Electronic Supplementary Information

Engineering bistetrazoles: (E)-5,5'-(ethene-1,2-diyl)bis(1H-tetrazol-1-ol) as a new planar high-energy-density material

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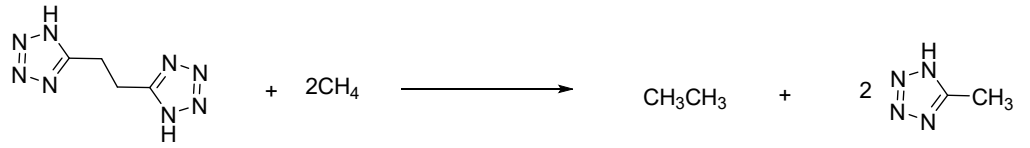
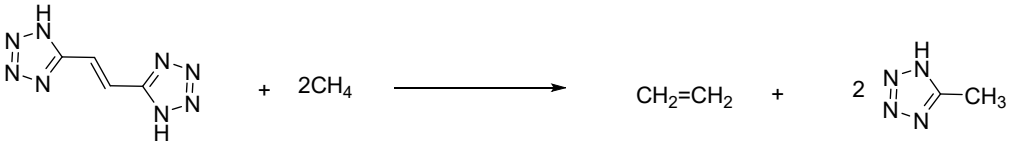
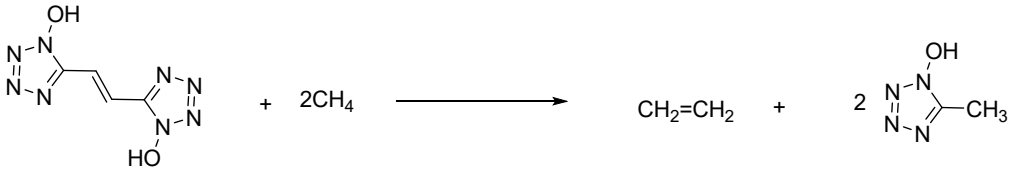
Isodesmic reactions



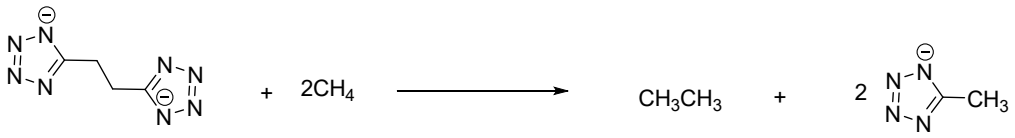
Compound 4



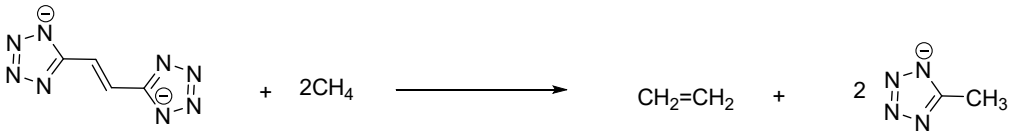
Compound 5



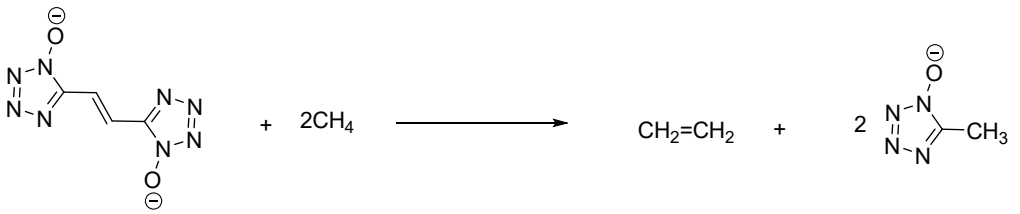
Compound 6



Compound 4_dianion



Compound 5_dianion



Compound 6_dianion

Scheme S1: Isodesmic reactions for compounds **4, 5** and **6** and their corresponding dianions.

Experimental section

All compounds should be synthesized in milligram amounts. The investigated compounds are energetic materials which show increased sensitivities toward various stimuli (e.g., higher temperatures, impact, and friction). Proper safety precautions such as leather gloves, face shield, and eye protection must be worn at all times while synthesizing and handling these materials.

General methods

All reagents (analytical grade) were purchased from AK Scientific or VWR and were used as supplied. ^{1}H, ^{13}C NMR and ^{15}N NMR spectra were recorded using a 500 MHz (Bruker AVANCE 500) NMR spectrometer operating at 500.19, 125.78 MHz, and 50.69 MHz, respectively. Chemical shifts in the ^{1}H and ^{13}C NMR spectra are reported relative to Me_4Si and ^{15}N NMR spectra to $MeNO_2$ as an external standard. The decomposition points (onset temperature) were obtained on a differential scanning calorimeter (TA Instruments Company, Model: Q2000) at a scan rate of 5 °C min^{-1}. Infra-red spectra were recorded on a FT-IR spectrometer (Thermo Nicolet AVATAR 370) as thin films using KBr plates. The room temperature densities were measured at 25 °C by employing a gas pycnometer (Micromeritics AccuPyc II 1340). The impact and friction sensitivities were determined by using a standard BAM drop hammer and BAM friction tester. Elemental analyses were carried out on a Vario Micro cube Elementar Analyser.

Colorless block-shaped crystals of **6, 7** and **8** with dimensions 0.21 × 0.16 × 0.05 mm^3, 0.14 × 0.09 × 0.03 mm^3 and 0.17 × 0.12 × 0.07 mm^3, respectively, and colorless cube-shaped crystals of **9** with dimensions 0.09 × 0.06 × 0.03 mm^3 were selected and mounted on a nylon loop with Paratone oil on a XtaLAB Synergy, Dualflex, HyPix diffractometer. The crystals were kept at a steady T = 100 K during data collection. The structures were solved with the ShelXT[1] solution program using dual methods and by using Olex2.[2] The model was refined with ShelXL[3] using full matrix least squares minimization on F^2.

Theoretical study

The HOFs (heat of formation) of compounds **5**, **6** and **7** were calculated by using isodesmic reactions. The single crystal structures were used for the geometric optimization and frequency analyses using the B3LYP functional with the 6-31+G** basis set. The single-point energies were obtained at the MP2/6-311++G** level.[4] The atomization energies for cations were calculated by using the G^2*ab initio* method.[5] All of the optimized structures were characterized to be true local energy minima on the potential energy surface without imaginary frequencies. In case of the energetic salts, the solid-phase heats of formation were obtained based on a Born–Haber energy cycle.[6] All calculated gas-phase enthalpies for covalent materials are converted to solid phase values by subtracting the empirical heat of sublimation obtained based on Trouton's rule.[7]

Synthesis of compound 3

Compound **2** (1.00 g, 12.8 mmol) was reacted with hydroxylamine (2 eq., 50% in water) in EtOH for 24h to give the diamidooxime derivative as white crystalline solid. The diamidooxime was dissolved in 6M HCl at 0 °C and $NaNO_2$ (2.2 eq.) was added while maintaining the temperature below 2 °C. The reaction mixture is stirred for 12h and the resulting mixture was extracted with ethyl acetate to give the dichlorooxime derivative as a white solid. Next, the dichlorooxime derivative was reacted with NaN_3 (2 eq.) in EtOH to give **3** as a white solid. T_d = 181 °C (onset); ^{1}H NMR (300 MHz, ppm, d_6-DMSO): 12.02 (s, 2H), 6.26 (s, 2H); ^{13}C NMR (75 MHz, ppm, d_6-DMSO): 154.7, 20.8; Elemental analysis: Calcd (%) for $C_4H_4N_8O_2$ (196.13): C, 24.50; H, 2.06; N, 57.13; Found: C, 24.78; H, 2.28; N, 57.97.

Synthesis of compound 4

To a 200 mL round-bottomed flask was added **1** (1.00 g, 12.5 mmol), sodium azide (1.70 g, 26.2 mmol), zinc chloride (0.85 g, 6.2 mmol), and water (30 mL). The reaction mixture was stirred at reflux for 24 h. After cooling, HCl (3M, 20 mL) was added to the reaction mixture with vigorous stirring. The reaction mixture was heated at 50 °C, cooled and extracted with

ethyl acetate (2 x 30 mL). The organic phase was dried over sodium sulfate and the solvent was removed under reduced pressure to obtain **4** as a white solid. Yield: 1.66 g (80%); T_d = 253 °C (onset); ^{1}H NMR (300 MHz, ppm, d_6-DMSO): 3.38 (s, 4H), ^{13}C NMR (75 MHz, ppm, d_6-DMSO): 154.7, 20.8; IR (ν, cm^{-1}): 3102, 3043, 2868, 1548, 1428, 1369, 1244, 1213, 1072, 1009, 859, 758; Elemental analysis: Calcd (%) for $C_4H_6N_8$ (166.14): C, 28.92; H, 3.64; N, 67.44; Found: C, 29.44; H, 3.66; N, 68.07.

Synthesis of compound 5

To a 200 mL round-bottomed flask was added **2** (1.00 g, 12.8 mmol), sodium azide (1.75 g, 26.9 mmol), zinc chloride (0.87 g, 6.4 mmol), and water (30 mL). The reaction mixture was stirred at reflux for 24 h. After cooling, HCl (3M, 20 mL) was added to the reaction mixture with vigorous stirring. The reaction mixture was heated at 50 °C (until the white solid dissolved) and allowed to cool to room temperature. The crystalline compound was filtered and dried to give **5** as a light-yellow solid. Yield: 1.85 g (88%); T_d = 275 °C (onset); ^{1}H NMR (300 MHz, ppm, d_6-DMSO): 7.66 (s, 2H), ^{13}C NMR (75 MHz, ppm, d_6-DMSO): 153.5, 119.5; IR (ν, cm^{-1}): 3158, 3024, 2885, 2762, 2709, 2634, 2496, 1585, 1413, 1260, 1113, 1060, 997, 899, 808, 697; Elemental analysis: Calcd (%) for $C_4H_4N_8$ (164.13): C, 29.27; H, 2.46; N, 68.27; Found: C 29.15, H 2.54, N 66.70.

Synthesis of compound 6

Compound **3** (1.0 g, 5.1 mmol) was dissolved in diethyl ether (100 mL). Gaseous HCl was passed through the reaction mixture until saturation was reached at 0–5 °C. The reaction flask was sealed and after stirring overnight at room temperature the solvent was removed. The off-white powder was purified by washing with water (3 x 30 mL) to give **6** as an off-white solid. Yield: 0.90 g (90%); T_d = 226 °C (onset); ^{1}H NMR (300 MHz, ppm, d_6-DMSO): 7.62 (s, 2H), ^{13}C NMR (75 MHz, ppm, d_6-DMSO): 144.0, 116.8; IR (ν, cm^{-1}): 3067, 1840, 1582, 1457, 1273,

1203, 966, 775, 699; Elemental analysis: Calcd (%) for $C_4H_4N_8O_2$ (196.13): C, 24.50; H, 2.06; N, 57.13; Found: C 23.94, H 2.38, N 55.39.

General procedure for the synthesis of energetic salts

Hydroxylamine (2.0 mmol) was added to a suspension of **4, 5** or **6** (1.0 mmol) in CH_3CN (50 mL). The reaction mixture was heated to 50 °C and stirred for 30 min. The precipitate was collected by filtration to give the product, which was purified further by washing with CH_3CN (3 x 10 mL).

Dihydroxylammonium 5,5'-(ethane-1,2-diyl)ditetrazol-1-ide (7): Isolated yield: 88%; $T_{dec.}$ (onset) = 255 °C; ^{1}H NMR (300 MHz, ppm, d_6-DMSO): 9.22 (bs, 6H), 3.25 (s, 4H); ^{13}C NMR (75 MHz, ppm, d_6-DMSO): 157.3, 22.5; IR (ν, cm^{-1}): 2978, 2714, 1652, 1541, 1472, 1434, 1411, 1396, 1333, 1281, 1205, 1164, 1146, 1086, 1043, 996, 890, 755, 721, 700; Elemental analysis: Calcd (%) for $C_4H_{12}N_{10}O_2$ (232.20): C, C, 20.69; H, 5.21; N, 60.32; Found: C 20.87, H 4.36, N 59.82.

Dihydroxylammonium (E)-5,5'-(ethene-1,2-diyl)ditetrazol-1-ide (8): Isolated yield: 91%; $T_{dec.}$ (onset) = 288 °C; ^{1}H NMR (500 MHz, d_6-DMSO): 8.99 (bs, 6H), 7.47 (s, 2H); ^{13}C NMR (126 MHz, d_6-DMSO): 157.1, 118.9; IR (ν, cm^{-1}): 2965, 2725, 2152, 1623, 1495, 1399, 1237, 1151, 983, 844, 748; Elemental analysis: Calcd (%) for $C_4H_{10}N_{10}O_2$ (230.19): C, 20.87; H, 4.38; N, 60.85; Found: C 21.18, H 3.75, N 59.75.

Dihydroxylammonium (E)-5,5'-(ethene-1,2-diyl)bis(1H-tetrazol-1-olate) (9): Isolated yield: 93%; $T_{dec.}$ (onset) = 230 °C; ^{1}H NMR (500 MHz, d_6-DMSO): 10.02 (bs, 6H), 7.72 (s, 2H); ^{13}C NMR (126 MHz, d_6-DMSO): 141.5, 114.6; IR (ν, cm^{-1}): 2966, 2699, 1608, 1533, 1429, 1308, 1243, 1176, 997, 957, 831, 786, 703; Elemental analysis: Calcd (%) for $C_4H_{10}N_{10}O_4$ (262.19): C, 18.32; H, 3.84; N, 53.42; Found: C 18.24, H 3.91, N 53.23.

References

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6. H. D. B. Jenkins, D. Tudela and L. Glasser, *Inorg. Chem.* 2002, **41**, 2364–2367.

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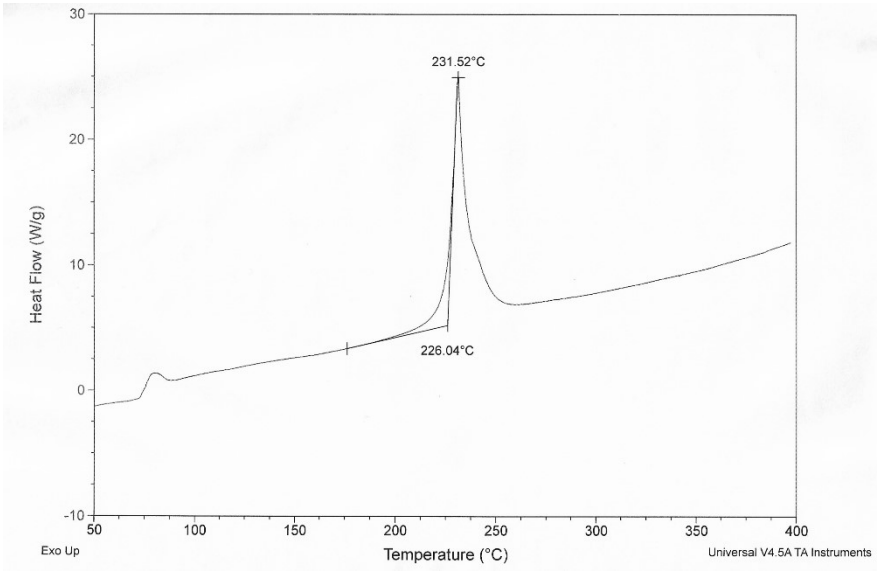

Figure S1: DSC analysis of compound **6** at 5 °C/min.

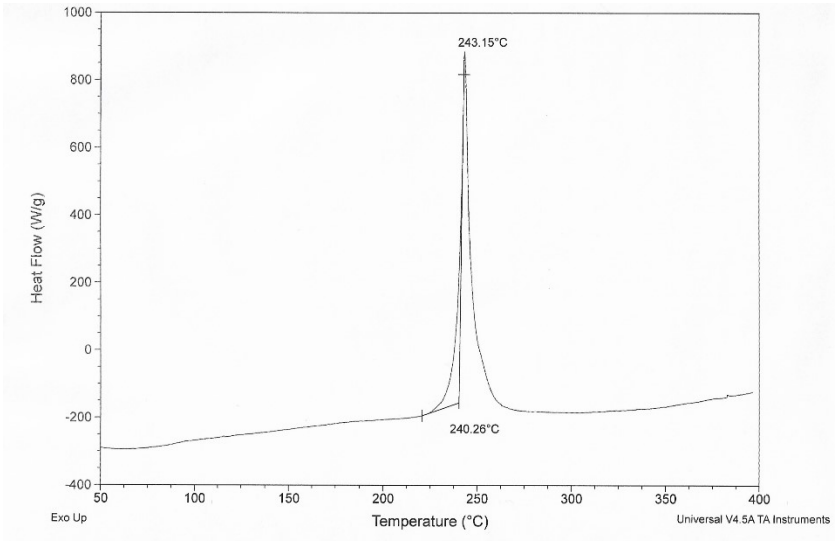

Figure S2: DSC analysis of compound **6** at 10 °C/min.

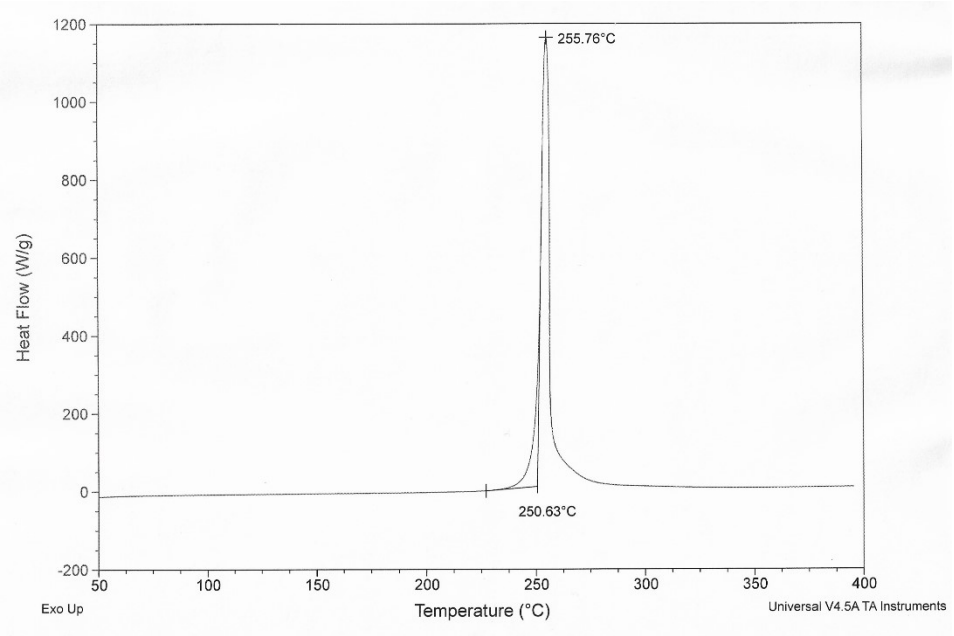

Figure S3: DSC analysis of compound **6** at 20 °C/min.

Table S1: Dv and Dp of compounds **4-9** calculated using EXPLO5 v6.01.

	ρ^a (g cm^{-3})	$\Delta H_f{}^b$ (kJmol^{-1})/kJg^{-1}	P^c (GPa)	$D_v{}^d$ (m s^{-1})
4	*1.50*	584.2/3.52	17.5	7309
5	*1.72*	790.9/4.82	26.5	8466
6	*1.86*	776.9/3.96	35.3	9230
7	*1.47*	369.2/1.59	18.9	7595
8	*1.56*	597.7/2.60	23.3	8146
9	*1.63*	553.3/2.11	27.1	8499

[a] Density – gas pycnometer at 298 K. [b] Calculated molar enthalpy of formation. [c] Calculated detonation pressure.

[d] Calculated detonation velocity.

Crystal Structure Data

Table S2: Crystal data and structure refinement for compounds **6**, **7, 8** and **9**.

Compound	**6**	**7**	**8**	**9**
CCDC #	2160643	2160646	2160645	2160644
Formula	$C_4H_4N_8O_2$	$C_4H_{12}N_{10}O_2$	$C_4H_{10}N_{10}O_2$	$C_2H_5N_5O_2$
$d_{calc.}$/ g cm^{-3}	1.905	1.506	1.585	1.668
μ/mm^{-1}	1.377	1.057	1.121	1.269
Formula Weight	196.15	232.24	230.22	131.11
Color	colorless	colorless	colorless	colorless
Shape	block-shaped	block-shaped	block-shaped	cube-shaped
Size/mm^3	0.21×0.16×0.05	0.17×0.12×0.07	0.14×0.09×0.03	0.09×0.06×0.03
T/K	99.99(10)	100.00(10)	100.00(10)	100(2)
Crystal System	tetragonal	orthorhombic	triclinic	monoclinic
Flack Parameter	-0.1(2)	0.11(9)	-	-
Hooft Parameter	-0.1(2)	0.09(6)	-	-
Space Group	$I4_1cd$	$Ima2$	P-1	$P2_1/c$
a/Å	10.60713(10)	7.45690(10)	4.3728(2)	6.9233(2)
b/Å	10.60713(10)	17.0704(2)	7.3072(4)	10.6988(3)
c/Å	12.1560(2)	8.04400(10)	8.3883(4)	7.0551(2)
α/°	90	90	66.474(5)	90
β/°	90	90	81.732(4)	92.465(3)
γ/°	90	90	79.997(4)	90
V/Å^3	1367.69(4)	1023.94(2)	241.19(2)	522.10(3)
Z	8	4	1	4
Z'	0.5	0.5	0.5	1
Wavelength/Å	1.54184	1.54184	1.54184	1.54184
Radiation type	Cu K_α	Cu K_α	Cu K_α	Cu K_α
Θ_{min}/°	8.358	5.182	5.772	6.399
Θ_{max}/°	76.324	77.305	76.203	76.915
Measured Refl's.	6016	5541	2089	2902
Indep't Refl's	703	1083	947	1010
Refl's I≥2 σ(I)	683	1077	861	914
R_{int}	0.0369	0.0237	0.0270	0.0270
Parameters	66	124	89	102
Restraints	1	1	0	0
Largest Peak	0.55	0.227	0.291	0.456
Deepest Hole	-0.31	-0.145	-0.271	-0.194
GooF	1.169	1.087	1.094	1.056
wR_2 (all data)	0.1058	0.0549	0.0976	0.1006
wR_2	0.1064	0.0548	0.0949	0.0972
R_1 (all data)	0.0384	0.0209	0.0386	0.0401
R_1	0.0369	0.0208	0.0359	0.0365

Table S3: Bond Lengths in Å for **6**.

Atom	Atom	Length/Å
O1	N1	1.300(3)
N1	N2	1.354(4)
N1	C1	1.340(4)
N2	N3	1.298(3)
N3	N4	1.341(3)
N4	C1	1.350(3)
C1	C2	1.437(4)
C2	C2[1]	1.341(5)

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

Table S4: Bond Angles in ° for **6.**

Atom	Atom	Atom	Angle/°
O1	N1	N2	121.3(2)
O1	N1	C1	128.6(2)
C1	N1	N2	110.1(2)
N3	N2	N1	107.6(2)
N2	N3	N4	107.9(2)
N3	N4	C1	110.3(2)
N1	C1	N4	104.1(2)
N1	C1	C2	128.7(2)
N4	C1	C2	127.3(2)
C2[1]	C2	C1	122.8(3)

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

Table S5: Torsion Angles in ° for **6**.

A	B	C	D	Angle/°
O1	N1	N2	N3	179.9(6)
O1	N1	C1	N4	179.6(6)
O1	N1	C1	C2	1.0(9)
N1	N2	N3	N4	0.2(7)
N1	C1	C2	C2[1]	-0.8(7)
N2	N1	C1	N4	-1.4(6)
N2	N1	C1	C2	180.0(5)
N2	N3	N4	C1	-1.1(9)
N3	N4	C1	N1	1.6(8)
N3	N4	C1	C2	-179.8(5)
N4	C1	C2	C2[1]	-179.1(5)
C1	N1	N2	N3	0.8(6)

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

Table S6: Hydrogen Bonds for **6.**

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
C2	H2	O1[1]	0.95	2.29	2.962(3)	127.5

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

Table S7: Bond Lengths in Å for **7**.

Atom	Atom	Length/Å
N1	N2	1.342(3)
N1	C1	1.323(3)
N2	N3	1.293(3)
N3	N4	1.349(3)
N4	C1	1.329(3)
N5	N6	1.345(2)
N5	C4	1.331(2)
N6	N6[1]	1.308(2)
C1	C2	1.498(3)
C2	C3	1.527(3)
C3	C4	1.501(3)
O1	N7	1.420(2)
O2	N8[1]	1.496(2)
O2	N8	1.496(2)
N8	N8[2]	1.393(4)

[1]3/2-x,+y,+z; [2]2-x,1-y,+z

Table S8: Bond Angles in ° for **7**.

Atom	Atom	Atom	Angle/°
C1	N1	N2	106.14(2)
N3	N2	N1	108.83(2)
N2	N3	N4	109.5(2)
C1	N4	N3	105.17(2)
C4	N5	N6	105.16(1)
N6[1]	N6	N5	109.26(7)
N1	C1	N4	110.34(2)
N1	C1	C2	123.89(2)
N4	C1	C2	125.77(2)
C1	C2	C3	113.15(2)
C4	C3	C2	110.39(2)
N5[1]	C4	N5	111.15(2)
N5[1]	C4	C3	124.40(8)
N5	C4	C3	124.40(8)
N8	O2	N8[1]	111.7(2)

Atom	Atom	Atom	Angle/°
N8[2]	N8	O2	154.74(1)

[1]3/2-x,+y,+z; [2]2-x,1-y,+z

Table S9: Torsion Angles in ° for **7**.

Atom	Atom	Atom	Atom	Angle/°
N1	N2	N3	N4	0.000(1)
N1	C1	C2	C3	180.000(1)
N2	N1	C1	N4	0.000(1)
N2	N1	C1	C2	180.000(1)
N2	N3	N4	C1	0.000(1)
N3	N4	C1	N1	0.000(1)
N3	N4	C1	C2	180.000(1)
N4	C1	C2	C3	0.000(1)
N6	N5	C4	N5[1]	0.6(2)
N6	N5	C4	C3	178.00(2)
C1	N1	N2	N3	0.000(1)
C1	C2	C3	C4	180.000(1)
C2	C3	C4	N5	-88.55(2)
C2	C3	C4	N5[1]	88.55(2)
C4	N5	N6	N6[1]	-0.34(1)
N8[1]	O2	N8	N8[2]	128.8(5)

[1]3/2-x,+y,+z; [2]2-x,1-y,+z

Table S10: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **7** U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H2	6430(30)	6299(11)	5200(30)	22(5)
H3	8560(30)	6463(12)	8140(30)	34(6)
H1	7500	1650(30)	3570(50)	52(11)
H7A	7500	3150(20)	3900(40)	21(7)
H7B	6480(30)	2786(11)	2610(30)	19(5)
H2A	7500	4640(20)	2600(50)	38(9)
H8A	10380(40)	4580(14)	1060(40)	61(8)
H8B	8750(50)	4860(20)	-380(50)	24(11)

Table S11: Bond Lengths in Å for **8**.

Atom	Atom	Length/Å
N1	N2	1.3407(2)
N1	C1	1.3440(2)
N2	N3	1.3116(2)
N3	N4	1.3504(2)
N4	C1	1.3382(2)
C1	C2	1.4561(2)
C2	C2[1]	1.337(3)
O1	N5	1.4197(2)

[1]-x,-y,1-z

Table S12: Bond Angles in ° for **8**.

Atom	Atom	Atom	Angle/°
N2	N1	C1	105.16(11)
N3	N2	N1	109.65(11)
N2	N3	N4	109.28(10)
C1	N4	N3	105.07(11)
N1	C1	C2	125.13(12)
N4	C1	N1	110.84(12)
N4	C1	C2	124.01(12)
C2[1]	C2	C1	122.76(16)

[1]-x,-y,1-z

Table S13: Torsion Angles in ° for **8**.

Atom	Atom	Atom	Atom	Angle/°
N1	N2	N3	N4	-0.34(14)
N1	C1	C2	C2[1]	-3.2(2)
N2	N1	C1	N4	-0.84(14)
N2	N1	C1	C2	177.43(12)
N2	N3	N4	C1	-0.18(14)
N3	N4	C1	N1	0.64(14)
N3	N4	C1	C2	-177.65(12)
N4	C1	C2	C2[1]	174.80(15)
C1	N1	N2	N3	0.71(14)

[1]-x,-y,1-z

Table S14: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **8**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H2	761.47	-1527.34	4349.99	15
H1	970(50)	5020(40)	3190(30)	41(6)
H5A	-3080(40)	8050(30)	1660(20)	22(4)
H5B	-220(50)	7300(30)	700(30)	22(5)
H5C	-2700(50)	5930(30)	1540(30)	27(5)

Table S15: Hydrogen Bond information for **8**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
O1	H1	N1	0.89(3)	1.80(3)	2.6905(15)	177(2)
N5	H5A	N4[1]	0.96(2)	1.90(2)	2.8374(16)	164.2(17)
N5	H5B	N3[2]	0.91(2)	1.98(2)	2.8938(17)	175.0(17)
N5	H5C	N2[3]	0.92(2)	1.99(2)	2.8983(17)	167.4(18)

[1]-1+x,1+y,+z; [2]1-x,1-y,-z; [3]-1+x,+y,+z

Table S16: Bond Lengths in Å for **9**.

Atom	Atom	Length/Å
O1	N1	1.3342(17)
N1	N2	1.3351(18)
N1	C2	1.3435(19)
N2	N3	1.3104(19)
N3	N4	1.3490(18)
N4	C2	1.332(2)
C1	C1[1]	1.328(3)
C1	C2	1.446(2)
O2	N5	1.4194(17)

[1]1-x,1-y,2-z

Table S17: Bond Angles in ° for **9**.

Atom	Atom	Atom	Angle/°
O1	N1	N2	121.18(12)
O1	N1	C2	128.83(13)
N2	N1	C2	109.99(13)
N3	N2	N1	105.22(12)
N2	N3	N4	111.54(12)
C2	N4	N3	105.81(12)
C1[1]	C1	C2	121.75(19)
N1	C2	C1	124.01(14)
N4	C2	N1	107.44(13)
N4	C2	C1	128.56(13)

[1]1-x,1-y,2-z

Table S18: Torsion Angles in ° for **9**.

Atom	Atom	Atom	Atom	Angle/°
O1	N1	N2	N3	179.11(12)
O1	N1	C2	N4	-178.89(13)
O1	N1	C2	C1	1.5(2)
N1	N2	N3	N4	-0.07(16)
N2	N1	C2	N4	0.27(16)
N2	N1	C2	C1	-179.33(13)
N2	N3	N4	C2	0.24(16)
N3	N4	C2	N1	-0.30(16)
N3	N4	C2	C1	179.27(14)
C1[1]	C1	C2	N1	-167.11(18)
C1[1]	C1	C2	N4	13.4(3)
C2	N1	N2	N3	-0.12(16)

[1]1-x,1-y,2-z

Table S19: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **9**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H1	7000(30)	5275(17)	10040(30)	20(4)
H2	9380(40)	4530(30)	7600(40)	57(7)
H5A	10200(30)	2220(20)	6860(30)	38(6)
H5B	8300(30)	2845(19)	6120(30)	26(5)
H5C	10220(30)	3310(20)	5480(30)	37(6)

Table S20: Hydrogen Bond information for **9**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
O2	H2	O1	0.93(3)	1.69(3)	2.6219(15)	178(2)
N5	H5A	O1[1]	0.94(3)	1.82(3)	2.7418(18)	166(2)
N5	H5B	N3[2]	0.92(2)	1.96(2)	2.8161(19)	153.6(18)
N5	H5C	O1[3]	0.90(2)	1.95(2)	2.8493(17)	174(2)

[1]2-x,-1/2+y,3/2-z; [2]1-x,1-y,1-z; [3]2-x,1-y,1-z