6)	-0.7(7)
N6	23.6(9)	47.4(9)	23.6(7)	-4.3(6)	-0.4(6)	-1.6(6)
C1	20.3(9)	29.2(8)	24.6(8)	-1.1(6)	-1.8(7)	-0.6(6)
C2	20.0(9)	35.4(9)	24.2(8)	-1.5(6)	2.5(7)	0.4(7)
C3	21(1)	44.6(10)	25.7(9)	0.6(7)	-1.5(7)	0.4(7)
N3	21.5(9)	48.6(9)	24.9(8)	1.6(6)	0.9(6)	-0.9(6)

Table S14 Bond Lengths for **6**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C1	1.319(2)	N4	C2	1.387(2)
O1	N6	1.237(2)	N2	C1	1.332(2)
O2	N6	1.2337(19)	N2	N3	1.376(2)
O3	N6	1.2746(19)	C2	C3	1.443(3)
N4	N5	1.4030(19)	C2	N3	1.308(2)
N4	C1	1.348(2)	C3	C3[1]	1.321(4)

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

Table S15 Bond Angles for **6**.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C1	N4	N5	121.44(14)	N1	C1	N2	128.84(17)
C1	N4	C2	107.42(14)	N2	C1	N4	105.80(15)
C2	N4	N5	131.14(14)	N4	C2	C3	123.08(15)
C1	N2	N3	111.85(15)	N3	C2	N4	110.24(16)
O1	N6	O3	118.84(15)	N3	C2	C3	126.68(17)
O2	N6	O1	121.91(16)	C3[1]	C3	C2	122.6(2)
O2	N6	O3	119.24(15)	C2	N3	N2	104.69(14)
N1	C1	N4	125.35(16)				

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

Table S16 Torsion Angles for **6**.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
N4	C2	C3	C3[1]	-167.59(11)	C1	N2	N3	C2	0.5(2)
N4	C2	N3	N2	-0.86(18)	C2	N4	C1	N1	178.55(17)
N5	N4	C1	N1	-2.4(3)	C2	N4	C1	N2	-0.51(18)
N5	N4	C1	N2	178.54(15)	C3	C2	N3	N2	178.85(17)
N5	N4	C2	C3	2.2(3)	N3	N2	C1	N1	-179.02(18)
N5	N4	C2	N3	-178.03(17)	N3	N2	C1	N4	-0.01(19)
C1	N4	C2	C3	-178.83(16)	N3	C2	C3	C3[1]	12.7(2)
C1	N4	C2	N3	0.89(19)					

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

Table S17 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **6**.

Atom	x	y	z	U(eq)
H1A	8933	-136	1973	42
H1B	8471	265	1003	42
H2	7913	-805	3498	36
H5A	6637	-645	276	40
H5B	6419	1308	536	40
H3	5122	-493	1474	37

Table S18. Atomic coordinates (Å x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **7**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	6564(5)	7221(4)	3788(1)	33(1)
O(2)	4478(5)	9281(4)	4368(1)	34(1)
O(3)	1468(4)	9484(4)	4018(1)	28(1)
O(4)	-429(5)	8633(4)	1861(1)	31(1)
O(5)	1390(5)	7247(4)	1279(1)	33(1)
O(6)	8852(4)	5985(4)	2939(2)	35(1)
O(7)	7534(5)	5460(4)	2017(2)	36(1)
N(1)	3176(5)	9064(5)	3953(2)	24(1)
N(2)	1102(6)	7926(5)	1778(2)	25(1)
N(3)	7468(6)	6069(5)	2544(2)	27(1)
C(1)	5436(7)	7482(6)	3321(2)	25(1)
C(2)	3623(6)	8319(6)	3358(2)	22(1)
C(3)	2219(6)	8458(6)	2872(2)	20(1)
C(4)	2598(6)	7832(6)	2286(2)	22(1)
C(5)	4329(6)	7079(6)	2187(2)	22(1)

C(6)	5701(6)	6911(6)	2682(2)	23(1)
N(4)	9967(5)	6382(5)	4312(2)	24(1)
N(5)	11721(5)	5614(5)	4333(2)	28(1)
N(6)	11467(5)	7086(5)	5169(2)	23(1)
N(7)	11858(6)	7855(5)	5744(2)	35(1)
N(8)	8324(5)	8175(5)	4937(2)	28(1)
C(7)	9787(6)	7284(6)	4813(2)	23(1)
C(8)	12613(6)	6063(6)	4866(2)	25(1)
C(9)	14506(6)	5554(6)	5121(2)	25(1)

Table S19. Bond lengths [Å] and angles [°] for **7**.

O(1)-C(1)	1.241(5)
O(2)-N(1)	1.232(4)
O(3)-N(1)	1.235(4)
O(4)-N(2)	1.238(5)
O(5)-N(2)	1.236(5)
O(6)-N(3)	1.231(5)
O(7)-N(3)	1.239(5)
N(1)-C(2)	1.463(5)
N(2)-C(4)	1.446(5)
N(3)-C(6)	1.459(6)
C(1)-C(2)	1.448(7)
C(1)-C(6)	1.458(6)
C(2)-C(3)	1.373(6)
C(3)-H(3)	0.9500
C(3)-C(4)	1.390(6)
C(4)-C(5)	1.381(6)
C(5)-H(5)	0.9500
C(5)-C(6)	1.375(6)
N(4)-H(4)	0.8800
N(4)-N(5)	1.376(5)
N(4)-C(7)	1.339(6)
N(5)-C(8)	1.314(6)
N(6)-N(7)	1.406(5)
N(6)-C(7)	1.350(5)
N(6)-C(8)	1.378(6)
N(7)-H(7A)	0.8637
N(7)-H(7B)	0.8639
N(8)-H(8A)	0.8800
N(8)-H(8B)	0.8800
N(8)-C(7)	1.311(6)
C(8)-C(9)	1.446(6)

C(9)-C(9)#1	1.314(9)
C(9)-H(9)	0.9500

O(2)-N(1)-O(3)	121.5(4)
O(2)-N(1)-C(2)	120.6(4)
O(3)-N(1)-C(2)	117.8(3)
O(4)-N(2)-C(4)	119.5(4)
O(5)-N(2)-O(4)	122.6(4)
O(5)-N(2)-C(4)	117.8(4)
O(6)-N(3)-O(7)	121.4(4)
O(6)-N(3)-C(6)	120.5(4)
O(7)-N(3)-C(6)	118.0(4)
O(1)-C(1)-C(2)	123.5(4)
O(1)-C(1)-C(6)	124.6(4)
C(2)-C(1)-C(6)	111.9(4)
C(1)-C(2)-N(1)	119.5(4)
C(3)-C(2)-N(1)	115.6(4)
C(3)-C(2)-C(1)	124.9(4)
C(2)-C(3)-H(3)	120.9
C(2)-C(3)-C(4)	118.3(4)
C(4)-C(3)-H(3)	120.9
C(3)-C(4)-N(2)	118.8(4)
C(5)-C(4)-N(2)	119.5(4)
C(5)-C(4)-C(3)	121.7(4)
C(4)-C(5)-H(5)	120.2
C(6)-C(5)-C(4)	119.5(4)
C(6)-C(5)-H(5)	120.2
C(1)-C(6)-N(3)	120.2(4)
C(5)-C(6)-N(3)	116.2(4)
C(5)-C(6)-C(1)	123.6(4)
N(5)-N(4)-H(4)	123.7
C(7)-N(4)-H(4)	123.7
C(7)-N(4)-N(5)	112.7(4)
C(8)-N(5)-N(4)	104.0(4)
C(7)-N(6)-N(7)	122.4(4)
C(7)-N(6)-C(8)	108.2(4)
C(8)-N(6)-N(7)	129.4(4)
N(6)-N(7)-H(7A)	108.9
N(6)-N(7)-H(7B)	109.9
H(7A)-N(7)-H(7B)	109.0
H(8A)-N(8)-H(8B)	120.0
C(7)-N(8)-H(8A)	120.0
C(7)-N(8)-H(8B)	120.0
N(4)-C(7)-N(6)	104.7(4)

N(8)-C(7)-N(4)	128.5(4)
N(8)-C(7)-N(6)	126.9(4)
N(5)-C(8)-N(6)	110.5(4)
N(5)-C(8)-C(9)	126.1(4)
N(6)-C(8)-C(9)	123.4(4)
C(8)-C(9)-H(9)	118.1
C(9)#1-C(9)-C(8)	123.8(5)
C(9)#1-C(9)-H(9)	118.1

Symmetry transformations used to generate equivalent atoms:

#1 -x+3,-y+1,-z+1

Table S20. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **7**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	28(2)	47(2)	22(2)	-3(2)	-11(1)	10(2)
O(2)	33(2)	46(3)	22(2)	-9(2)	-16(2)	13(2)
O(3)	23(2)	39(2)	21(2)	-2(2)	-2(1)	1(2)
O(4)	22(2)	43(2)	27(2)	-5(2)	-12(1)	11(2)
O(5)	38(2)	41(2)	18(2)	-10(2)	-12(1)	11(2)
O(6)	19(2)	57(3)	29(2)	-8(2)	-13(1)	8(2)
O(7)	36(2)	54(3)	18(2)	-8(2)	-7(1)	12(2)
N(1)	24(2)	31(3)	15(2)	1(2)	-6(2)	4(2)
N(2)	23(2)	36(3)	15(2)	0(2)	-10(2)	2(2)
N(3)	20(2)	37(3)	23(2)	1(2)	-3(2)	1(2)
C(1)	22(3)	35(3)	17(2)	1(2)	-7(2)	-2(2)
C(2)	20(2)	31(3)	15(2)	-2(2)	-4(2)	-3(2)
C(3)	12(2)	28(3)	21(2)	1(2)	-3(2)	6(2)
C(4)	20(2)	32(3)	13(2)	-1(2)	-11(2)	-1(2)
C(5)	18(2)	29(3)	17(2)	0(2)	-5(2)	-4(2)
C(6)	16(2)	32(3)	20(2)	0(2)	-5(2)	2(2)
N(4)	17(2)	39(3)	15(2)	-2(2)	-9(2)	4(2)
N(5)	19(2)	42(3)	20(2)	-1(2)	-7(2)	8(2)
N(6)	20(2)	31(3)	17(2)	-1(2)	-5(2)	4(2)
N(7)	25(2)	51(3)	28(2)	-15(2)	-11(2)	12(2)
N(8)	18(2)	45(3)	20(2)	-3(2)	-9(2)	7(2)
C(7)	13(2)	37(3)	17(2)	3(2)	-3(2)	0(2)
C(8)	23(3)	33(3)	17(2)	0(2)	-2(2)	2(2)
C(9)	17(2)	39(3)	18(2)	-2(2)	-5(2)	4(2)

Table S21. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **7**.

	x	y	z	U(eq)
H(3)	1019	8969	2935	25
H(5)	4571	6681	1780	26
H(4)	9061	6290	4002	29
H(7A)	13010	8258	5736	42
H(7B)	10993	8550	5787	42
H(8A)	7288	8230	4672	34
H(8B)	8377	8719	5286	34
H(9)	15068	6051	5484	30

Table S22. Torsion angles [°] for **7**.

O(1)-C(1)-C(2)-N(1)	7.7(8)
O(1)-C(1)-C(2)-C(3)	-170.8(5)
O(1)-C(1)-C(6)-N(3)	-5.2(8)
O(1)-C(1)-C(6)-C(5)	172.8(5)
O(2)-N(1)-C(2)-C(1)	16.7(7)
O(2)-N(1)-C(2)-C(3)	-164.6(4)
O(3)-N(1)-C(2)-C(1)	-164.5(4)
O(3)-N(1)-C(2)-C(3)	14.2(6)
O(4)-N(2)-C(4)-C(3)	4.3(7)
O(4)-N(2)-C(4)-C(5)	-178.1(4)
O(5)-N(2)-C(4)-C(3)	-173.6(4)
O(5)-N(2)-C(4)-C(5)	4.0(7)
O(6)-N(3)-C(6)-C(1)	-8.8(7)
O(6)-N(3)-C(6)-C(5)	173.1(5)
O(7)-N(3)-C(6)-C(1)	171.9(4)
O(7)-N(3)-C(6)-C(5)	-6.2(6)
N(1)-C(2)-C(3)-C(4)	177.2(4)
N(2)-C(4)-C(5)-C(6)	-176.1(4)
C(1)-C(2)-C(3)-C(4)	-4.2(8)
C(2)-C(1)-C(6)-N(3)	178.4(4)
C(2)-C(1)-C(6)-C(5)	-3.6(7)
C(2)-C(3)-C(4)-N(2)	177.9(4)
C(2)-C(3)-C(4)-C(5)	0.3(7)
C(3)-C(4)-C(5)-C(6)	1.5(7)
C(4)-C(5)-C(6)-N(3)	178.4(4)

C(4)-C(5)-C(6)-C(1)	0.4(8)
C(6)-C(1)-C(2)-N(1)	-175.8(4)
C(6)-C(1)-C(2)-C(3)	5.6(7)
N(4)-N(5)-C(8)-N(6)	-0.3(5)
N(4)-N(5)-C(8)-C(9)	178.3(5)
N(5)-N(4)-C(7)-N(6)	-0.3(5)
N(5)-N(4)-C(7)-N(8)	179.4(5)
N(5)-C(8)-C(9)-C(9)#1	-7.5(10)
N(6)-C(8)-C(9)-C(9)#1	171.0(6)
N(7)-N(6)-C(7)-N(4)	179.6(4)
N(7)-N(6)-C(7)-N(8)	-0.1(8)
N(7)-N(6)-C(8)-N(5)	-179.3(4)
N(7)-N(6)-C(8)-C(9)	2.0(8)
C(7)-N(4)-N(5)-C(8)	0.4(5)
C(7)-N(6)-C(8)-N(5)	0.1(6)
C(7)-N(6)-C(8)-C(9)	-178.5(4)
C(8)-N(6)-C(7)-N(4)	0.1(5)
C(8)-N(6)-C(7)-N(8)	-179.6(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x+3,-y+1,-z+1

Table S23. Hydrogen bonds for **7** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(4)-H(4)...O(1)	0.88	1.93	2.627(5)	135.4
N(8)-H(8A)...O(1)	0.88	2.11	2.785(5)	133.2

Symmetry transformations used to generate equivalent atoms:

#1 -x+3,-y+1,-z+1

Table S24. 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)
O(1)	5301(5)	1403(10)	5478(2)	75(2)
O(2)	3471(6)	-131(12)	5812(2)	95(2)
O(3)	3404(5)	276(10)	6680(2)	71(2)
O(4)	4289(4)	4431(9)	7200(2)	51(1)

O(5)	5916(5)	7565(10)	7795(2)	69(1)
O(6)	6647(5)	10207(9)	7281(2)	71(1)
O(7)	7456(4)	8348(10)	6450(2)	58(1)
O(8)	8079(8)	5810(20)	5630(3)	137(2)
O(9)	6773(8)	4100(20)	5086(3)	143(2)
N(1)	3817(4)	943(10)	6281(2)	48(1)
N(2)	6147(4)	8132(10)	7335(2)	43(1)
N(3)	7099(6)	4991(15)	5538(3)	80(2)
C(1)	5452(5)	3013(12)	5912(2)	46(1)
C(2)	4736(5)	2847(11)	6334(2)	41(1)
C(3)	4934(5)	4534(11)	6835(2)	38(1)
C(4)	5891(5)	6410(10)	6853(2)	38(1)
C(5)	6599(5)	6613(11)	6431(2)	43(1)
C(6)	6374(5)	4872(12)	5965(2)	48(1)
N(4)	3371(5)	701(12)	7949(2)	56(1)
N(5)	4639(5)	4122(12)	8367(2)	52(1)
N(6)	5017(5)	5216(11)	8902(2)	56(1)
N(7)	3824(4)	1886(9)	8933(2)	42(1)
N(8)	3054(6)	71(12)	9110(2)	58(1)
C(7)	3912(5)	2157(12)	8377(2)	42(1)
C(8)	4509(5)	3819(12)	9236(2)	44(1)
C(9)	4616(5)	4194(14)	9852(2)	49(1)

Table S25. Bond lengths [Å] and angles [°] for **8**.

O(1)-H(1)	0.8200
O(1)-C(1)	1.311(7)
O(2)-N(1)	1.238(6)
O(3)-N(1)	1.188(6)
O(4)-C(3)	1.238(6)
O(5)-N(2)	1.211(6)
O(6)-N(2)	1.233(6)
O(7)-H(7)	0.90(12)
O(7)-C(5)	1.313(7)
O(8)-N(3)	1.162(9)
O(9)-N(3)	1.160(9)
N(1)-C(2)	1.417(7)
N(2)-C(4)	1.436(7)
N(3)-C(6)	1.425(7)
C(1)-C(2)	1.408(7)
C(1)-C(6)	1.404(8)
C(2)-C(3)	1.458(7)
C(3)-C(4)	1.445(7)
C(4)-C(5)	1.403(7)
C(5)-C(6)	1.412(8)
N(4)-H(4A)	0.90(10)
N(4)-H(4B)	0.97(9)
N(4)-C(7)	1.316(8)
N(5)-H(5)	0.81(8)
N(5)-N(6)	1.379(7)
N(5)-C(7)	1.310(8)
N(6)-C(8)	1.290(8)
N(7)-N(8)	1.400(7)
N(7)-C(7)	1.351(6)
N(7)-C(8)	1.377(8)
N(8)-H(8A)	0.95(12)
N(8)-H(8B)	1.10(11)
C(8)-C(9)	1.458(7)
C(9)-C(9)#1	1.303(13)
C(9)-H(9)	1.00(7)
C(1)-O(1)-H(1)	109.5
C(5)-O(7)-H(7)	106(7)
O(2)-N(1)-C(2)	119.1(5)
O(3)-N(1)-O(2)	119.0(5)
O(3)-N(1)-C(2)	121.8(5)
O(5)-N(2)-O(6)	119.3(5)

O(5)-N(2)-C(4)	121.7(5)
O(6)-N(2)-C(4)	118.9(4)
O(8)-N(3)-C(6)	122.5(6)
O(9)-N(3)-O(8)	115.7(6)
O(9)-N(3)-C(6)	121.6(7)
O(1)-C(1)-C(2)	121.3(5)
O(1)-C(1)-C(6)	119.0(5)
C(6)-C(1)-C(2)	119.7(5)
N(1)-C(2)-C(3)	118.7(4)
C(1)-C(2)-N(1)	119.3(5)
C(1)-C(2)-C(3)	121.9(5)
O(4)-C(3)-C(2)	122.1(5)
O(4)-C(3)-C(4)	123.0(5)
C(4)-C(3)-C(2)	114.8(4)
N(2)-C(4)-C(3)	118.2(4)
C(5)-C(4)-N(2)	118.1(5)
C(5)-C(4)-C(3)	123.7(5)
O(7)-C(5)-C(4)	123.0(5)
O(7)-C(5)-C(6)	118.7(5)
C(4)-C(5)-C(6)	118.3(5)
C(1)-C(6)-N(3)	118.9(5)
C(1)-C(6)-C(5)	121.5(5)
C(5)-C(6)-N(3)	119.5(6)
H(4A)-N(4)-H(4B)	120(8)
C(7)-N(4)-H(4A)	122(7)
C(7)-N(4)-H(4B)	116(5)
N(6)-N(5)-H(5)	112(6)
C(7)-N(5)-H(5)	136(6)
C(7)-N(5)-N(6)	112.4(5)
C(8)-N(6)-N(5)	104.1(5)
C(7)-N(7)-N(8)	122.2(5)
C(7)-N(7)-C(8)	107.1(5)
C(8)-N(7)-N(8)	130.4(4)
N(7)-N(8)-H(8A)	110(7)
N(7)-N(8)-H(8B)	89(6)
H(8A)-N(8)-H(8B)	144(8)
N(4)-C(7)-N(7)	125.8(6)
N(5)-C(7)-N(4)	128.8(5)
N(5)-C(7)-N(7)	105.5(5)
N(6)-C(8)-N(7)	110.9(5)
N(6)-C(8)-C(9)	125.9(6)
N(7)-C(8)-C(9)	123.2(5)
C(8)-C(9)-H(9)	114(4)
C(9)#1-C(9)-C(8)	122.8(7)

C(9)#1-C(9)-H(9) 123(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+2

Table S26. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **8**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	91(4)	85(4)	54(3)	-34(2)	29(2)	-23(3)
O(2)	130(5)	108(5)	51(3)	-29(3)	25(3)	-72(4)
O(3)	86(3)	85(4)	45(2)	-7(2)	22(2)	-41(3)
O(4)	50(2)	70(3)	37(2)	-12(2)	18(2)	-13(2)
O(5)	89(3)	86(3)	37(2)	-20(2)	25(2)	-31(3)
O(6)	102(4)	58(3)	52(3)	-8(2)	10(2)	-22(3)
O(7)	51(3)	68(3)	59(3)	-7(2)	19(2)	-16(2)
O(8)	126(4)	197(5)	109(4)	-45(4)	71(4)	-61(4)
O(9)	130(4)	217(6)	100(4)	-45(4)	68(4)	-56(4)
N(1)	55(3)	55(3)	33(2)	-7(2)	11(2)	-10(2)
N(2)	38(2)	52(3)	38(2)	-6(2)	4(2)	-1(2)
N(3)	79(4)	122(5)	53(3)	-32(3)	43(3)	-38(4)
C(1)	51(3)	54(3)	35(3)	-5(2)	15(2)	-4(3)
C(2)	38(3)	54(3)	31(2)	-4(2)	9(2)	-7(3)
C(3)	37(3)	47(3)	32(3)	0(2)	9(2)	-3(2)
C(4)	37(3)	48(3)	31(3)	-2(2)	9(2)	-2(2)
C(5)	38(3)	54(3)	40(3)	0(2)	13(2)	-3(3)
C(6)	47(3)	65(4)	36(3)	0(2)	18(2)	-1(3)
N(4)	57(3)	78(4)	35(3)	-15(2)	15(2)	-7(3)
N(5)	49(3)	82(4)	27(2)	-4(2)	13(2)	-9(3)
N(6)	56(3)	79(4)	34(2)	-7(2)	14(2)	-19(3)
N(7)	39(2)	56(3)	31(2)	0(2)	12(2)	4(2)
N(8)	71(4)	59(3)	48(3)	1(2)	20(3)	-9(3)
C(7)	34(3)	59(4)	36(3)	-3(2)	13(2)	9(3)
C(8)	38(3)	62(4)	32(3)	-5(2)	9(2)	2(3)
C(9)	47(3)	74(4)	26(3)	-3(2)	8(2)	-3(3)

Table S27. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **8**.

	x	y	z	U(eq)
H(1)	5352	-82	5599	112
H(7)	7380(100)	9400(200)	6730(50)	130(40)
H(4A)	3600(90)	700(200)	7610(40)	110(30)
H(4B)	2600(80)	-30(160)	7990(30)	80(20)
H(5)	4950(70)	4830(150)	8130(30)	70(20)
H(8A)	3510(100)	-1300(200)	9300(40)	130(40)
H(8B)	2430(100)	1700(200)	9160(40)	130(40)
H(9)	4040(60)	3150(120)	10020(30)	55(17)

Table S28. Torsion angles [°] for **8**.

O(1)-C(1)-C(2)-N(1)	-1.5(9)
O(1)-C(1)-C(2)-C(3)	176.7(6)
O(1)-C(1)-C(6)-N(3)	1.5(10)
O(1)-C(1)-C(6)-C(5)	-178.4(6)
O(2)-N(1)-C(2)-C(1)	-16.4(9)
O(2)-N(1)-C(2)-C(3)	165.3(6)
O(3)-N(1)-C(2)-C(1)	160.5(6)
O(3)-N(1)-C(2)-C(3)	-17.8(9)
O(4)-C(3)-C(4)-N(2)	3.7(8)
O(4)-C(3)-C(4)-C(5)	-177.5(5)
O(5)-N(2)-C(4)-C(3)	25.4(8)
O(5)-N(2)-C(4)-C(5)	-153.5(5)
O(6)-N(2)-C(4)-C(3)	-156.8(5)
O(6)-N(2)-C(4)-C(5)	24.4(8)
O(7)-C(5)-C(6)-N(3)	1.7(9)
O(7)-C(5)-C(6)-C(1)	-178.4(6)
O(8)-N(3)-C(6)-C(1)	-154.5(10)
O(8)-N(3)-C(6)-C(5)	25.4(13)
O(9)-N(3)-C(6)-C(1)	20.0(13)
O(9)-N(3)-C(6)-C(5)	-160.1(9)
N(1)-C(2)-C(3)-O(4)	-3.4(9)
N(1)-C(2)-C(3)-C(4)	179.9(5)
N(2)-C(4)-C(5)-O(7)	-2.1(8)
N(2)-C(4)-C(5)-C(6)	178.1(5)
C(1)-C(2)-C(3)-O(4)	178.3(5)
C(1)-C(2)-C(3)-C(4)	1.6(8)
C(2)-C(1)-C(6)-N(3)	179.2(6)

C(2)-C(1)-C(6)-C(5)	-0.6(9)
C(2)-C(3)-C(4)-N(2)	-179.6(5)
C(2)-C(3)-C(4)-C(5)	-0.8(8)
C(3)-C(4)-C(5)-O(7)	179.2(5)
C(3)-C(4)-C(5)-C(6)	-0.6(8)
C(4)-C(5)-C(6)-N(3)	-178.5(6)
C(4)-C(5)-C(6)-C(1)	1.4(9)
C(6)-C(1)-C(2)-N(1)	-179.2(5)
C(6)-C(1)-C(2)-C(3)	-1.0(9)
N(5)-N(6)-C(8)-N(7)	-0.1(7)
N(5)-N(6)-C(8)-C(9)	-179.5(5)
N(6)-N(5)-C(7)-N(4)	178.9(6)
N(6)-N(5)-C(7)-N(7)	-1.5(7)
N(6)-C(8)-C(9)-C(9)#1	-9.7(12)
N(7)-C(8)-C(9)-C(9)#1	170.9(8)
N(8)-N(7)-C(7)-N(4)	-4.7(9)
N(8)-N(7)-C(7)-N(5)	175.7(5)
N(8)-N(7)-C(8)-N(6)	-174.5(6)
N(8)-N(7)-C(8)-C(9)	4.9(9)
C(7)-N(5)-N(6)-C(8)	1.0(7)
C(7)-N(7)-C(8)-N(6)	-0.9(6)
C(7)-N(7)-C(8)-C(9)	178.6(5)
C(8)-N(7)-C(7)-N(4)	-179.0(6)
C(8)-N(7)-C(7)-N(5)	1.4(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+2

Table S29. Hydrogen bonds for **8** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(7)-H(7)...O(6)	0.90(12)	1.72(11)	2.525(6)	148(11)
N(5)-H(5)...O(4)	0.81(8)	2.19(8)	2.728(6)	124(7)
N(5)-H(5)...O(5)	0.81(8)	2.04(8)	2.806(7)	157(8)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+2

Table S30. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **9·3H$_2$O**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	6727(2)	2751(1)	5841(1)	20(1)
N(2)	7156(2)	3749(1)	7356(1)	19(1)
N(3)	10065(1)	2905(1)	6760(1)	15(1)
N(4)	12135(2)	2591(1)	6823(1)	21(1)
N(5)	8686(2)	1278(1)	4147(1)	23(1)
C(1)	8469(2)	2235(1)	5472(1)	16(1)
C(2)	9190(2)	3812(1)	7894(1)	14(1)
C(3)	10461(2)	4696(1)	9436(1)	15(1)
O(1)	5489(1)	3555(1)	2026(1)	30(1)
O(2)	4990(1)	3119(1)	-246(1)	31(1)
O(3)	-2901(1)	-65(1)	-3263(1)	26(1)
O(4)	-4672(1)	-122(1)	-1698(1)	27(1)
N(6)	1174(2)	2343(1)	1481(1)	20(1)
N(7)	849(1)	1546(1)	-998(1)	17(1)
N(8)	4340(2)	3023(1)	749(1)	21(1)
N(9)	-2985(2)	263(1)	-1988(1)	18(1)
C(4)	2090(2)	2265(1)	396(1)	18(1)
C(5)	-1087(2)	1119(1)	-779(1)	16(1)
C(6)	-923(2)	1596(1)	718(1)	19(1)
O(5)	3421(2)	3678(1)	4545(1)	27(1)
O(6)	394(4)	5210(3)	5599(3)	37(1)

Table S31. Bond lengths [Å] and angles [°] for **9·3H$_2$O**.

N(1)-H(1)	0.866(19)
N(1)-N(2)	1.3860(12)
N(1)-C(1)	1.3349(14)
N(2)-C(2)	1.3081(14)
N(3)-N(4)	1.4000(13)
N(3)-C(1)	1.3527(12)
N(3)-C(2)	1.3897(13)
N(4)-H(4A)	0.903(18)
N(4)-H(4B)	0.89(2)
N(5)-H(5A)	0.863(18)
N(5)-H(5B)	0.870(19)

N(5)-C(1)	1.3234(13)
C(2)-C(3)	1.4504(13)
C(3)-C(3)#1	1.3406(19)
C(3)-H(3)	0.989(16)
O(1)-N(8)	1.2321(12)
O(2)-N(8)	1.2345(14)
O(3)-N(9)	1.2378(12)
O(4)-N(9)	1.2426(13)
N(6)-C(4)	1.3503(14)
N(6)-C(6)	1.3527(14)
N(7)-C(4)	1.3303(13)
N(7)-C(5)	1.3594(14)
N(8)-C(4)	1.4442(14)
N(9)-C(5)	1.4217(13)
C(5)-C(6)	1.3963(14)
C(6)-H(6)	0.939(16)
O(5)-H(5AA)	0.8701
O(5)-H(5BB)	0.865(18)
O(5)-H(5C)	0.92(4)
O(6)-O(6)#2	1.118(5)
O(6)-H(6A)	0.865(18)
O(6)-H(6B)	0.90(5)

N(2)-N(1)-H(1)	118.5(12)
C(1)-N(1)-H(1)	128.6(12)
C(1)-N(1)-N(2)	111.89(9)
C(2)-N(2)-N(1)	104.46(9)
C(1)-N(3)-N(4)	122.23(8)
C(1)-N(3)-C(2)	107.42(9)
C(2)-N(3)-N(4)	130.25(8)
N(3)-N(4)-H(4A)	104.3(11)
N(3)-N(4)-H(4B)	107.3(13)
H(4A)-N(4)-H(4B)	111.9(16)
H(5A)-N(5)-H(5B)	121.1(16)
C(1)-N(5)-H(5A)	120.8(12)
C(1)-N(5)-H(5B)	117.6(11)
N(1)-C(1)-N(3)	105.68(9)
N(5)-C(1)-N(1)	129.30(10)

N(5)-C(1)-N(3)	125.01(10)
N(2)-C(2)-N(3)	110.53(9)
N(2)-C(2)-C(3)	127.28(9)
N(3)-C(2)-C(3)	122.19(9)
C(2)-C(3)-H(3)	118.1(9)
C(3)#1-C(3)-C(2)	122.40(12)
C(3)#1-C(3)-H(3)	119.5(9)
C(4)-N(6)-C(6)	102.39(9)
C(4)-N(7)-C(5)	99.64(9)
O(1)-N(8)-O(2)	123.80(10)
O(1)-N(8)-C(4)	118.42(10)
O(2)-N(8)-C(4)	117.78(9)
O(3)-N(9)-O(4)	123.06(9)
O(3)-N(9)-C(5)	119.74(9)
O(4)-N(9)-C(5)	117.20(9)
N(6)-C(4)-N(8)	120.77(9)
N(7)-C(4)-N(6)	118.74(9)
N(7)-C(4)-N(8)	120.39(9)
N(7)-C(5)-N(9)	121.26(9)
N(7)-C(5)-C(6)	112.05(9)
C(6)-C(5)-N(9)	126.68(10)
N(6)-C(6)-C(5)	107.19(10)
N(6)-C(6)-H(6)	123.0(9)
C(5)-C(6)-H(6)	129.8(9)
H(5AA)-O(5)-H(5BB)	100.9
H(5AA)-O(5)-H(5C)	113.0
O(6)#2-O(6)-H(6A)	55(2)
O(6)#2-O(6)-H(6B)	149(3)
H(6A)-O(6)-H(6B)	109(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z+2 #2 -x,-y+1,-z+1

Table S32. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **9·3H$_2$O.** The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	14(1)	27(1)	12(1)	6(1)	1(1)	5(1)
N(2)	16(1)	23(1)	13(1)	6(1)	2(1)	6(1)
N(3)	12(1)	18(1)	12(1)	6(1)	2(1)	4(1)
N(4)	14(1)	29(1)	18(1)	10(1)	4(1)	10(1)
N(5)	19(1)	28(1)	12(1)	4(1)	2(1)	5(1)
C(1)	15(1)	18(1)	14(1)	7(1)	2(1)	2(1)
C(2)	14(1)	15(1)	12(1)	6(1)	3(1)	3(1)
C(3)	14(1)	15(1)	13(1)	6(1)	2(1)	2(1)
O(1)	20(1)	32(1)	26(1)	9(1)	-5(1)	2(1)
O(2)	19(1)	40(1)	38(1)	26(1)	4(1)	0(1)
O(3)	25(1)	30(1)	16(1)	9(1)	1(1)	3(1)
O(4)	14(1)	35(1)	28(1)	16(1)	2(1)	-1(1)
N(6)	19(1)	21(1)	17(1)	9(1)	1(1)	4(1)
N(7)	14(1)	17(1)	19(1)	9(1)	2(1)	3(1)
N(8)	16(1)	20(1)	25(1)	11(1)	0(1)	3(1)
N(9)	15(1)	18(1)	18(1)	8(1)	1(1)	3(1)
C(4)	14(1)	17(1)	20(1)	9(1)	1(1)	2(1)
C(5)	13(1)	17(1)	16(1)	8(1)	1(1)	3(1)
C(6)	18(1)	22(1)	18(1)	10(1)	4(1)	5(1)
O(5)	26(1)	29(1)	22(1)	12(1)	-1(1)	6(1)
O(6)	35(1)	35(1)	35(1)	11(1)	9(1)	13(1)

Table S33. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **9·3H$_2$O**.

	x	y	z	U(eq)
H(1)	5520(30)	2670(20)	5260(20)	39(5)
H(4A)	12330(30)	2290(20)	7512(19)	37(5)
H(4B)	13080(30)	3450(20)	7110(20)	42(5)
H(5A)	7570(30)	800(20)	3381(19)	37(5)
H(5B)	9950(30)	1060(20)	4100(19)	34(4)
H(3)	12060(30)	4853(17)	9650(16)	24(4)
H(6)	-2000(30)	1464(18)	1177(17)	26(4)
H(5AA)	2909	3237	3584	41
H(5BB)	2420(40)	4150(30)	4840(30)	20(7)
H(6A)	-880(30)	5300(30)	5270(30)	19(7)
H(6B)	990(80)	6000(50)	6530(50)	65(13)
H(5C)	4460(80)	4570(50)	4940(50)	60(13)

Table S34. Torsion angles [°] for **9·3H$_2$O.**

N(1)-N(2)-C(2)-N(3)	1.02(12)
N(1)-N(2)-C(2)-C(3)	-179.85(10)
N(2)-N(1)-C(1)-N(3)	-0.15(12)
N(2)-N(1)-C(1)-N(5)	-179.81(11)
N(2)-C(2)-C(3)-C(3)#1	15.7(2)
N(3)-C(2)-C(3)-C(3)#1	-165.32(12)
N(4)-N(3)-C(1)-N(1)	177.58(10)
N(4)-N(3)-C(1)-N(5)	-2.73(16)
N(4)-N(3)-C(2)-N(2)	-177.64(10)
N(4)-N(3)-C(2)-C(3)	3.18(16)
C(1)-N(1)-N(2)-C(2)	-0.55(12)
C(1)-N(3)-C(2)-N(2)	-1.16(12)
C(1)-N(3)-C(2)-C(3)	179.66(9)
C(2)-N(3)-C(1)-N(1)	0.75(11)
C(2)-N(3)-C(1)-N(5)	-179.56(10)
O(1)-N(8)-C(4)-N(6)	10.22(16)

O(1)-N(8)-C(4)-N(7)	-173.48(10)
O(2)-N(8)-C(4)-N(6)	-168.76(10)
O(2)-N(8)-C(4)-N(7)	7.54(16)
O(3)-N(9)-C(5)-N(7)	-2.16(15)
O(3)-N(9)-C(5)-C(6)	179.06(10)
O(4)-N(9)-C(5)-N(7)	177.82(10)
O(4)-N(9)-C(5)-C(6)	-0.96(16)
N(7)-C(5)-C(6)-N(6)	-0.28(13)
N(9)-C(5)-C(6)-N(6)	178.59(10)
C(4)-N(6)-C(6)-C(5)	0.35(12)
C(4)-N(7)-C(5)-N(9)	-178.87(10)
C(4)-N(7)-C(5)-C(6)	0.07(12)
C(5)-N(7)-C(4)-N(6)	0.19(12)
C(5)-N(7)-C(4)-N(8)	-176.19(9)
C(6)-N(6)-C(4)-N(7)	-0.36(13)
C(6)-N(6)-C(4)-N(8)	176.00(10)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z+2 #2 -x,-y+1,-z+1

Table S35. Hydrogen bonds for **9·3H$_2$O** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(5)	0.866(19)	2.033(19)	2.8127(14)	149.5(17)
O(5)-H(5AA)...N(6)	0.87	1.99	2.8516(13)	168.2
O(6)-H(6A)...O(5)#2	0.865(18)	2.03(2)	2.828(3)	154(3)
O(5)-H(5C)...O(5)#3	0.92(4)	1.88(4)	2.799(2)	172(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z+2 #2 -x,-y+1,-z+1 #3 -x+1,-y+1,-z+1

Table S36. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **10**. U(eq) is defined as one third of of the trace of the orthogonalised U^{IJ} tensor.

Atom	x	y	z	U(eq)
C1	4961.3(16)	9101(4)	4731.1(14)	17.5(6)
C2	5479.0(16)	7875(4)	2508.0(15)	15.0(5)
C3	5282.0(16)	9111(4)	3855.2(14)	15.1(5)

C4	1429.2(17)	10130(4)	4805.2(15)	18.8(5)
C5	1996.8(16)	8286(4)	4652.1(14)	16.0(5)
C6	2159.5(17)	7287(4)	5495.1(15)	18.3(6)
N1	5790.9(14)	10681(3)	3512.5(12)	17.2(5)
N2	5919.2(15)	9865(3)	2673.2(12)	18.2(5)
N3	5074.9(14)	7359(3)	3253.8(12)	15.0(4)
N4	5436.1(16)	6625(4)	1781.0(14)	23.5(5)
N5	4563.7(16)	5374(3)	3423.5(14)	23.3(5)
N6	1715.0(15)	8466(3)	6093.9(13)	22.6(5)
N7	1253.7(14)	10235(3)	5657.6(13)	24.1(5)
N8	970.8(15)	11798(4)	4181.4(15)	26.2(5)
N9	2362.7(15)	7644(4)	3822.6(13)	21.7(5)
N10	2757.3(14)	5342(3)	5770.3(14)	25.2(5)
O1	587.2(14)	13447(3)	4493.6(13)	40.0(5)
O2	990.7(13)	11467(3)	3377.2(11)	33.4(5)
O3	2954.7(13)	8911(3)	3539.2(11)	31.6(5)
O4	2049.7(14)	5882(3)	3464.4(11)	35.2(5)
O5	3228.2(14)	4515(3)	5206.8(12)	38.0(5)
O6	2776.8(14)	4652(3)	6533.6(12)	39.6(5)

Table S37. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **10**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11}+2hka^*b^*U^{12}+\ldots]$.

Atom	U11	U22	U33	U23	U13	U12
C1	17.0(13)	19.7(13)	15.8(13)	-0.3(9)	2.4(11)	-2.6(11)
C2	15.2(12)	15.3(13)	14.7(12)	-1.1(10)	2.2(10)	1.9(10)
C3	17.0(13)	14.1(13)	14.1(12)	-2.3(10)	1.6(10)	1.6(10)
C4	19.2(13)	18.4(13)	18.4(13)	3.7(11)	0.7(10)	1.2(11)
C5	15.0(12)	19.0(14)	13.7(13)	-2(1)	1.2(10)	-1.5(10)
C6	17.0(13)	19.5(14)	18.3(13)	1.5(11)	2.1(10)	3.6(11)
N1	21.9(11)	19.0(11)	10.9(10)	-2.8(8)	3.0(8)	-1.8(9)
N2	21.7(11)	20.6(12)	13.8(11)	-2.4(9)	7.2(8)	-5(1)
N3	19(1)	11.7(10)	14.9(10)	-0.1(9)	4.5(8)	-1.6(9)
N4	32.1(13)	22.6(13)	18.1(12)	-5.8(10)	11.6(10)	-8.4(10)
N5	26.8(13)	16.3(12)	27.7(12)	-0.2(10)	6.8(10)	-3.6(10)
N6	23.4(12)	25.1(12)	19.8(11)	1.4(10)	4.8(9)	3(1)

N7	26.7(12)	24.3(12)	22.5(12)	1.3(10)	7.4(9)	6.9(10)
N8	20.6(12)	24.5(13)	32.6(14)	6.6(10)	1(1)	-2.3(10)
N9	21.6(11)	26.0(13)	17.7(11)	1.1(10)	3.1(9)	2.1(10)
N10	21.5(12)	27.8(13)	26.4(13)	4(1)	4.1(10)	3(1)
O1	42.2(12)	25.7(11)	55.0(13)	11.5(10)	17.4(10)	15(1)
O2	38.0(12)	34.1(11)	25.3(11)	9.6(8)	-5.7(9)	-6.7(9)
O3	26.9(10)	40.5(12)	29.3(11)	5.0(9)	10.6(8)	-7.9(9)
O4	49.2(12)	31.6(11)	26.5(10)	-12.9(9)	11.5(9)	-9.8(10)
O5	44.0(12)	39.9(12)	32.1(11)	3.5(9)	12.3(10)	22.9(10)
O6	43.4(12)	48.6(13)	28.5(11)	23.1(10)	11.5(9)	16.9(10)

Table S38. Bond Lengths for **10**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C1[1]	1.333(4)	C6	N6	1.344(3)
C1	C3	1.442(3)	C6	N10	1.434(3)
C2	N4	1.316(3)	N1	N2	1.385(2)
C2	N2	1.329(3)	N3	N5	1.404(3)
C2	N3	1.347(3)	N6	N7	1.343(3)
C3	N1	1.303(3)	N8	O2	1.229(2)
C3	N3	1.380(3)	N8	O1	1.229(2)
C4	N7	1.337(3)	N9	O3	1.214(2)
C4	C5	1.371(3)	N9	O4	1.223(2)
C4	N8	1.442(3)	N10	O6	1.216(2)
C5	C6	1.389(3)	N10	O5	1.228(2)
C5	N9	1.454(3)			

[1]1-X,2-Y,1-Z

Table S39. Bond Angles for **10**.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C11	C1	C3	122.9(3)	C3	N1	N2	104.42(17)
N4	C2	N2	128.6(2)	C2	N2	N1	111.89(18)
N4	C2	N3	126.0(2)	C2	N3	C3	107.86(18)
N2	C2	N3	105.44(19)	C2	N3	N5	127.25(18)
N1	C3	N3	110.37(18)	C3	N3	N5	124.84(18)
N1	C3	C1	127.1(2)	C6	N6	N7	107.27(18)

N3	C3	C1	122.5(2)	C4	N7	N6	107.57(19)
N7	C4	C5	112.0(2)	O2	N8	O1	124.8(2)
N7	C4	N8	118.4(2)	O2	N8	C4	117.8(2)
C5	C4	N8	129.5(2)	O1	N8	C4	117.5(2)
C4	C5	C6	102.00(19)	O3	N9	O4	125.2(2)
C4	C5	N9	128.0(2)	O3	N9	C5	117.1(2)
C6	C5	N9	130.0(2)	O4	N9	C5	117.7(2)
N6	C6	C5	111.2(2)	O6	N10	O5	124.9(2)
N6	C6	N10	120.5(2)	O6	N10	C6	118.8(2)
C5	C6	N10	128.2(2)	O5	N10	C6	116.3(2)

[1]1-X,2-Y,1-Z

Table S40. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **10**.

Atom	x	y	z	U(eq)
H1	4683	7755	4934	21
H2A	6274(16)	10540(40)	2314(15)	22
H4A	5072(19)	5450(40)	1738(16)	28
H4B	5667(18)	7270(40)	1337(17)	28
H5A	4980(16)	4260(30)	3389(16)	28
H5B	3958(13)	5330(40)	3079(14)	28

Table S41. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **11**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	3983(1)	8025(2)	5799(1)	21(1)
N(2)	3516(1)	7754(2)	5411(1)	22(1)
N(3)	4237(1)	10843(2)	5454(1)	16(1)
N(4)	4517(1)	12805(2)	5324(1)	21(1)
N(5)	3394(1)	9858(3)	4818(1)	22(1)
N(6)	6237(1)	11746(2)	7423(1)	15(1)
N(7)	5829(1)	12027(2)	7028(1)	16(1)
N(8)	5946(1)	8702(2)	7185(1)	13(1)
N(9)	5908(1)	6539(2)	7170(1)	16(1)
N(10)	6644(1)	8906(2)	7868(1)	16(1)

C(1)	3683(1)	9480(3)	5210(1)	18(1)
C(2)	4413(1)	9868(3)	5822(1)	16(1)
C(3)	4951(1)	10725(2)	6181(1)	16(1)
C(4)	5218(1)	9503(2)	6497(1)	15(1)
C(5)	5665(1)	10156(2)	6888(1)	14(1)
C(6)	6311(1)	9749(2)	7520(1)	13(1)
O(1)	8527(1)	9707(2)	6970(1)	22(1)
O(2)	6569(1)	5603(2)	5619(1)	32(1)
O(3)	6674(2)	3945(3)	6188(1)	54(1)
N(11)	8219(1)	9859(2)	6265(1)	20(1)
N(12)	7735(1)	8676(2)	5966(1)	19(1)
N(13)	7615(1)	7166(2)	6581(1)	16(1)
N(14)	6838(1)	5457(3)	5979(1)	27(1)
C(7)	8150(1)	8970(2)	6638(1)	16(1)
C(8)	7410(1)	7141(2)	6178(1)	17(1)

Table S42. Bond lengths [Å] and angles [°] for **11**.

N(1)-N(2)	1.3941(18)
N(1)-C(2)	1.317(2)
N(2)-C(1)	1.329(2)
N(3)-N(4)	1.4003(19)
N(3)-C(1)	1.365(2)
N(3)-C(2)	1.3786(19)
N(4)-H(4A)	0.93(2)
N(4)-H(4B)	0.90(3)
N(5)-H(5A)	0.88(3)
N(5)-H(5B)	0.87(3)
N(5)-C(1)	1.352(2)
N(6)-H(6)	0.83(3)
N(6)-N(7)	1.3875(17)
N(6)-C(6)	1.337(2)
N(7)-C(5)	1.311(2)
N(8)-N(9)	1.4041(18)
N(8)-C(5)	1.3935(19)
N(8)-C(6)	1.3568(18)
N(9)-H(9A)	0.87(2)
N(9)-H(9B)	0.93(2)
N(10)-H(10A)	0.84(3)
N(10)-H(10B)	0.87(3)
N(10)-C(6)	1.3226(19)
C(2)-C(3)	1.447(2)
C(3)-H(3)	0.96(3)
C(3)-C(4)	1.340(2)
C(4)-H(4)	0.94(2)
C(4)-C(5)	1.445(2)
O(1)-C(7)	1.2661(19)
O(2)-N(14)	1.2275(19)
O(3)-N(14)	1.229(2)
N(11)-H(11)	0.89(3)
N(11)-N(12)	1.3669(19)
N(11)-C(7)	1.376(2)
N(12)-C(8)	1.306(2)
N(13)-C(7)	1.363(2)
N(13)-C(8)	1.3483(19)
N(14)-C(8)	1.447(2)
C(2)-N(1)-N(2)	108.49(13)
C(1)-N(2)-N(1)	106.53(13)
C(1)-N(3)-N(4)	122.61(13)

C(1)-N(3)-C(2)	105.93(13)
C(2)-N(3)-N(4)	131.46(13)
N(3)-N(4)-H(4A)	108.3(14)
N(3)-N(4)-H(4B)	108.4(18)
H(4A)-N(4)-H(4B)	109(2)
H(5A)-N(5)-H(5B)	114(2)
C(1)-N(5)-H(5A)	113.3(15)
C(1)-N(5)-H(5B)	116.8(16)
N(7)-N(6)-H(6)	122.4(17)
C(6)-N(6)-H(6)	125.5(17)
C(6)-N(6)-N(7)	111.77(12)
C(5)-N(7)-N(6)	104.69(12)
C(5)-N(8)-N(9)	130.12(12)
C(6)-N(8)-N(9)	122.54(12)
C(6)-N(8)-C(5)	107.34(13)
N(8)-N(9)-H(9A)	107.0(16)
N(8)-N(9)-H(9B)	110.1(14)
H(9A)-N(9)-H(9B)	106(2)
H(10A)-N(10)-H(10B)	124(2)
C(6)-N(10)-H(10A)	119.0(16)
C(6)-N(10)-H(10B)	117.0(18)
N(2)-C(1)-N(3)	110.06(13)
N(2)-C(1)-N(5)	126.46(15)
N(5)-C(1)-N(3)	123.43(15)
N(1)-C(2)-N(3)	108.99(13)
N(1)-C(2)-C(3)	124.64(14)
N(3)-C(2)-C(3)	126.34(14)
C(2)-C(3)-H(3)	119.1(14)
C(4)-C(3)-C(2)	119.99(15)
C(4)-C(3)-H(3)	120.9(14)
C(3)-C(4)-H(4)	118.2(13)
C(3)-C(4)-C(5)	126.42(15)
C(5)-C(4)-H(4)	115.3(13)
N(7)-C(5)-N(8)	110.38(13)
N(7)-C(5)-C(4)	129.30(14)
N(8)-C(5)-C(4)	120.26(13)
N(6)-C(6)-N(8)	105.82(13)
N(10)-C(6)-N(6)	128.67(14)
N(10)-C(6)-N(8)	125.50(14)
N(12)-N(11)-H(11)	116.2(17)
N(12)-N(11)-C(7)	111.27(13)
C(7)-N(11)-H(11)	132.4(17)
C(8)-N(12)-N(11)	100.59(12)
C(8)-N(13)-C(7)	101.91(13)

O(2)-N(14)-O(3)	124.48(17)
O(2)-N(14)-C(8)	118.94(15)
O(3)-N(14)-C(8)	116.57(15)
O(1)-C(7)-N(11)	125.56(15)
O(1)-C(7)-N(13)	126.88(14)
N(13)-C(7)-N(11)	107.56(13)
N(12)-C(8)-N(13)	118.67(14)
N(12)-C(8)-N(14)	120.16(14)
N(13)-C(8)-N(14)	121.17(14)

Symmetry transformations used to generate equivalent atoms:

Table S43. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **11**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	26(1)	20(1)	15(1)	3(1)	-4(1)	-8(1)
N(2)	28(1)	21(1)	15(1)	3(1)	-6(1)	-10(1)
N(3)	20(1)	15(1)	13(1)	3(1)	-2(1)	-5(1)
N(4)	27(1)	15(1)	20(1)	4(1)	-1(1)	-6(1)
N(5)	28(1)	24(1)	14(1)	4(1)	-6(1)	-9(1)
N(6)	20(1)	12(1)	12(1)	-1(1)	-1(1)	-2(1)
N(7)	20(1)	14(1)	12(1)	0(1)	-2(1)	-1(1)
N(8)	17(1)	10(1)	11(1)	-1(1)	-1(1)	-1(1)
N(9)	23(1)	10(1)	15(1)	-1(1)	0(1)	-1(1)
N(10)	23(1)	12(1)	12(1)	-1(1)	-3(1)	0(1)
C(1)	18(1)	20(1)	15(1)	1(1)	-3(1)	-5(1)
C(2)	18(1)	16(1)	14(1)	3(1)	-1(1)	-3(1)
C(3)	18(1)	16(1)	15(1)	1(1)	-1(1)	-4(1)
C(4)	19(1)	15(1)	13(1)	-1(1)	0(1)	-2(1)
C(5)	15(1)	13(1)	12(1)	2(1)	1(1)	-1(1)
C(6)	13(1)	13(1)	12(1)	-2(1)	1(1)	0(1)
O(1)	37(1)	14(1)	13(1)	0(1)	-4(1)	1(1)
O(2)	42(1)	31(1)	22(1)	-2(1)	-9(1)	-12(1)
O(3)	78(1)	44(1)	38(1)	12(1)	-6(1)	-43(1)
N(11)	31(1)	14(1)	13(1)	2(1)	-3(1)	-6(1)
N(12)	25(1)	17(1)	14(1)	1(1)	-1(1)	-5(1)
N(13)	19(1)	15(1)	13(1)	2(1)	1(1)	-1(1)
N(14)	30(1)	27(1)	22(1)	1(1)	-2(1)	-14(1)
C(7)	21(1)	13(1)	14(1)	2(1)	0(1)	3(1)
C(8)	18(1)	16(1)	16(1)	1(1)	-1(1)	-3(1)

Table S44. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for **11**.

	x	y	z	U(eq)
H(4A)	4160(18)	13780(40)	5464(7)	26(6)
H(4B)	5200(20)	12980(40)	5383(8)	43(7)
H(5A)	2812(19)	9230(40)	4731(7)	28(6)
H(5B)	3432(19)	11130(40)	4737(7)	33(6)
H(6)	6355(18)	12720(40)	7580(7)	31(6)
H(9A)	6283(18)	6150(40)	6975(7)	25(6)
H(9B)	5232(18)	6100(30)	7098(7)	24(5)
H(10A)	6640(18)	7610(40)	7891(7)	28(6)
H(10B)	6877(19)	9740(40)	8060(7)	35(6)
H(3)	5119(18)	12170(40)	6188(7)	32(6)
H(4)	5091(16)	8070(30)	6470(6)	19(5)
H(11)	8470(20)	11070(40)	6188(8)	40(7)

Table S45. Torsion angles [°] for **11**.

N(1)-N(2)-C(1)-N(3)	0.01(19)
N(1)-N(2)-C(1)-N(5)	177.56(17)
N(1)-C(2)-C(3)-C(4)	13.0(3)
N(2)-N(1)-C(2)-N(3)	0.24(19)
N(2)-N(1)-C(2)-C(3)	178.50(15)
N(3)-C(2)-C(3)-C(4)	-169.02(16)
N(4)-N(3)-C(1)-N(2)	-179.33(15)
N(4)-N(3)-C(1)-N(5)	3.0(3)
N(4)-N(3)-C(2)-N(1)	179.16(16)
N(4)-N(3)-C(2)-C(3)	0.9(3)
N(6)-N(7)-C(5)-N(8)	0.71(16)
N(6)-N(7)-C(5)-C(4)	177.93(15)
N(7)-N(6)-C(6)-N(8)	-0.01(17)
N(7)-N(6)-C(6)-N(10)	-178.74(15)
N(9)-N(8)-C(5)-N(7)	-179.71(15)
N(9)-N(8)-C(5)-C(4)	2.8(2)
N(9)-N(8)-C(6)-N(6)	179.50(13)
N(9)-N(8)-C(6)-N(10)	-1.7(2)
C(1)-N(3)-C(2)-N(1)	-0.23(18)
C(1)-N(3)-C(2)-C(3)	-178.45(15)
C(2)-N(1)-N(2)-C(1)	-0.16(19)
C(2)-N(3)-C(1)-N(2)	0.13(19)

C(2)-N(3)-C(1)-N(5)	-177.51(16)
C(2)-C(3)-C(4)-C(5)	-173.66(14)
C(3)-C(4)-C(5)-N(7)	5.7(3)
C(3)-C(4)-C(5)-N(8)	-177.27(15)
C(5)-N(8)-C(6)-N(6)	0.44(16)
C(5)-N(8)-C(6)-N(10)	179.22(14)
C(6)-N(6)-N(7)-C(5)	-0.44(17)
C(6)-N(8)-C(5)-N(7)	-0.75(17)
C(6)-N(8)-C(5)-C(4)	-178.26(13)
O(2)-N(14)-C(8)-N(12)	-7.8(3)
O(2)-N(14)-C(8)-N(13)	172.06(16)
O(3)-N(14)-C(8)-N(12)	170.91(19)
O(3)-N(14)-C(8)-N(13)	-9.2(3)
N(11)-N(12)-C(8)-N(13)	0.3(2)
N(11)-N(12)-C(8)-N(14)	-179.83(15)
N(12)-N(11)-C(7)-O(1)	179.83(15)
N(12)-N(11)-C(7)-N(13)	0.35(19)
C(7)-N(11)-N(12)-C(8)	-0.39(18)
C(7)-N(13)-C(8)-N(12)	-0.1(2)
C(7)-N(13)-C(8)-N(14)	-179.97(15)
C(8)-N(13)-C(7)-O(1)	-179.61(16)
C(8)-N(13)-C(7)-N(11)	-0.14(17)

Symmetry transformations used to generate equivalent atoms:

Table S46. Hydrogen bonds for **11** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(6)-H(6)...O(1)#1	0.83(3)	1.97(3)	2.7866(18)	168(2)
N(10)-H(10A)...O(1)#2	0.84(3)	1.96(3)	2.7875(19)	169(2)
N(11)-H(11)...N(1)#3	0.89(3)	1.96(3)	2.794(2)	155(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+3/2,y+1/2,-z+3/2 #2 -x+3/2,y-1/2,-z+3/2

#3 x+1/2,y+1/2,z

Table S47. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **14**·**2H$_2$O**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)

N(6)	3151(3)	6588(2)	5467(2)	27(1)
N(7)	4943(3)	7485(2)	4846(2)	26(1)
N(8)	3686(3)	6924(2)	2966(2)	22(1)
N(9)	3299(4)	6848(2)	1512(2)	31(1)
N(10)	6864(3)	8436(2)	2388(2)	28(1)
C(2)	5297(3)	7680(2)	3348(2)	22(1)
C(3)	2414(4)	6262(2)	4304(2)	24(1)
C(4)	584(4)	5323(2)	4346(2)	27(1)
N(1)	982(3)	10533(2)	1743(2)	30(1)
N(2)	2537(3)	11402(2)	837(2)	31(1)
N(3)	3621(3)	12058(2)	1651(2)	29(1)
N(4)	2798(3)	11634(2)	3124(2)	27(1)
N(5)	-204(3)	9910(2)	4368(2)	25(1)
C(1)	1197(4)	10705(2)	3132(2)	24(1)
O(1)	7939(4)	4746(3)	1183(2)	58(1)

Table S48. Bond lengths [Å] and angles [°] for **14**·**2H$_2$O**.

N(6)-N(7)	1.396(3)
N(6)-C(3)	1.315(3)
N(7)-H(7)	0.85(3)
N(7)-C(2)	1.331(3)
N(8)-N(9)	1.404(2)
N(8)-C(2)	1.371(3)
N(8)-C(3)	1.393(2)
N(9)-H(9A)	0.92(3)
N(9)-H(9B)	0.89(3)
N(10)-H(10A)	0.84(3)
N(10)-H(10B)	0.84(3)
N(10)-C(2)	1.324(3)
C(3)-C(4)	1.456(3)
C(4)-C(4)#1	1.342(4)
C(4)-H(4)	0.95(2)
N(1)-N(2)	1.353(3)
N(1)-C(1)	1.340(3)
N(2)-N(3)	1.328(3)

N(3)-N(4)	1.351(2)
N(4)-C(1)	1.347(3)
N(5)-N(5)#2	1.267(3)
N(5)-C(1)	1.415(3)
O(1)-H(1A)	0.88(4)
O(1)-H(1B)	0.89(8)

C(3)-N(6)-N(7)	104.95(16)
N(6)-N(7)-H(7)	115(2)
C(2)-N(7)-N(6)	111.62(17)
C(2)-N(7)-H(7)	133(2)
C(2)-N(8)-N(9)	127.56(17)
C(2)-N(8)-C(3)	107.26(16)
C(3)-N(8)-N(9)	125.15(17)
N(8)-N(9)-H(9A)	104.5(16)
N(8)-N(9)-H(9B)	109(2)
H(9A)-N(9)-H(9B)	114(3)
H(10A)-N(10)-H(10B)	118(3)
C(2)-N(10)-H(10A)	119.0(19)
C(2)-N(10)-H(10B)	123(2)
N(7)-C(2)-N(8)	105.92(18)
N(10)-C(2)-N(7)	128.48(19)
N(10)-C(2)-N(8)	125.61(19)
N(6)-C(3)-N(8)	110.23(18)
N(6)-C(3)-C(4)	126.78(19)
N(8)-C(3)-C(4)	122.97(19)
C(3)-C(4)-H(4)	117.1(14)
C(4)#1-C(4)-C(3)	121.6(3)
C(4)#1-C(4)-H(4)	121.3(14)
C(1)-N(1)-N(2)	103.58(17)
N(3)-N(2)-N(1)	110.43(17)
N(2)-N(3)-N(4)	108.88(18)
C(1)-N(4)-N(3)	104.41(16)
N(5)#2-N(5)-C(1)	113.1(2)
N(1)-C(1)-N(4)	112.70(18)
N(1)-C(1)-N(5)	117.87(19)
N(4)-C(1)-N(5)	129.43(19)
H(1A)-O(1)-H(1B)	99(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1 #2 -x,-y+2,-z+1

Table S49. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **14·2H$_2$O**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(6)	30(1)	22(1)	23(1)	2(1)	-1(1)	-2(1)
N(7)	31(1)	26(1)	19(1)	-1(1)	-3(1)	-4(1)
N(8)	28(1)	20(1)	18(1)	-1(1)	-3(1)	-6(1)
N(9)	38(1)	34(1)	22(1)	-7(1)	-6(1)	-8(1)
N(10)	32(1)	32(1)	23(1)	-4(1)	-3(1)	-14(1)
C(2)	24(1)	18(1)	22(1)	-2(1)	-4(1)	-2(1)
C(3)	25(1)	18(1)	22(1)	2(1)	2(1)	0(1)
C(4)	27(1)	20(1)	30(1)	-1(1)	-2(1)	-1(1)
N(1)	40(1)	29(1)	21(1)	-3(1)	-4(1)	-8(1)
N(2)	42(1)	33(1)	20(1)	-2(1)	-4(1)	-12(1)
N(3)	42(1)	30(1)	18(1)	-3(1)	-2(1)	-11(1)
N(4)	35(1)	26(1)	18(1)	-2(1)	-2(1)	-5(1)
N(5)	31(1)	20(1)	22(1)	-3(1)	-4(1)	-1(1)
C(1)	29(1)	21(1)	19(1)	-1(1)	0(1)	-1(1)
O(1)	63(1)	68(2)	34(1)	-10(1)	-9(1)	12(1)

Table S50. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2 x\ 10^3$) for **14·2H$_2$O**.

	x	y	z	U(eq)
H(7)	5590(60)	7780(30)	5480(40)	61(9)
H(9A)	4760(50)	6410(30)	1070(30)	44(7)
H(9B)	2780(60)	7810(40)	1040(40)	75(10)
H(10A)	7020(50)	8380(30)	1470(30)	49(8)
H(10B)	7760(50)	8940(30)	2670(30)	52(8)
H(4)	300(40)	5150(30)	3400(30)	32(6)

H(1A)	7560(70)	3870(40)	1760(40)	79(13)
H(1B)	8760(130)	4340(80)	400(90)	250(40)

Table S51. Torsion angles [°] for **14·2H$_2$O**.

N(6)-N(7)-C(2)-N(8)	1.1(2)
N(6)-N(7)-C(2)-N(10)	-178.86(18)
N(6)-C(3)-C(4)-C(4)#1	0.4(4)
N(7)-N(6)-C(3)-N(8)	0.1(2)
N(7)-N(6)-C(3)-C(4)	178.68(17)
N(8)-C(3)-C(4)-C(4)#1	178.8(2)
N(9)-N(8)-C(2)-N(7)	177.34(18)
N(9)-N(8)-C(2)-N(10)	-2.7(3)
N(9)-N(8)-C(3)-N(6)	-177.79(17)
N(9)-N(8)-C(3)-C(4)	3.5(3)
C(2)-N(8)-C(3)-N(6)	0.6(2)
C(2)-N(8)-C(3)-C(4)	-178.11(17)
C(3)-N(6)-N(7)-C(2)	-0.7(2)
C(3)-N(8)-C(2)-N(7)	-0.97(19)
C(3)-N(8)-C(2)-N(10)	178.94(18)
N(1)-N(2)-N(3)-N(4)	0.0(2)
N(2)-N(1)-C(1)-N(4)	0.1(2)
N(2)-N(1)-C(1)-N(5)	-179.28(16)
N(2)-N(3)-N(4)-C(1)	0.1(2)
N(3)-N(4)-C(1)-N(1)	-0.1(2)
N(3)-N(4)-C(1)-N(5)	179.16(18)
N(5)#2-N(5)-C(1)-N(1)	177.03(19)
N(5)#2-N(5)-C(1)-N(4)	-2.2(3)
C(1)-N(1)-N(2)-N(3)	0.0(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1 #2 -x,-y+2,-z+1

Table S52. Hydrogen bonds for **14·2H$_2$O** [Å and °].

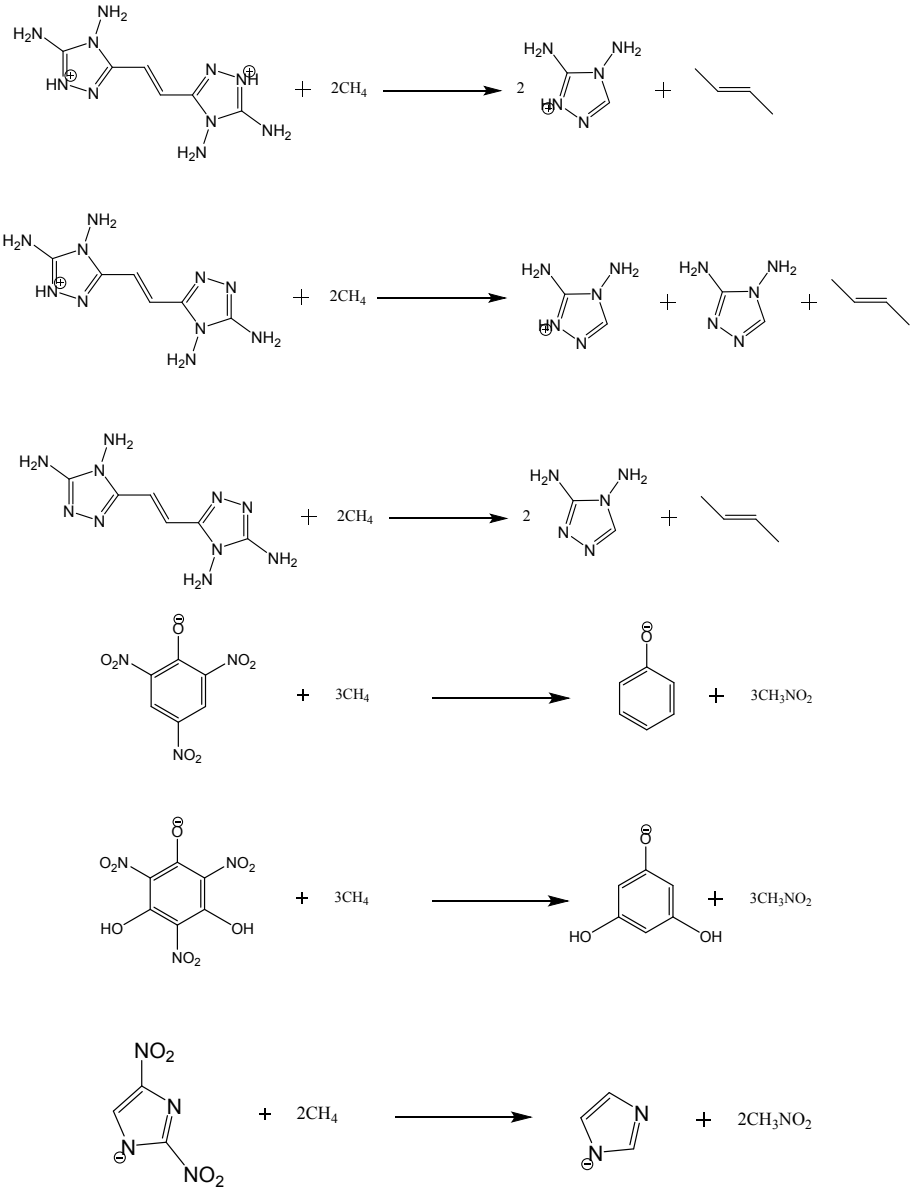
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

N(7)-H(7)...N(4)#3	0.85(3)	1.90(3)	2.753(3)	177(3)
N(10)-H(10A)...N(2)#4	0.84(3)	2.06(3)	2.890(3)	171(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1 #2 -x,-y+2,-z+1 #3 -x+1,-y+2,-z+1

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



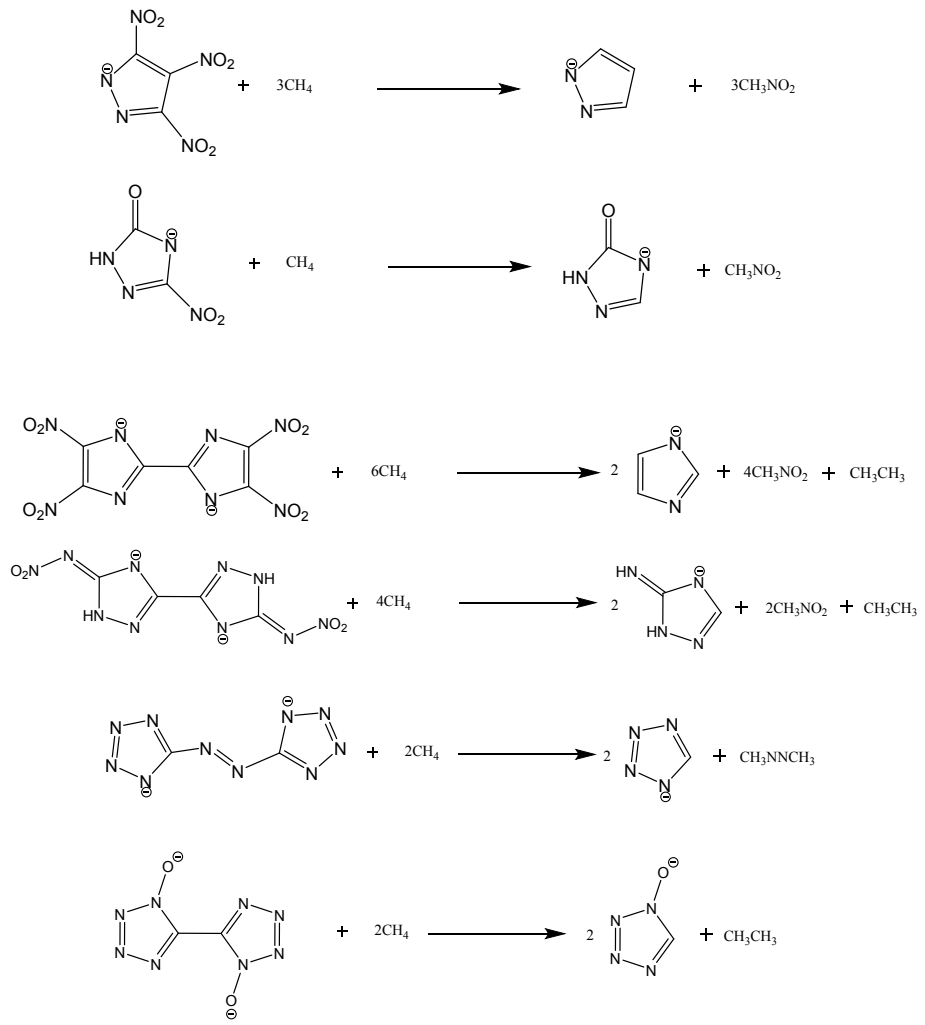


Figure S1. Isodesmic reactions for neutral molecules, cations and anions in **3**–**15**

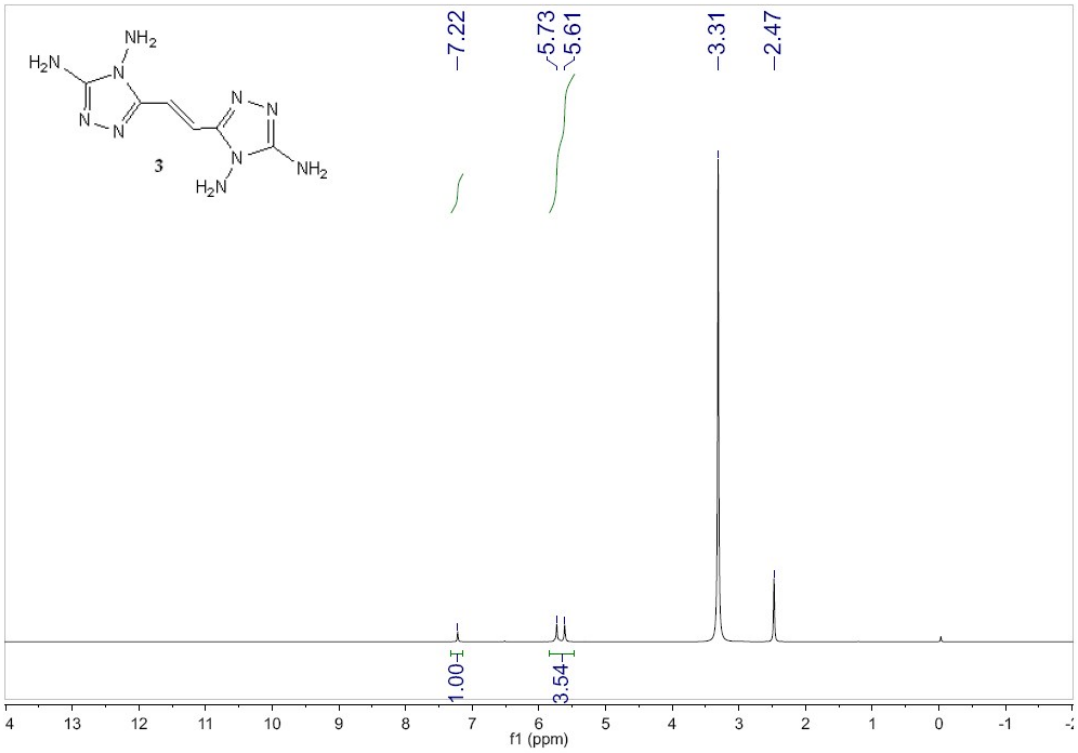


Figure S2. ^{1}H NMR spectra of **3**

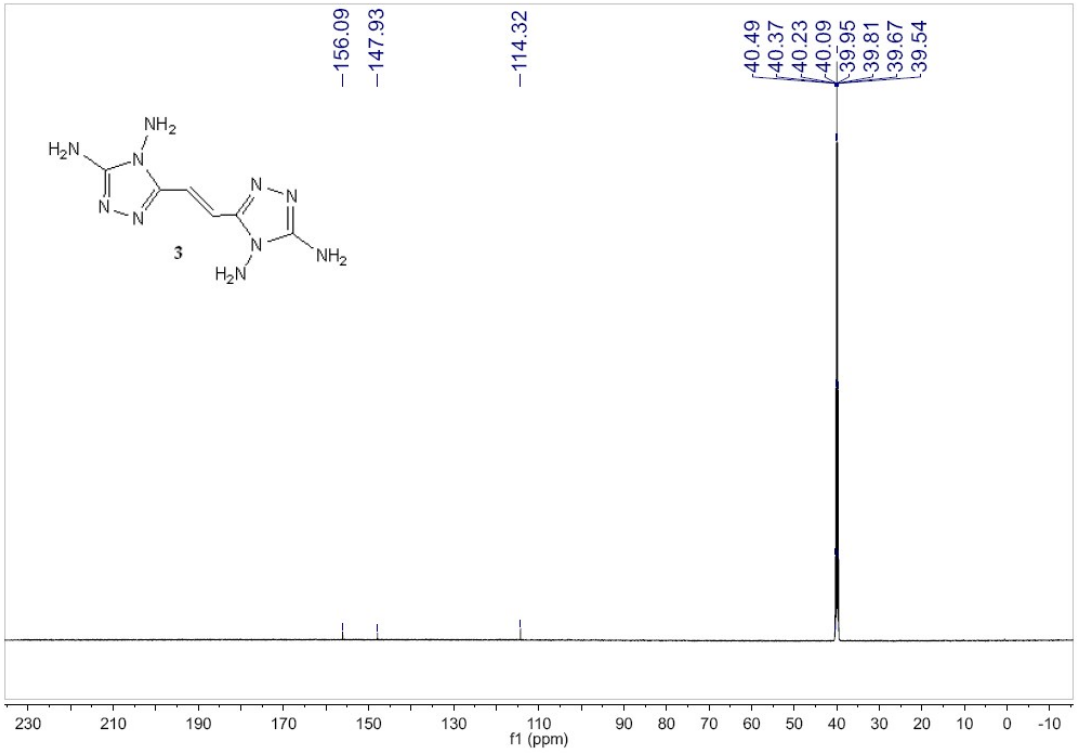


Figure S3. ^{13}C NMR spectra of **3**

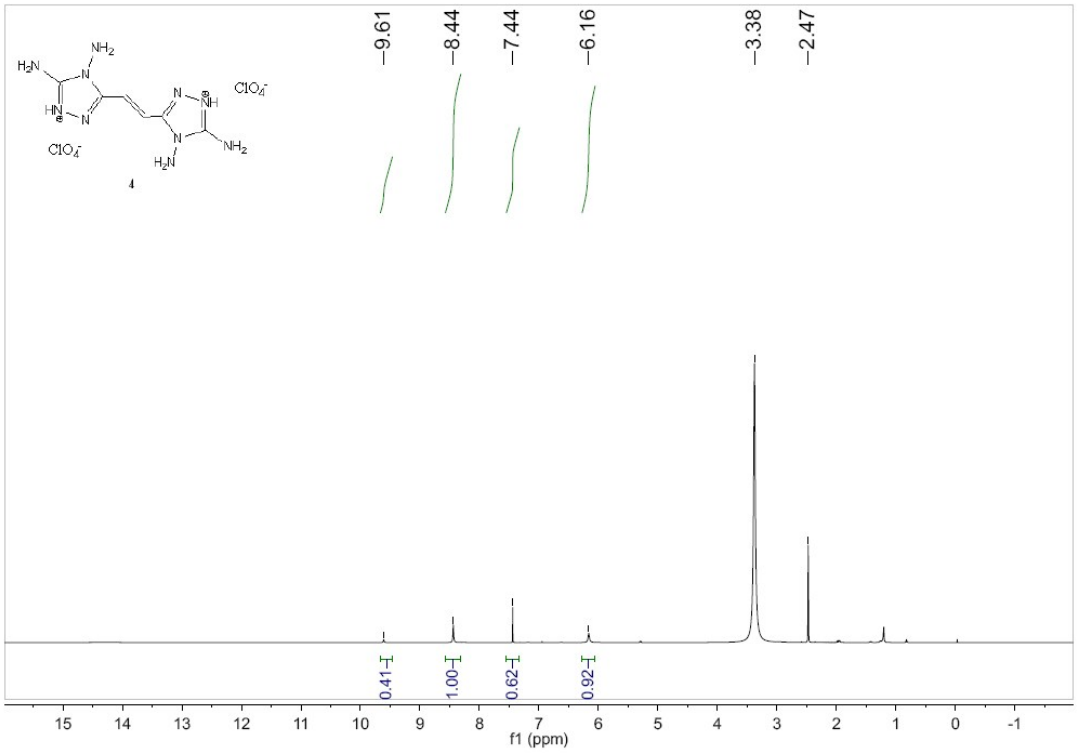


Figure S4. ^{1}H NMR spectra of **4**

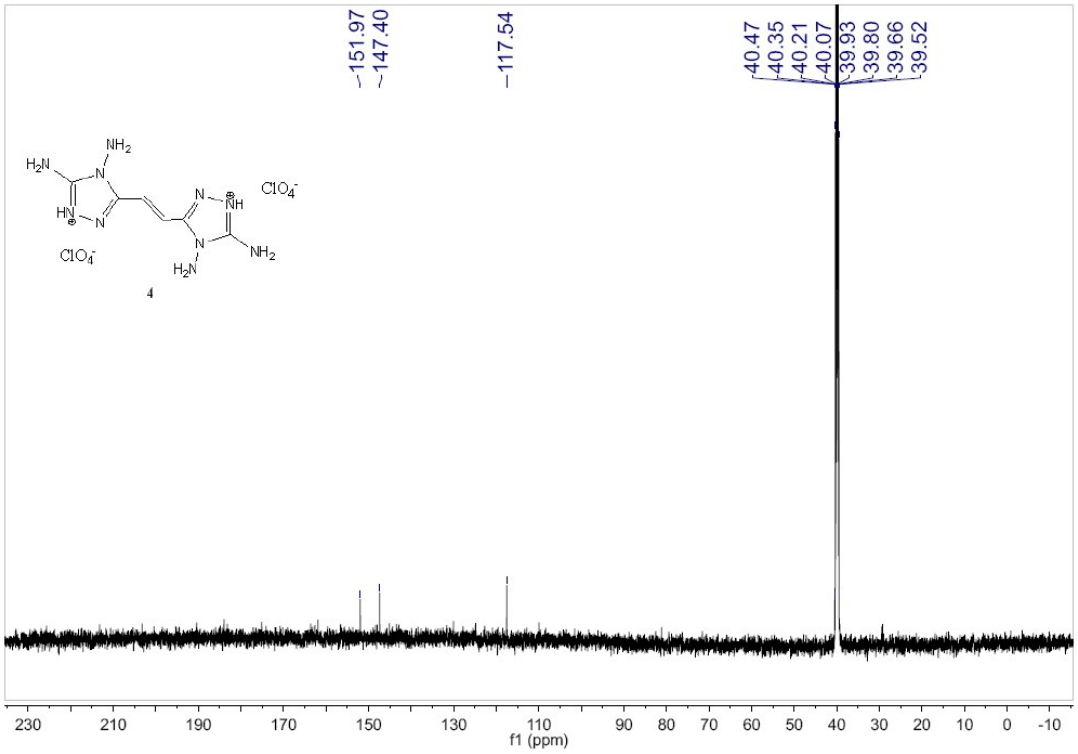


Figure S5. ^{13}C NMR spectra of **4**

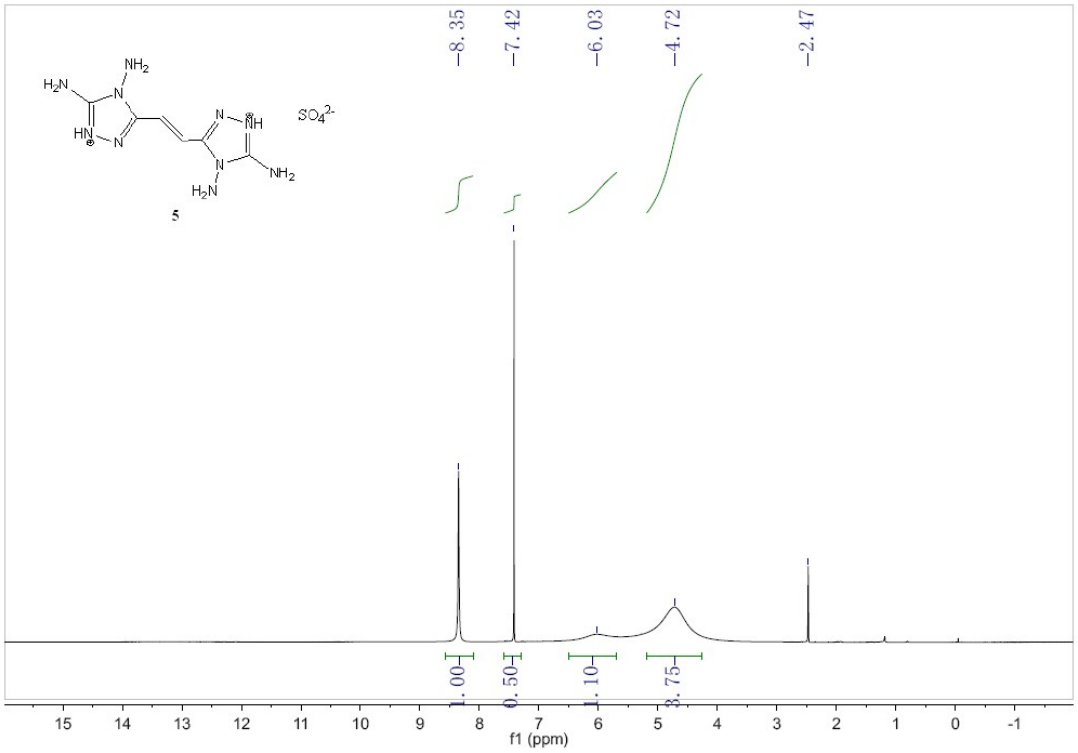


Figure S6. ^{1}H NMR spectra of **5**

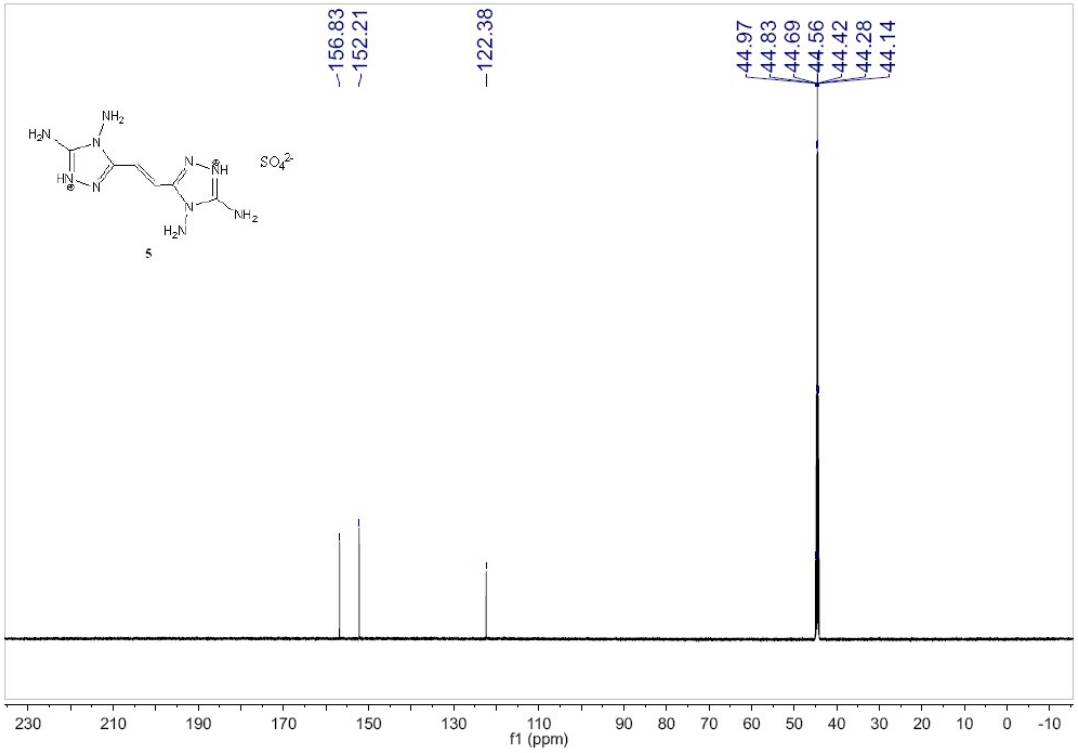


Figure S7. ^{13}C NMR spectra of **5**

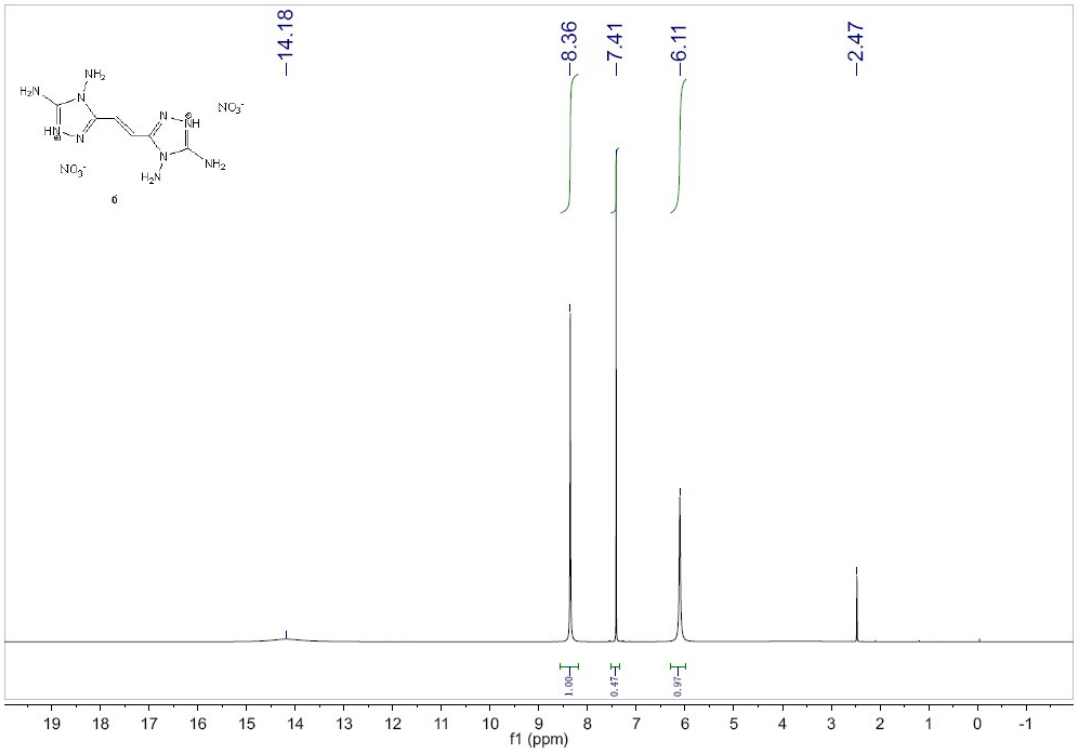


Figure S8. ^{1}H NMR spectra of **6**

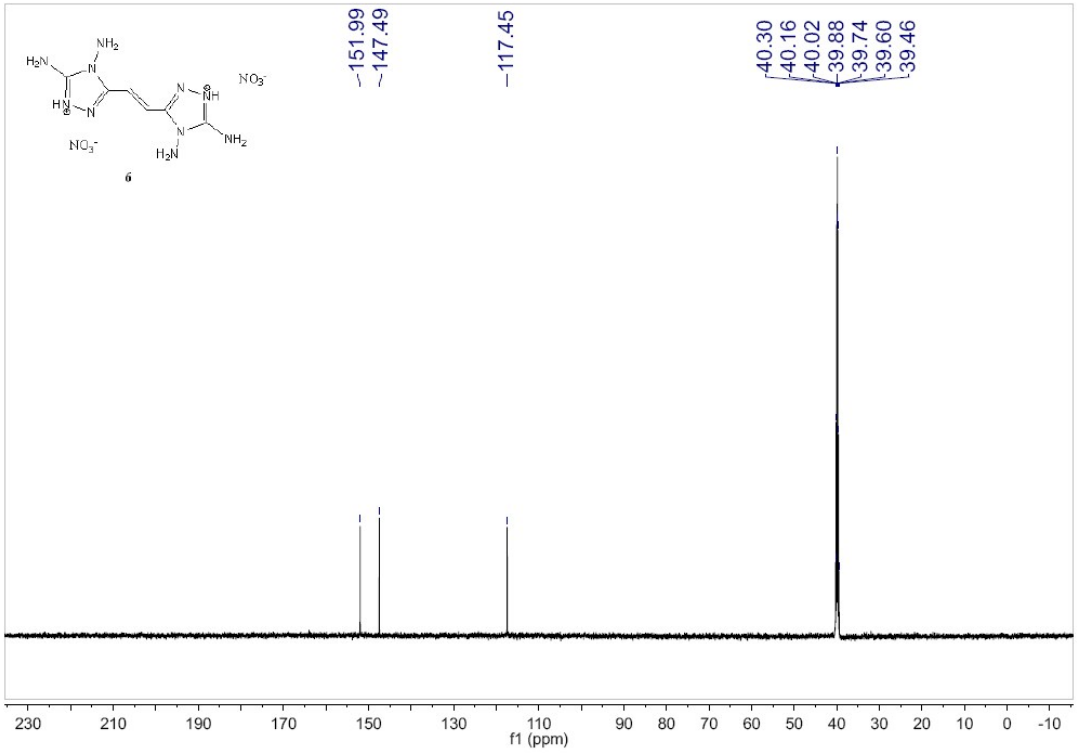


Figure S9. ^{13}C NMR spectra of **6**

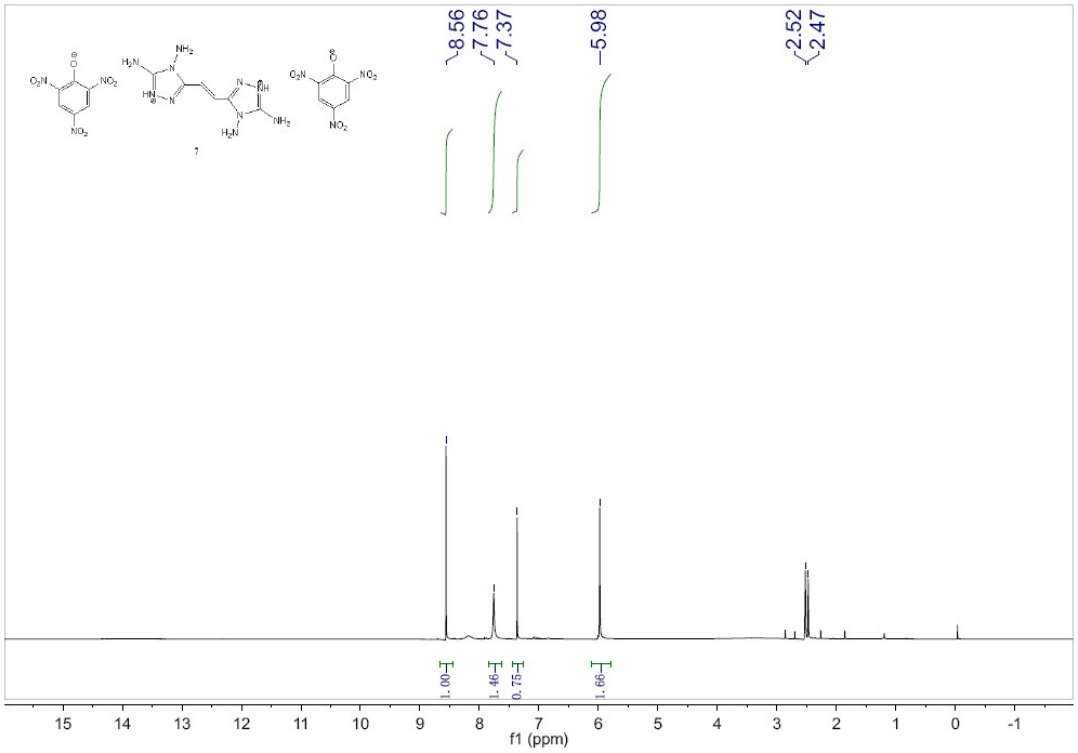


Figure S10. ^{1}H NMR spectra of **7**

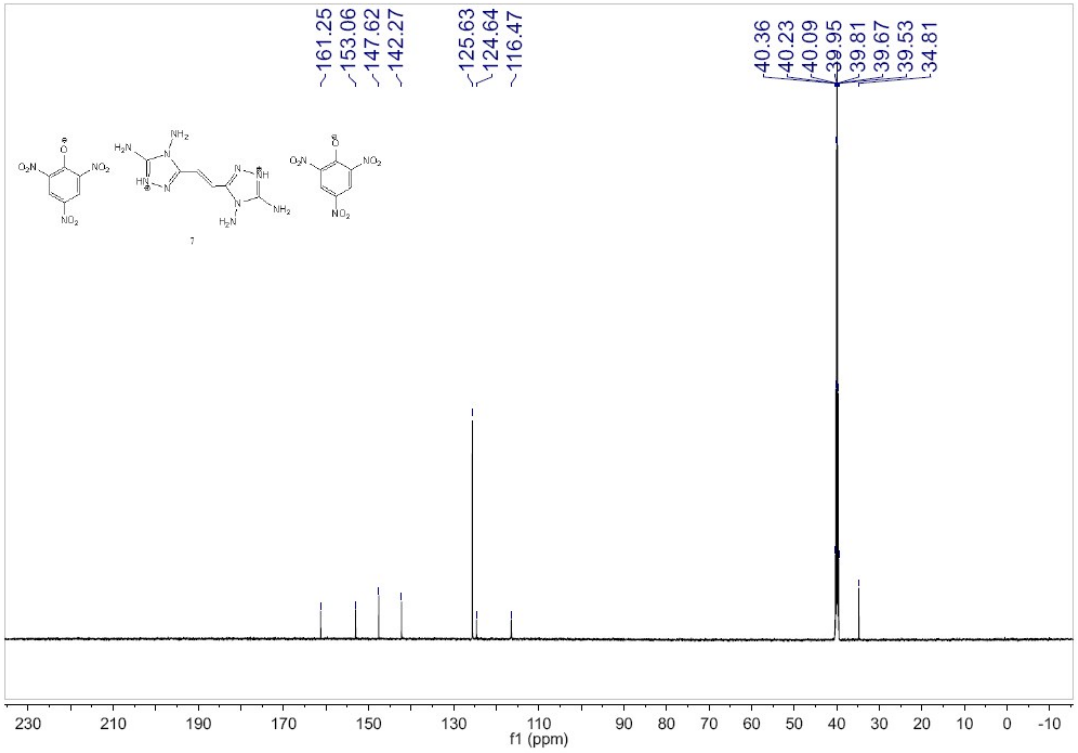


Figure S11. ^{13}C NMR spectra of **7**

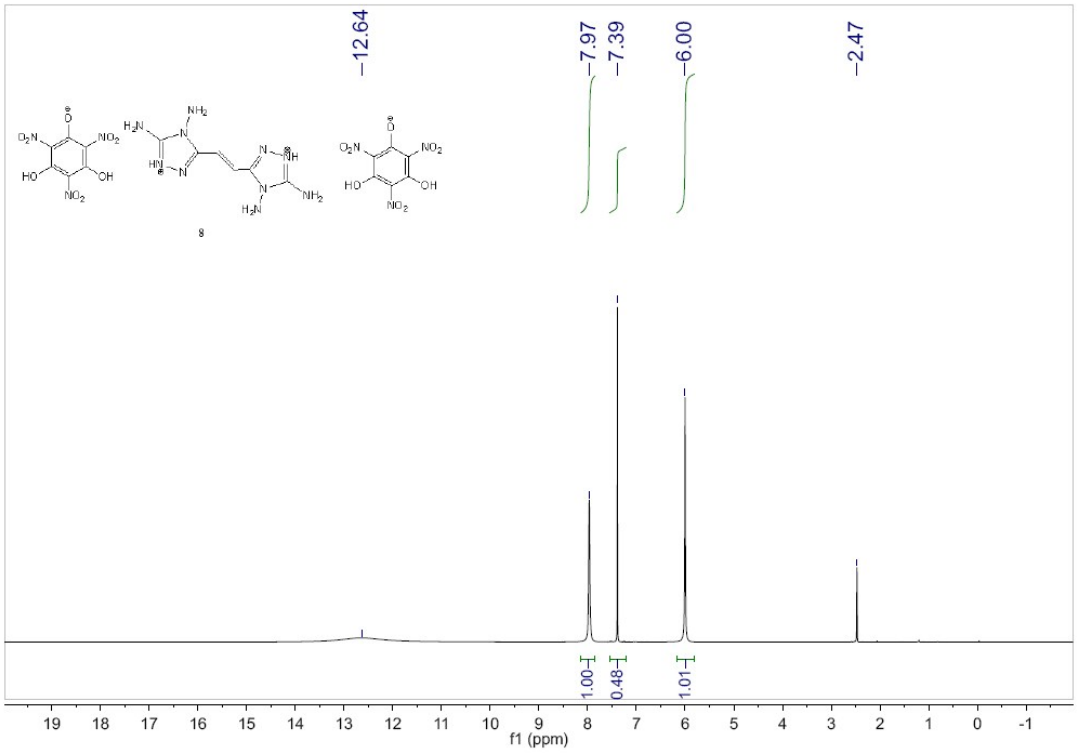


Figure S12. ^{1}H NMR spectra of **8**

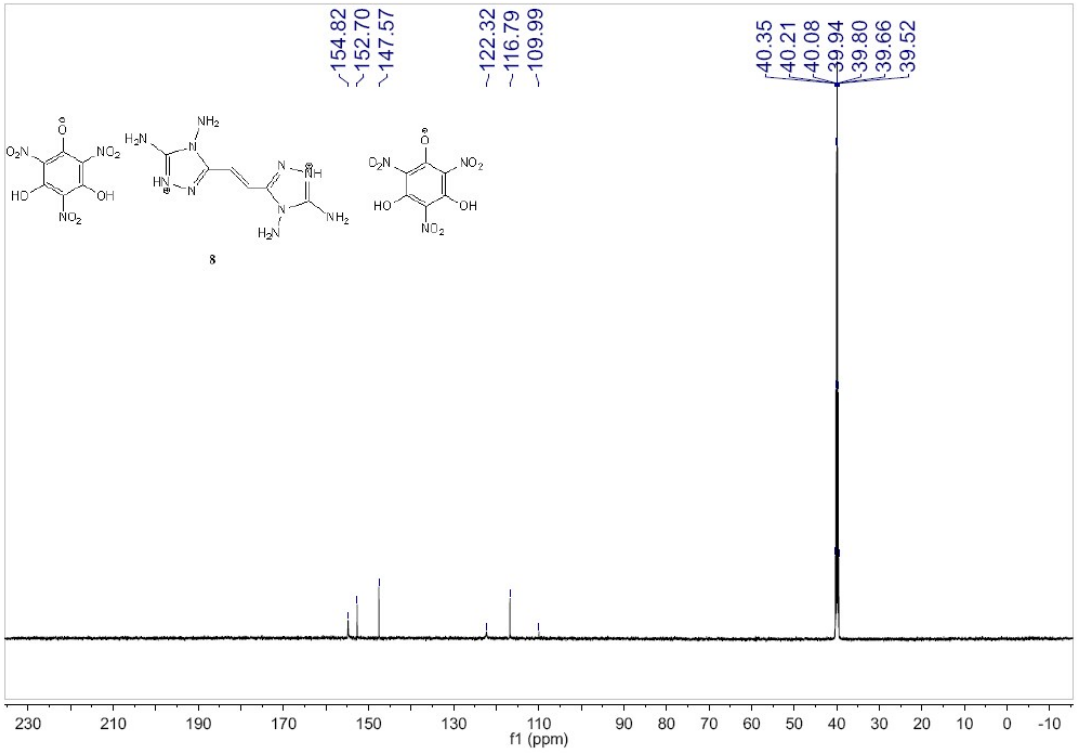


Figure S13. ^{13}C NMR spectra of **8**

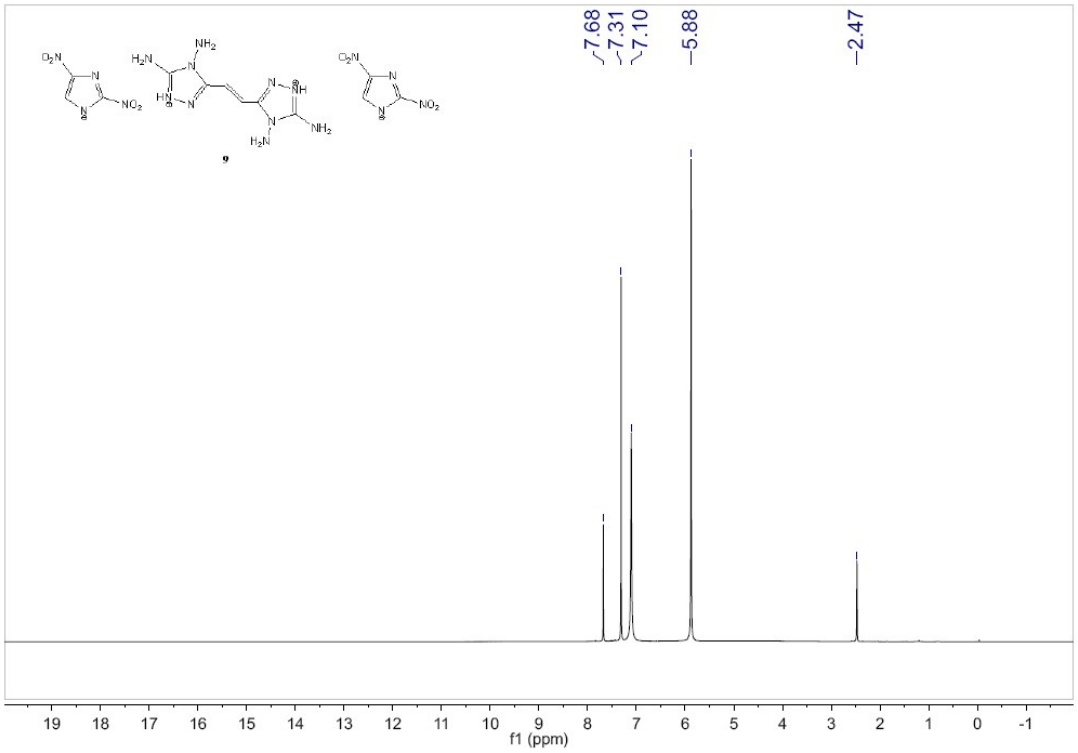


Figure S14. ^{1}H NMR spectra of **9**

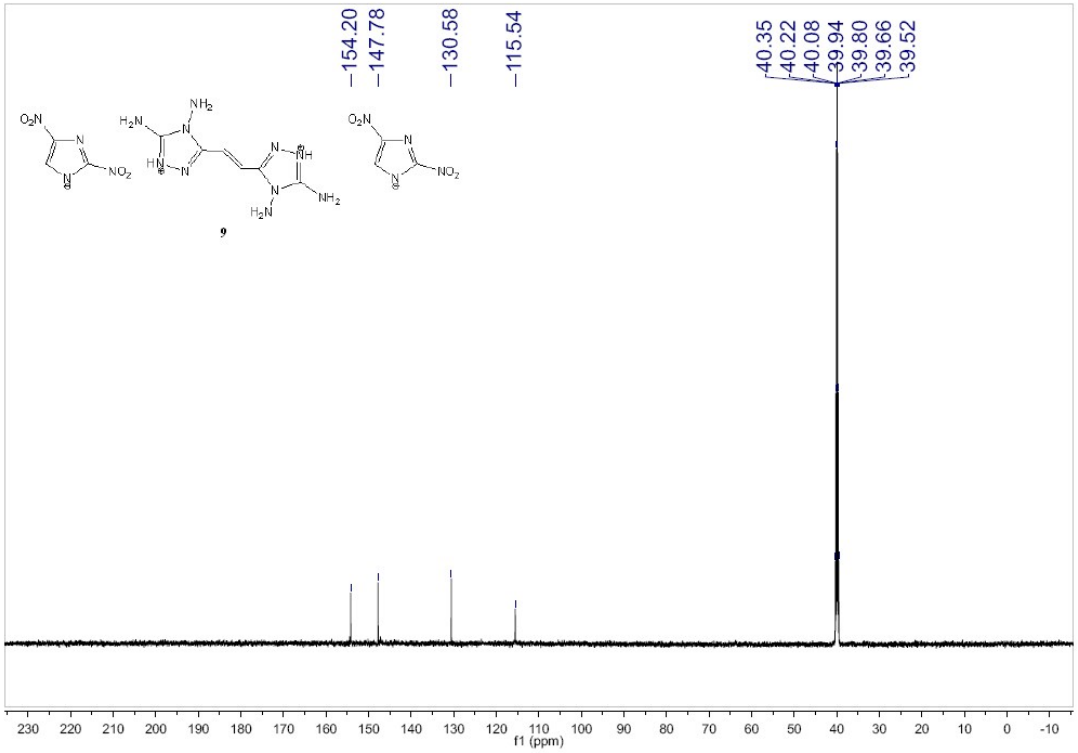


Figure S15. ^{13}C NMR spectra of **9**

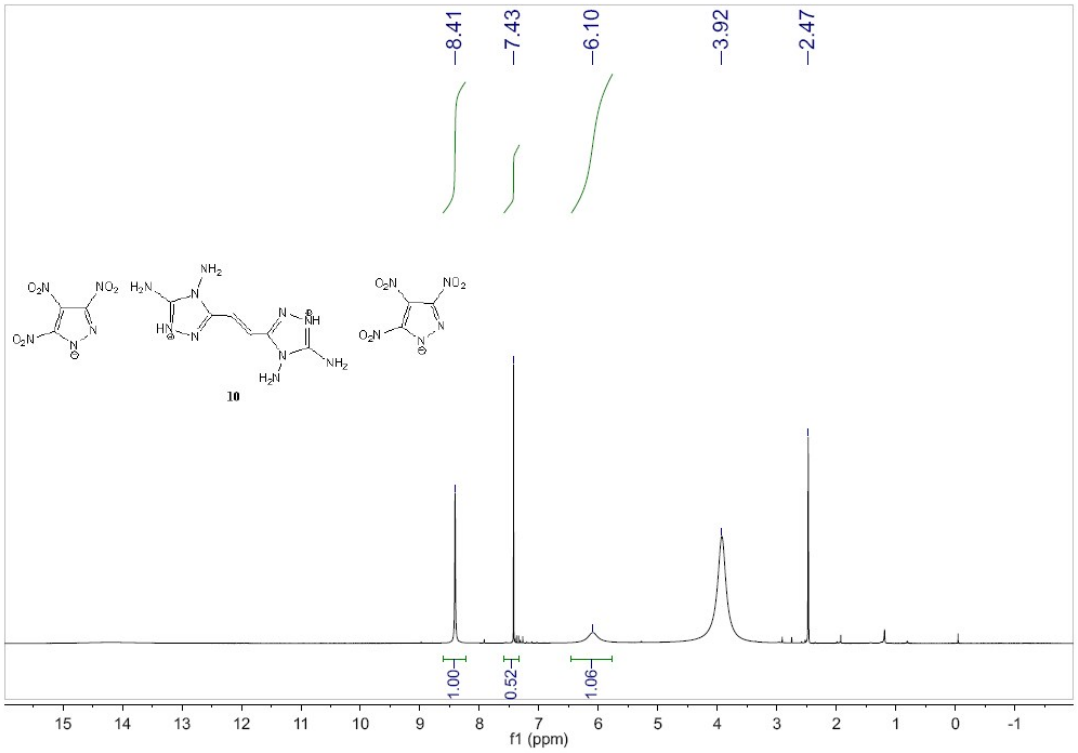


Figure S16. ^{1}H NMR spectra of **10**

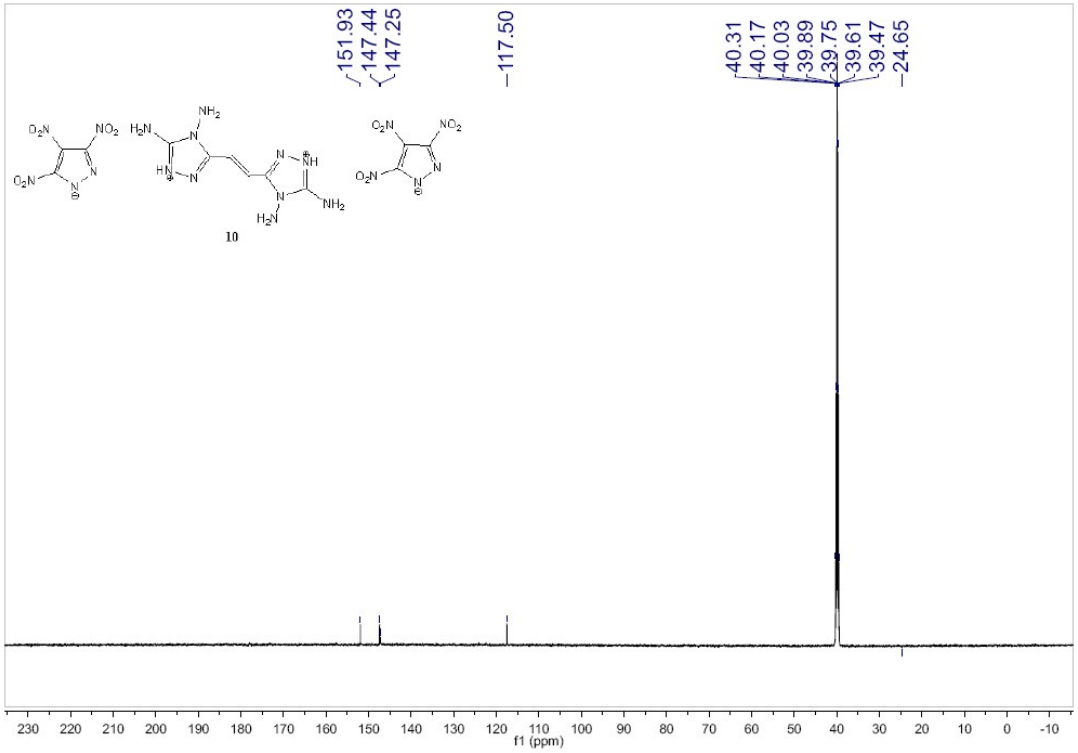


Figure S17. ^{13}C NMR spectra of **10**

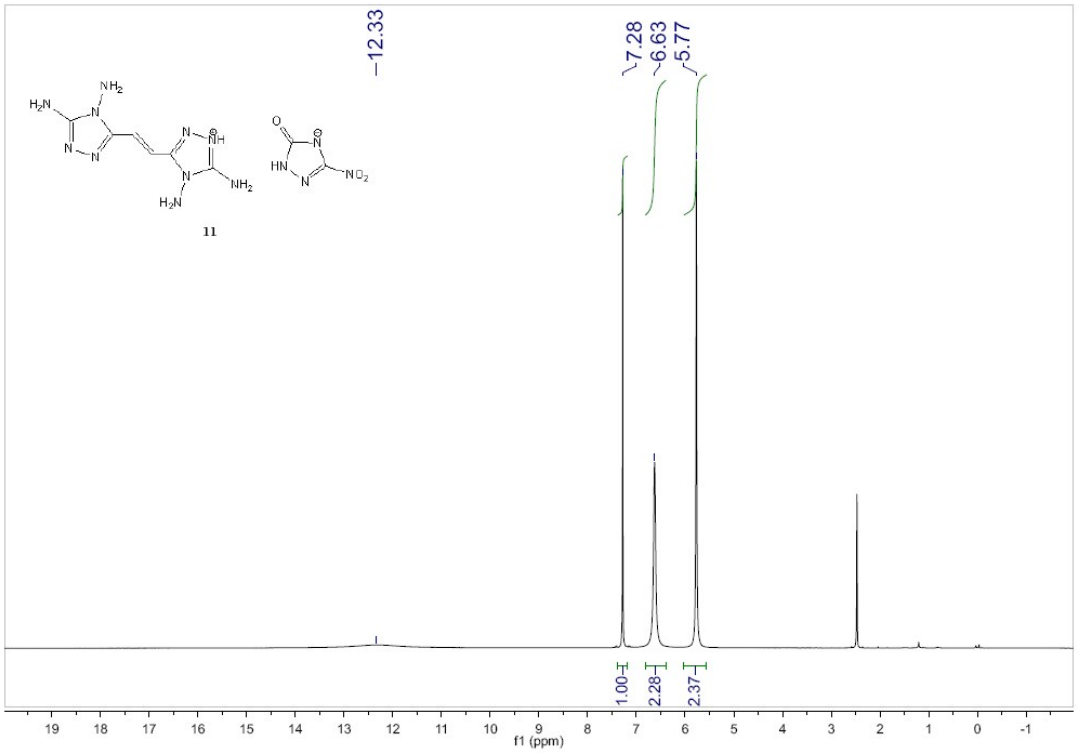


Figure S18. ^{1}H NMR spectra of **11**

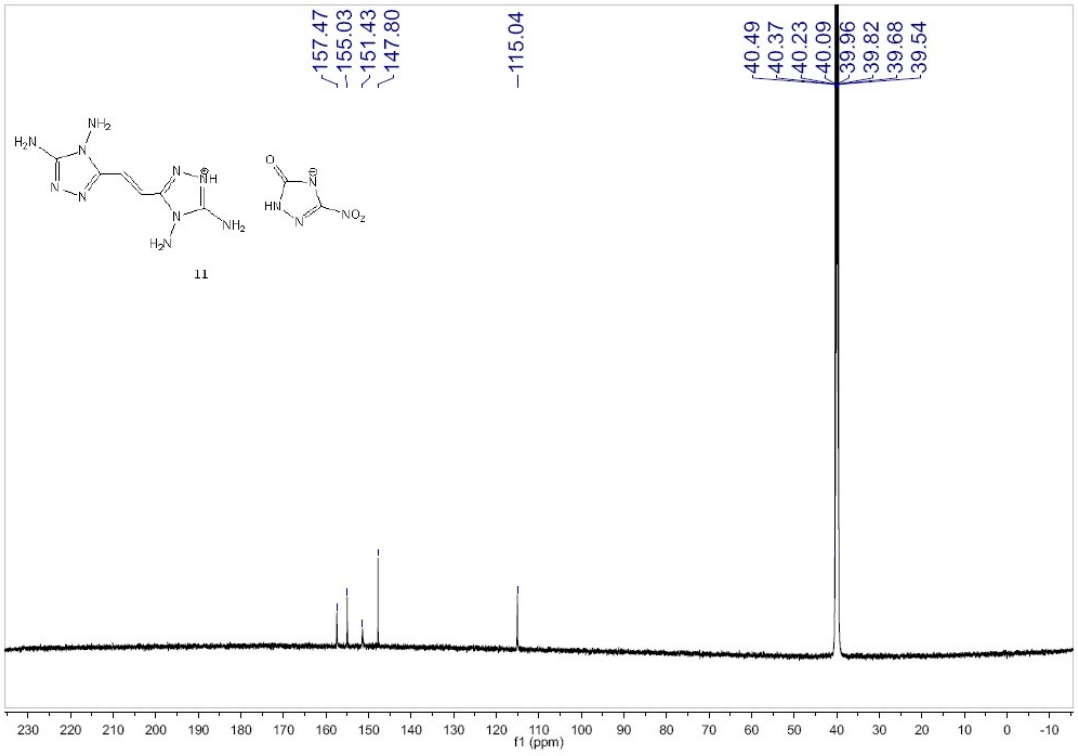


Figure S19. ^{13}C NMR spectra of **11**

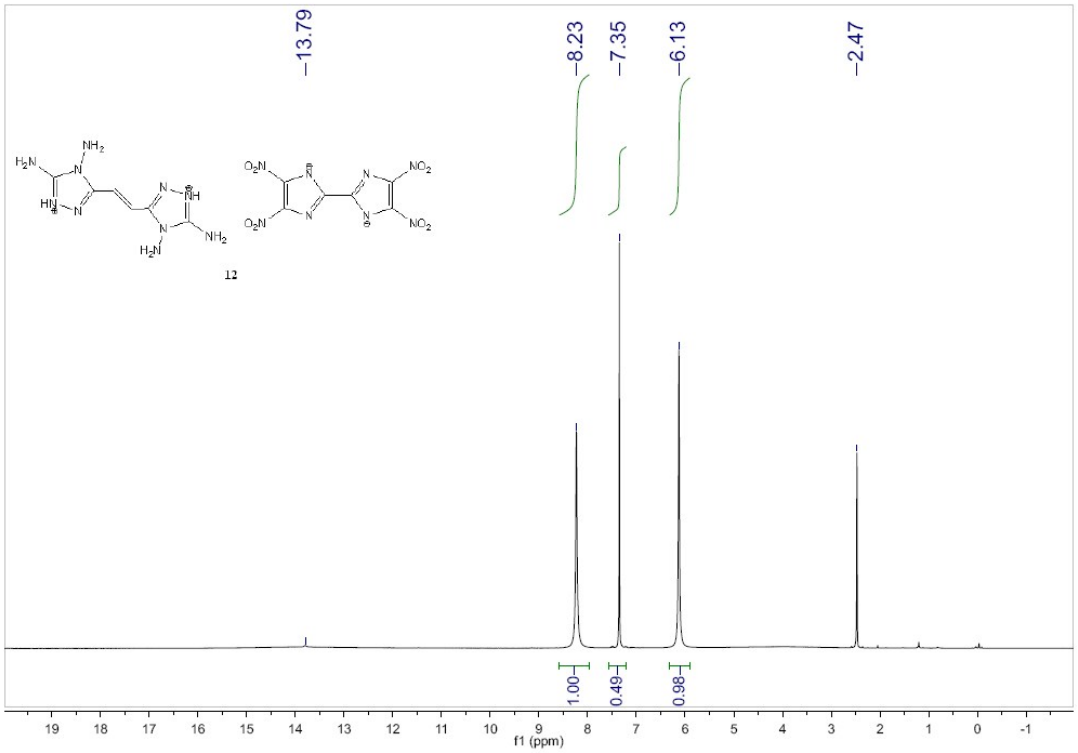


Figure S20. ^{1}H NMR spectra of **12**

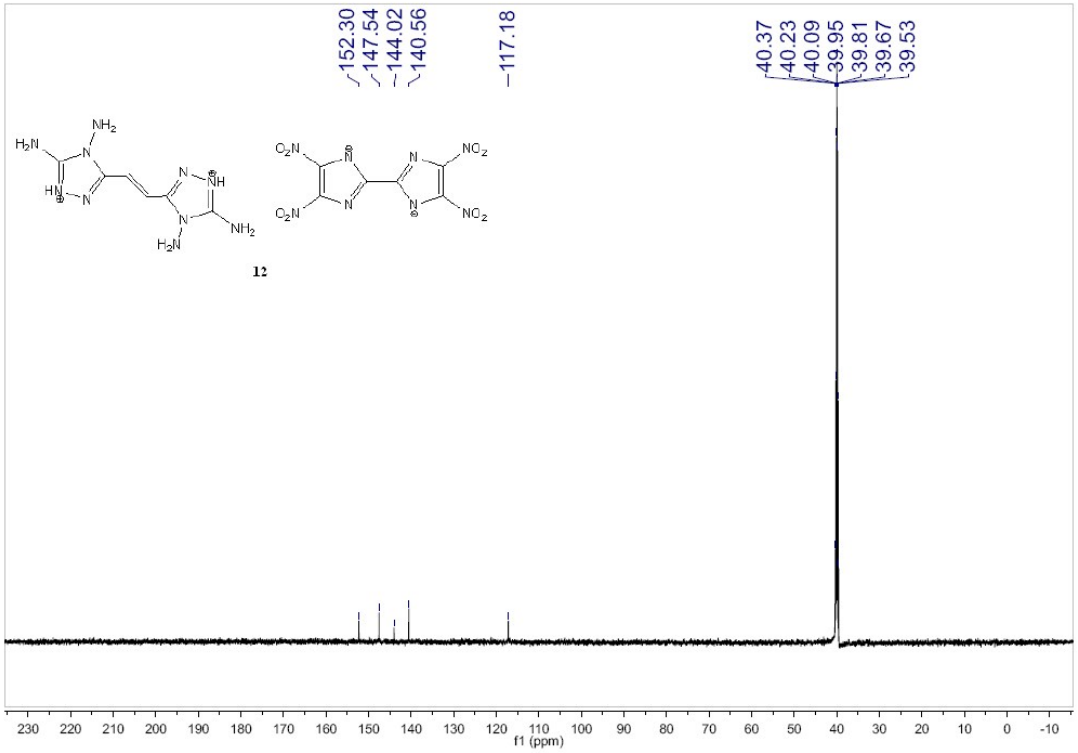


Figure S21. ^{13}C NMR spectra of **12**

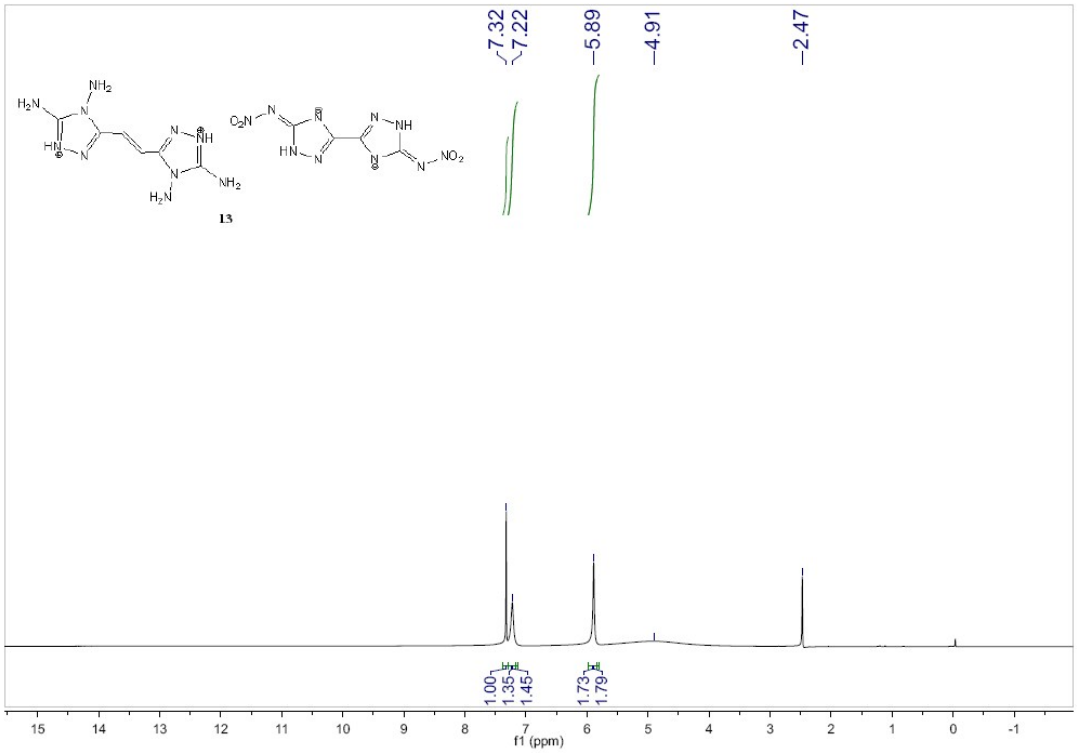


Figure S22. ^{1}H NMR spectra of **13**

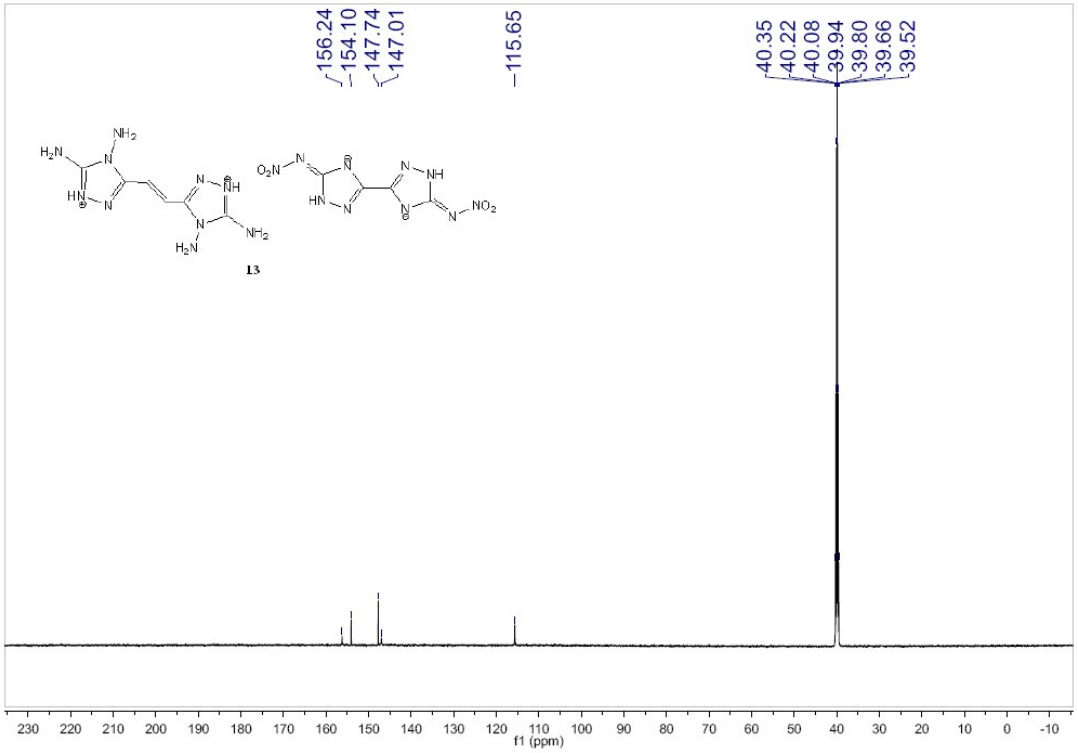


Figure S23. ^{13}C NMR spectra of **13**

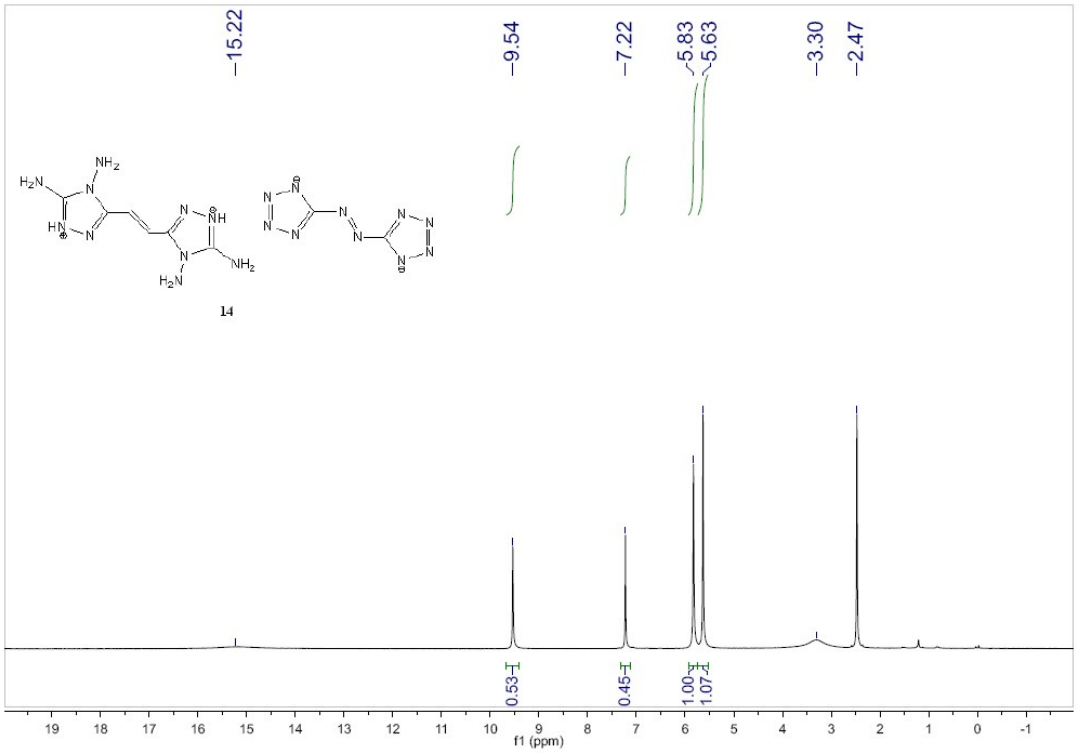


Figure S24. ^{1}H NMR spectra of **14**

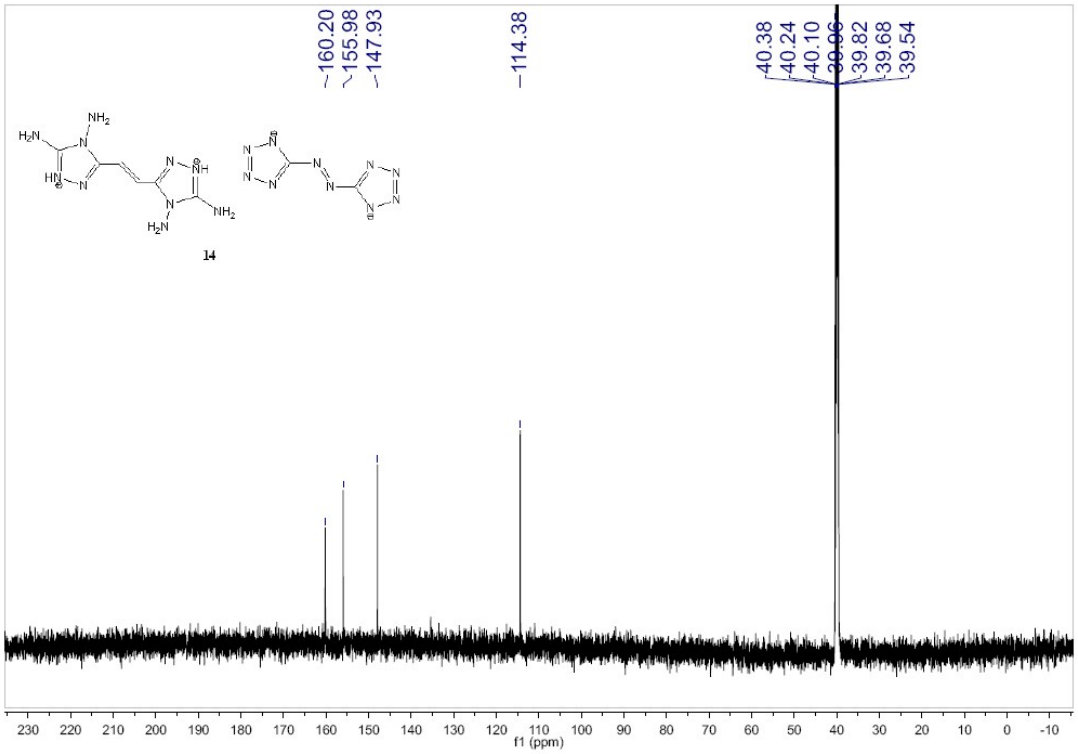


Figure S25. ^{13}C NMR spectra of **14**

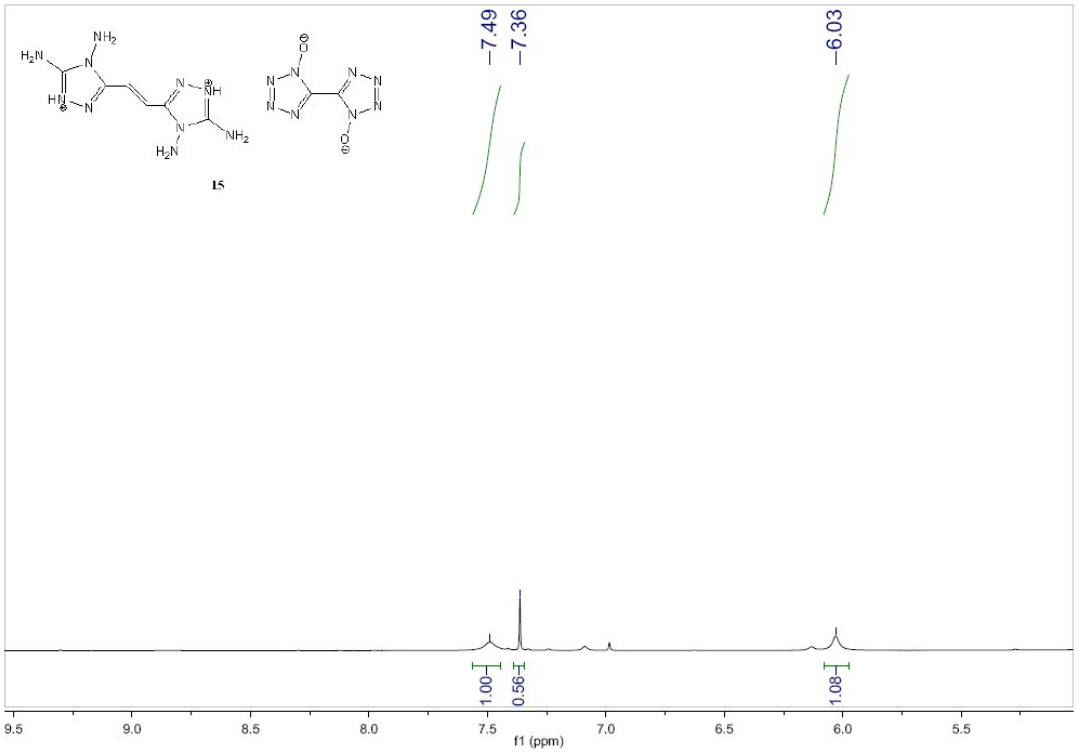


Figure S26. ^{1}H NMR spectra of **15**

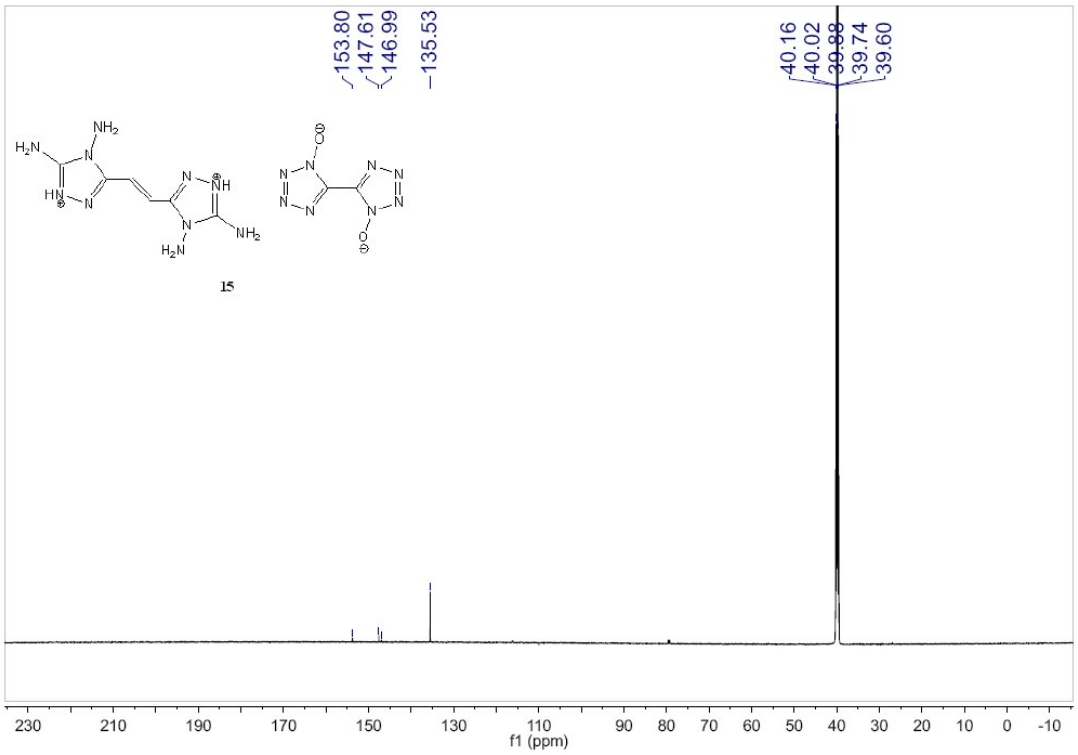


Figure S27. ^{13}C NMR spectra of **15**