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Supporting information

Preparation and characteristics of 1,2,4-oxadiazole-derived energetic ionic salts with nitrogen-linkages

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Contents

1. General Information

^{1}H NMR and ^{13}C NMR spectra were recorded on a 400 MHz (Buruker Avance 400) nuclear magnetic resonance spectrometers operating at 400 and 100 MHz, respectively, by using DMSO-d_6 as solvent and locking solvent. IR spectra were recorded using KBr pellets for solids on a Bruker ALPHA FT-IR-Spektrometer. Differential scanning calorimeter (Shimadzu TA-60ws) was employed to measure the melting points and composition temperatures at a scan rate of 5 ºC·min^{-1} in argon atomosphere. High resolution mass spectrometry was recorded on Bruker Apex IV FTMS.

2. Computation details

The heats of formation of **2-9** were computed by using the Gaussian09 (Revision B.01) suite of programs based on isodesmic reactions at the MP2 level of theory(Figure 1).[S1] The geometric optimization of molecules and frequency analysis were accomplished by using B3LYP with the 6-311+G** basis set. Based on a Born-Haber energy cycle (Scheme S1), the heat of formation of a salt can be simplified by the formula given in [Equation (1)]

$$\Delta H_f^\theta(\text{salts}, 298\,\text{K}) = \Delta H_f^\theta(\text{cation}, 298\,\text{K}) + \Delta H_f^\theta(\text{anion}, 298\,\text{K}) - \Delta H_L \qquad (1)$$

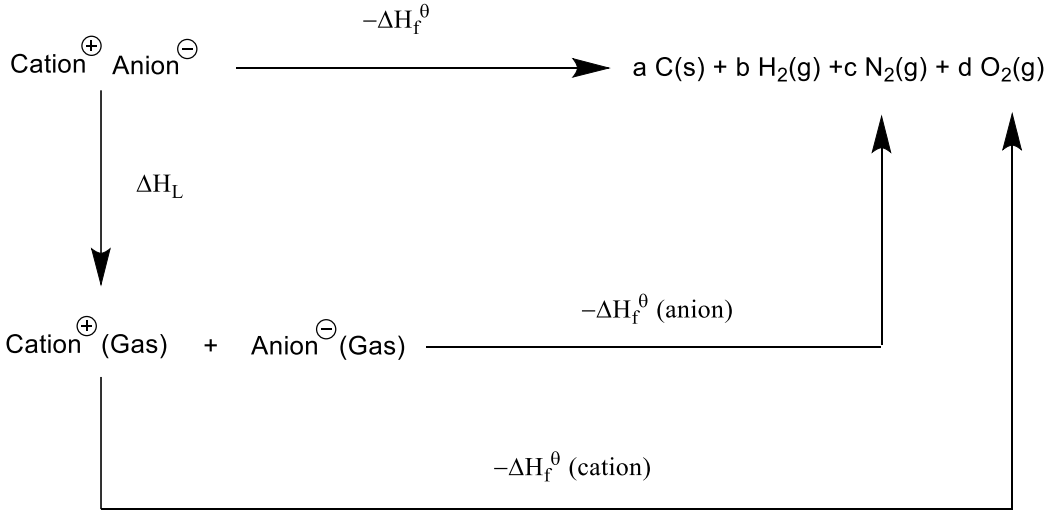
where ΔH_L is the lattice energy of the salts, which could be predicted by using the formula suggested by Jenkins et al.[S2][Eq. (2)]

$$\Delta H_L = U_{pot} + [\, p\,(n_M/2 - 2) + q\,(n_X/2 - 2)\,]\,RT \qquad (2)$$

In this equation, n_M and n_X depend on the nature of the ions Mp+ and Xq-, respectively, and are equal to three for monoatomic ions, five for linear polyatomic ions, and six for nonlinear polyatomic ions. The equation for lattice potential energy U_{pot} [Eq. (3)] has the form:

$$U_{pot}\,[\text{kJ mol}^{-1}] = \gamma\,(\rho_m / M_m)^{1/3} + \delta \qquad (3)$$

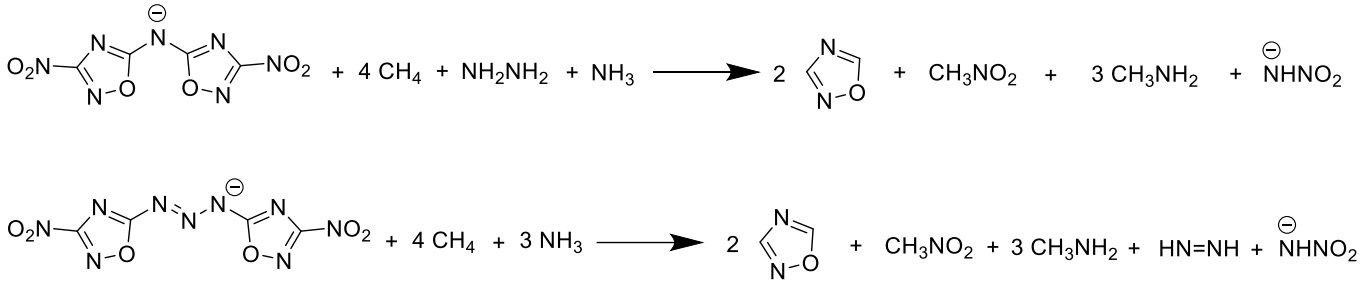
Where ρ_m [g cm^{-3}] is the density, M_m is the chemical formula mass of the ionic material, and values for the coefficients γ (kJ mol^{-1} cm) and δ (kJ mol^{-1}) are taken from the literature.[S2]



Scheme S1. Born-Haber cycle for the formation of energetic salts.

The heat of formation of bis(3-nitro-1,2,4-oxadiazol-5-yl)amide and sodium 1,3-bis(3-nitro-1,2,4-oxadiazol-5-yl)triaz-2-en-1-ide anion was determined by using an isodesmic reaction (Scheme S2). The heats of formation

of other compounds in Scheme S1 were determined from the NIST WebBook[S3] and literature references.[S4]



Scheme S2 Isodesmic reactions for anions of **2–9**

3. References

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[S3] P. J. Linstrom, W. G. Mallard, Eds., NIST Chemistry WebBook, NIST Standard Reference Database Number 69, June 2005, National Institute of Standards and Technology, Gaithersburg MD, 20899 (http://webbook.nist.gov).
[S4] K. Wang, D. A. Parrish and J. M. Shreeve. *Chem.–Eur. J.*, 2011, **17**, 14485-14492.
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4. X-ray Diffraction

Crystal data of **2**·DIOX were collected on a Rigaku Saturn 724 CCD diffractometer at 153 K and data of **2**·2H_2O, **2'**, **3**·DIOX, **4**·EtOAc, **5**, **7**·2DIOX were collected on a Bruker APEX-II CCD diffractometer at 296 K employing graphite-monochromated MoKa radiation (λ=0.71073 Å). The structure was solved by direct methods and refined by the least-squares method on F^2 using the SHELXTL-97 suite of programs.[S5] All non-hydrogen atoms were refined anisotropically. Details of the x-ray data collection and structure refinements are summarized in Table S1. Supplementary crystallographic data for this paper can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif with the CCDC number 1565962-8.

Table S1 Crystallographic data for **2**·2H_2O, **2**·DIOX, **2'**, **3**·DIOX, **4**·EtOAc, **5**, **7**·2DIOX

	2·2H_2O	**2**·DIOX	**2'**	**3**·DIOX	**4**·EtOAc	**5**	**7**·2DIXO
Formula	$C_4H_4N_7NaO_8$	$C_8H_8N_7NaO_8$	-	$C_8H_8N_9NaO_8$	$C_9H_{14}N_{10}O_8$	$C_5H_8N_{12}O_6$	$C_{11}H_{18}N_{12}O_9$
Mw[g mol^{-1}]	301.13	353.20	-	381.22	390.30	332.23	462.37
T[K]	296(2)	153(2)	296(2)	296(2)	296(2)	296(2)	296(2)
Crystal size[mm^3]	0.300 × 0.150 × 0.100	0.370 × 0.260 × 0.170	0.300 × 0.150 × 0.100	0.300 × 0.150 × 0.100	0.300 × 0.150 × 0.100	0.300 × 0.150 × 0.100	0.300 × 0.150 × 0.100
Crystal system	Monoclinic	Monoclinic	Cubic	Orthorhombic	Orthorhombic	Orthorhombic	Triclinic
Space group	$P2_1/n$	$P2_1/c$	*F d -3*	*Pbca*	*Pbcm*	$Pna2_1$	*P*-1
a[Å]	7.8182(4)	18.955(4)	37.2002(12)	9.438(2)	16.141(3)	12.6832(10)	8.9077(8)
b[Å]	12.4042(7)	9.9608(18)	37.2002(12)	34.981(8)	16.706(3)	14.8873(12)	11.0719(10)
c[Å]	12.0228(7)	15.930(3)	37.2002(12)	9.410(2)	6.4305(12)	6.9071(6)	11.9040(10)
α[°]	90	90	90	90	90	90	105.744(3)
β[°]	103.486(2)	111.912(2)	90	90	90	90	95.441(3)
γ[°]	90	90	90	90	90	90	109.541(3)
V[$Å^3$]	1133.80(11)	2790.5(10)	51480(5)	3106.7(12)	1734.0(6)	1304.19(19)	1042.38(16)
Z	4	8	16	8	4	4	2
ρ_{calc}[g cm^{-3}]	1.764	1.681	1.806	1.630	1.495	1.692	1.473
μ[mm^{-1}]	0.198	0.175	0.191	0.167	0.131	0.151	0.128
F[000]	608	1440	28305	1552	808	680	480
θ range[°]	2.394-31.612	2.350 -29.140	1.816-24.992	1.164-28.692	1.754-28.588	2.109-25.480	1.816-28.248
Reflections collected	15228 / 3497	24352 / 7478	11343/3797	31927 / 3879	20473 / 2390	12555 / 2429	12831 / 5143
Index ranges	-11<=h<=11, -17<=k<=17, -16<=l<=17	-25<=h<=25, -13<=k<=9, -21<=l<=21	0<=h<=44, 0<=h<=44, 0<=h<=44,	-12<=h<=12, -46<=k<=46, -12<=l<=12	-21<=h<=21, -22<=k<=22, -8<=l<=8	-15<=h<=15, -18<=k<=18, -8<=l<=8	-11<=h<=11, -14<=k<=14, -15<=l<=15
R_{int}	0.0208	0.0291	0.0126	0.0550	0.0717	0.0175	0.0173
Data/restraints/parameters	3497 / 1 / 181	7478 / 0 / 433	3797/0/318	3879 / 0 / 235	2390 / 0 / 165	2429 / 1 / 208	5143 / 0 / 289
Final *R* index[$I > 2\sigma(I)$]	R1 = 0.0363, wR_2 = 0.0948	R1 = 0.0485, wR2 = 0.1139	R1 = 0.0489, wR2 = 0.1121	R1 = 0.0762, wR2 = 0.1604	R1 = 0.0546, wR2 = 0.1307	R1 = 0.0292, wR2 = 0.0764	R1 = 0.0549, wR2 = 0.1594
Final *R* index[all data]	R_1 = 0.0519, wR_2 = 0.1052	R1 = 0.0616, wR2 = 0.1217	R1 = 0.0607, wR2 = 0.1193	R1 = 0.1033, wR2 = 0.1719	R1 = 0.0847, wR2 = 0.1486	R1 = 0.0309, wR2 = 0.0775	R1 = 0.0777, wR2 = 0.1793
GOF on F^2	0.998	1.129	1.089	1.105	1.054	1.044	1.049
CCDC	1565962	1565965	1565966	1565968	1565964	1565963	1565967

$R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|$. $wR_2 = [(w(F_o^2 - F_c^2)^2) / w(F_o^2)^2]^{1/2}$.

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **2**·2H_2O.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

x	y	z	U(eq)	
C(1)	-31(2)	10007(1)	1732(1)	36(1)
C(2)	2023(2)	9167(1)	978(1)	36(1)
C(3)	-2207(1)	9739(1)	2373(1)	35(1)
C(4)	2873(2)	7678(1)	580(1)	36(1)
N(1)	1358(1)	10071(1)	1285(1)	42(1)
N(2)	1685(1)	8131(1)	1079(1)	35(1)
N(3)	-1016(1)	9200(1)	1944(1)	35(1)
N(4)	3920(2)	8292(1)	178(1)	47(1)
N(5)	-2105(1)	10779(1)	2463(1)	43(1)
N(6)	3026(1)	6507(1)	503(1)	43(1)
N(7)	-3620(1)	9184(1)	2739(1)	44(1)
O(1)	-617(1)	10982(1)	2028(1)	46(1)
O(2)	3364(1)	9321(1)	438(1)	50(1)
O(3)	-4660(1)	9736(1)	3104(1)	61(1)
O(4)	3996(2)	6158(1)	-65(1)	72(1)
O(5)	-3671(2)	8209(1)	2643(1)	68(1)
O(6)	2173(2)	5966(1)	1019(1)	60(1)
O(7)	-1745(2)	6514(1)	-87(1)	72(1)
O(8)	1201(1)	6883(1)	3543(1)	43(1)
Na(1)	-691(1)	7127(1)	1746(1)	45(1)

Table S3. Bond lengths [A] and angles [deg] for **2**·2H_2O.

C(1)-N(1)	1.3222(16)
C(1)-N(3)	1.3236(15)
C(1)-O(1)	1.3689(14)
C(2)-N(1)	1.3232(15)
C(2)-N(2)	1.3233(14)
C(2)-O(2)	1.3701(14)
C(3)-N(5)	1.2953(15)
C(3)-N(3)	1.3430(14)
C(3)-N(7)	1.4542(15)
C(4)-N(4)	1.2914(16)
C(4)-N(2)	1.3408(14)

C(4)-N(6)	1.4618(16)
N(2)-Na(1)	2.5180(10)
N(3)-Na(1)	2.5999(10)
N(4)-O(2)	1.4076(15)
N(5)-O(1)	1.4049(14)
N(5)-Na(1)#1	2.7267(11)
N(6)-O(4)	1.2134(15)
N(6)-O(6)	1.2137(15)
N(7)-O(5)	1.2146(15)
N(7)-O(3)	1.2202(14)
O(3)-Na(1)#1	2.9799(13)
O(7)-Na(1)	2.2950(13)
O(7)-H(3)	0.8525
O(7)-H(4)	0.8485
O(8)-Na(1)	2.3362(11)
O(8)-H(1)	0.8512
O(8)-H(2)	0.8508
Na(1)-N(5)#2	2.7267(11)
Na(1)-O(3)#2	2.9799(13)

N(1)-C(1)-N(3)	133.94(11)
N(1)-C(1)-O(1)	114.16(10)
N(3)-C(1)-O(1)	111.89(10)
N(1)-C(2)-N(2)	134.27(11)
N(1)-C(2)-O(2)	114.05(10)
N(2)-C(2)-O(2)	111.68(10)
N(5)-C(3)-N(3)	119.55(11)
N(5)-C(3)-N(7)	118.85(10)
N(3)-C(3)-N(7)	121.60(10)
N(4)-C(4)-N(2)	119.09(11)
N(4)-C(4)-N(6)	119.57(10)
N(2)-C(4)-N(6)	121.33(10)
C(1)-N(1)-C(2)	118.38(10)
C(2)-N(2)-C(4)	101.12(9)
C(2)-N(2)-Na(1)	133.38(8)
C(4)-N(2)-Na(1)	125.08(8)
C(1)-N(3)-C(3)	100.60(9)
C(1)-N(3)-Na(1)	131.04(8)
C(3)-N(3)-Na(1)	128.23(8)
C(4)-N(4)-O(2)	101.30(9)
C(3)-N(5)-O(1)	100.80(9)
C(3)-N(5)-Na(1)#1	127.47(8)
O(1)-N(5)-Na(1)#1	131.72(7)
O(4)-N(6)-O(6)	125.50(12)
O(4)-N(6)-C(4)	117.46(12)
O(6)-N(6)-C(4)	117.03(10)
O(5)-N(7)-O(3)	125.71(11)

O(5)-N(7)-C(3)	116.95(11)
O(3)-N(7)-C(3)	117.34(11)
C(1)-O(1)-N(5)	107.16(8)
C(2)-O(2)-N(4)	106.81(9)
N(7)-O(3)-Na(1)#1	121.42(8)
Na(1)-O(7)-H(3)	122.8
Na(1)-O(7)-H(4)	133.6
H(3)-O(7)-H(4)	103.5
Na(1)-O(8)-H(1)	118.2
Na(1)-O(8)-H(2)	116.6
H(1)-O(8)-H(2)	99.3
O(7)-Na(1)-O(8)	148.57(4)
O(7)-Na(1)-N(2)	89.10(5)
O(8)-Na(1)-N(2)	90.21(4)
O(7)-Na(1)-N(3)	113.25(4)
O(8)-Na(1)-N(3)	95.61(3)
N(2)-Na(1)-N(3)	68.62(3)
O(7)-Na(1)-N(5)#2	90.99(5)
O(8)-Na(1)-N(5)#2	85.01(4)
N(2)-Na(1)-N(5)#2	170.97(4)
N(3)-Na(1)-N(5)#2	119.43(4)
O(7)-Na(1)-O(3)#2	74.69(4)
O(8)-Na(1)-O(3)#2	77.59(4)
N(2)-Na(1)-O(3)#2	116.56(3)
N(3)-Na(1)-O(3)#2	171.16(4)
N(5)#2-Na(1)-O(3)#2	54.90(3)

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

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for **2**·2H_2O.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	38(1)	26(1)	44(1)	-3(1)	12(1)	0(1)
C(2)	36(1)	36(1)	40(1)	-2(1)	16(1)	-5(1)
C(3)	35(1)	29(1)	42(1)	0(1)	11(1)	3(1)
C(4)	35(1)	38(1)	36(1)	-2(1)	12(1)	1(1)
N(1)	44(1)	31(1)	55(1)	-4(1)	22(1)	-6(1)
N(2)	34(1)	33(1)	41(1)	-1(1)	15(1)	-1(1)
N(3)	37(1)	26(1)	44(1)	-1(1)	15(1)	1(1)

N(4)	52(1)	45(1)	54(1)	-3(1)	31(1)	-1(1)
N(5)	42(1)	30(1)	60(1)	-2(1)	20(1)	2(1)
N(6)	38(1)	40(1)	50(1)	-3(1)	11(1)	6(1)
N(7)	42(1)	36(1)	56(1)	3(1)	18(1)	1(1)
O(1)	47(1)	26(1)	71(1)	-5(1)	26(1)	-2(1)
O(2)	56(1)	40(1)	65(1)	-2(1)	37(1)	-7(1)
O(3)	54(1)	56(1)	86(1)	3(1)	40(1)	8(1)
O(4)	74(1)	59(1)	98(1)	-13(1)	46(1)	15(1)
O(5)	68(1)	35(1)	112(1)	1(1)	42(1)	-8(1)
O(6)	64(1)	38(1)	85(1)	5(1)	31(1)	0(1)
O(7)	92(1)	48(1)	62(1)	-6(1)	-6(1)	12(1)
O(8)	46(1)	40(1)	47(1)	2(1)	21(1)	5(1)
Na(1)	46(1)	41(1)	48(1)	3(1)	13(1)	-6(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **2**·2H_2O.

x	y	z	U(eq)	
H(3)	-2238	6926	-637	86
H(4)	-1827	5894	-392	86
H(1)	1944	6370	3626	52
H(2)	723	6737	4092	52

Table S6. Torsion angles [deg] for **2**·2H_2O.

N(3)-C(1)-N(1)-C(2)	-1.7(2)
O(1)-C(1)-N(1)-C(2)	179.64(11)
N(2)-C(2)-N(1)-C(1)	-5.4(2)
O(2)-C(2)-N(1)-C(1)	174.84(11)
N(1)-C(2)-N(2)-C(4)	-179.79(14)
O(2)-C(2)-N(2)-C(4)	0.02(13)
N(1)-C(2)-N(2)-Na(1)	7.6(2)
O(2)-C(2)-N(2)-Na(1)	-172.55(8)
N(4)-C(4)-N(2)-C(2)	0.08(15)
N(6)-C(4)-N(2)-C(2)	178.83(11)
N(4)-C(4)-N(2)-Na(1)	173.48(9)
N(6)-C(4)-N(2)-Na(1)	-7.77(15)
N(1)-C(1)-N(3)-C(3)	-178.52(14)
O(1)-C(1)-N(3)-C(3)	0.20(13)
N(1)-C(1)-N(3)-Na(1)	5.4(2)

O(1)-C(1)-N(3)-Na(1)	-175.92(7)
N(5)-C(3)-N(3)-C(1)	-0.15(14)
N(7)-C(3)-N(3)-C(1)	179.68(11)
N(5)-C(3)-N(3)-Na(1)	176.12(9)
N(7)-C(3)-N(3)-Na(1)	-4.05(16)
N(2)-C(4)-N(4)-O(2)	-0.14(15)
N(6)-C(4)-N(4)-O(2)	-178.91(10)
N(3)-C(3)-N(5)-O(1)	0.03(15)
N(7)-C(3)-N(5)-O(1)	-179.80(10)
N(3)-C(3)-N(5)-Na(1)#1	178.90(8)
N(7)-C(3)-N(5)-Na(1)#1	-0.94(17)
N(4)-C(4)-N(6)-O(4)	-8.95(18)
N(2)-C(4)-N(6)-O(4)	172.31(12)
N(4)-C(4)-N(6)-O(6)	170.87(12)
N(2)-C(4)-N(6)-O(6)	-7.88(17)
N(5)-C(3)-N(7)-O(5)	-179.90(13)
N(3)-C(3)-N(7)-O(5)	0.27(18)
N(5)-C(3)-N(7)-O(3)	0.85(18)
N(3)-C(3)-N(7)-O(3)	-178.98(11)
N(1)-C(1)-O(1)-N(5)	178.79(10)
N(3)-C(1)-O(1)-N(5)	-0.20(14)
C(3)-N(5)-O(1)-C(1)	0.09(13)
Na(1)#1-N(5)-O(1)-C(1)	-178.70(8)
N(1)-C(2)-O(2)-N(4)	179.76(11)
N(2)-C(2)-O(2)-N(4)	-0.09(14)
C(4)-N(4)-O(2)-C(2)	0.13(13)
O(5)-N(7)-O(3)-Na(1)#1	-179.59(12)
C(3)-N(7)-O(3)-Na(1)#1	-0.42(16)

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

Table S7. Hydrogen bonds for **2**·2H_2O [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(7)-H(4)...O(6)#3	0.85	2.42	3.2644(16)	171.9
O(7)-H(3)...O(8)#4	0.85	2.02	2.8304(15)	158.2
O(8)-H(2)...N(4)#5	0.85	2.13	2.9537(14)	162.0
O(8)-H(1)...N(1)#6	0.85	2.07	2.9240(13)	175.7
O(7)-H(4)...O(6)#3	0.85	2.42	3.2644(16)	171.9
O(7)-H(3)...O(8)#4	0.85	2.02	2.8304(15)	158.2
O(8)-H(2)...N(4)#5	0.85	2.13	2.9537(14)	162.0
O(8)-H(1)...N(1)#6	0.85	2.07	2.9240(13)	175.7
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O(7)-H(3)...O(8)#4	0.85	2.02	2.8304(15)	158.2
O(8)-H(2)...N(4)#5	0.85	2.13	2.9537(14)	162.0
O(8)-H(1)...N(1)#6	0.85	2.07	2.9240(13)	175.7
O(7)-H(4)...O(6)#3	0.85	2.42	3.2644(16)	171.9
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O(8)-H(1)...N(1)#6	0.85	2.07	2.9240(13)	175.7
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O(8)-H(2)...N(4)#5	0.85	2.13	2.9537(14)	162.0
O(8)-H(1)...N(1)#6	0.85	2.07	2.9240(13)	175.7
O(7)-H(4)...O(6)#3	0.85	2.42	3.2644(16)	171.9
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O(7)-H(4)...O(6)#3	0.85	2.42	3.2644(16)	171.9
O(7)-H(3)...O(8)#4	0.85	2.02	2.8304(15)	158.2
O(8)-H(2)...N(4)#5	0.85	2.13	2.9537(14)	162.0
O(8)-H(1)...N(1)#6	0.85	2.07	2.9240(13)	175.7
O(7)-H(4)...O(6)#3	0.85	2.42	3.2644(16)	171.9
O(7)-H(3)...O(8)#4	0.85	2.02	2.8304(15)	158.2
O(8)-H(2)...N(4)#5	0.85	2.13	2.9537(14)	162.0
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O(8)-H(1)...N(1)#6	0.85	2.07	2.9240(13)	175.7
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O(7)-H(4)...O(6)#3	0.85	2.42	3.2644(16)	171.9
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O(8)-H(2)...N(4)#5	0.85	2.13	2.9537(14)	162.0
O(7)-H(3)...O(8)#4	0.85	2.02	2.8304(15)	158.2
O(7)-H(4)...O(6)#3	0.85	2.42	3.2644(16)	171.9
O(8)-H(1)...N(1)#6	0.85	2.07	2.9240(13)	175.7
O(8)-H(2)...N(4)#5	0.85	2.13	2.9537(14)	162.0
O(7)-H(3)...O(8)#4	0.85	2.02	2.8304(15)	158.2
O(7)-H(4)...O(6)#3	0.85	2.42	3.2644(16)	171.9
O(8)-H(1)...N(1)#6	0.85	2.07	2.9240(13)	175.7
O(8)-H(2)...N(4)#5	0.85	2.13	2.9537(14)	162.0
O(7)-H(3)...O(8)#4	0.85	2.02	2.8304(15)	158.2
O(8)-H(1)...N(1)#6	0.85	2.07	2.9240(13)	175.7
O(8)-H(2)...N(4)#5	0.85	2.13	2.9537(14)	162.0
O(7)-H(3)...O(8)#4	0.85	2.02	2.8304(15)	158.2
O(7)-H(4)...O(6)#3	0.85	2.42	3.2644(16)	171.9
O(8)-H(1)...N(1)#6	0.85	2.07	2.9240(13)	175.7
O(8)-H(2)...N(4)#5	0.85	2.13	2.9537(14)	162.0
O(7)-H(3)...O(8)#4	0.85	2.02	2.8304(15)	158.2
O(7)-H(4)...O(6)#3	0.85	2.42	3.2644(16)	171.9
O(8)-H(1)...N(1)#6	0.85	2.07	2.9240(13)	175.7
O(8)-H(2)...N(4)#5	0.85	2.13	2.9537(14)	162.0
O(7)-H(3)...O(8)#4	0.85	2.02	2.8304(15)	158.2
O(8)-H(1)...N(1)#6	0.85	2.07	2.9240(13)	175.7
O(8)-H(2)...N(4)#5	0.85	2.13	2.9537(14)	162.0
O(7)-H(3)...O(8)#4	0.85	2.02	2.8304(15)	158.2
O(7)-H(4)...O(6)#3	0.85	2.42	3.2644(16)	171.9
O(8)-H(1)...N(1)#6	0.85	2.07	2.9240(13)	175.7
O(8)-H(2)...N(4)#5	0.85	2.13	2.9537(14)	162.0
O(7)-H(3)...O(8)#4	0.85	2.02	2.8304(15)	158.2
O(7)-H(4)...O(6)#3	0.85	2.42	3.2644(16)	171.9
O(8)-H(1)...N(1)#6	0.85	2.07	2.9240(13)	175.7
O(8)-H(2)...N(4)#5	0.85	2.13	2.9537(14)	162.0
O(7)-H(3)...O(8)#4	0.85	2.02	2.8304(15)	158.2
O(7)-H(4)...O(6)#3	0.85	2.42	3.2644(16)	171.9
O(8)-H(1)...N(1)#6	0.85	2.07	2.9240(13)	175.7
O(8)-H(2)...N(4)#5	0.85	2.13	2.9537(14)	162.0
O(7)-H(3)...O(8)#4	0.85	2.02	2.8304(15)	158.2
O(7)-H(4)...O(6)#3	0.85	2.42	3.2644(16)	171.9
O(8)-H(1)...N(1)#6	0.85	2.07	2.9240(13)	175.7
O(8)-H(2)...N(4)#5	0.85	2.13	2.9537(14)	162.0
O(7)-H(3)...O(8)#4	0.85	2.02	2.8304(15)	158.2
O(7)-H(4)...O(6)#3	0.85	2.42	3.2644(16)	171.9

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

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **2**·DIOX.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

x	y	z	U(eq)	
Na(1)	3842(1)	7714(1)	7426(1)	24(1)
Na(2)	1096(1)	2906(1)	7583(1)	25(1)
O(1)	4225(1)	9603(1)	6048(1)	31(1)
O(2)	5639(1)	9019(1)	9036(1)	34(1)
O(3)	4620(1)	12233(1)	4347(1)	44(1)
O(4)	5614(1)	12736(1)	5536(1)	38(1)
O(5)	7058(1)	12569(1)	9408(1)	35(1)
O(6)	7264(1)	11481(1)	10659(1)	40(1)
O(7)	707(1)	-1180(1)	8780(1)	39(1)
O(8)	-681(1)	-216(1)	5827(1)	40(1)
O(9)	2302(1)	1094(1)	10602(1)	43(1)
O(10)	1947(1)	2576(1)	9522(1)	37(1)
O(11)	605(1)	3312(1)	5632(1)	48(1)
O(12)	-274(1)	2758(2)	4346(1)	61(1)
O(13)	3194(1)	9790(1)	7201(1)	31(1)
O(14)	2220(1)	11861(1)	7365(1)	28(1)
O(16)	1731(1)	4986(1)	7980(1)	31(1)
O(15)	2813(1)	6492(1)	7545(1)	37(1)
N(1)	4215(1)	10378(1)	5298(1)	31(1)
N(2)	5176(1)	11070(1)	6583(1)	22(1)
N(3)	4928(1)	9383(1)	7550(1)	27(1)
N(4)	5929(1)	10888(1)	8472(1)	23(1)
N(5)	6231(1)	9642(1)	9757(1)	33(1)
N(6)	5022(1)	12131(1)	5148(1)	30(1)
N(7)	6936(1)	11655(1)	9847(1)	27(1)
N(8)	1265(1)	-622(1)	9557(1)	37(1)
N(9)	967(1)	839(1)	8374(1)	25(1)
N(10)	4(1)	-624(1)	7320(1)	32(1)
N(11)	239(1)	1260(1)	6489(1)	26(1)
N(12)	-698(1)	715(2)	5147(1)	40(1)
N(13)	1915(1)	1470(1)	9838(1)	30(1)

N(14)	74(1)	2615(2)	5159(1)	40(1)
C(1)	4785(1)	11178(1)	5691(1)	23(1)
C(2)	4815(1)	10053(1)	6788(1)	23(1)
C(3)	5483(1)	9816(1)	8289(1)	24(1)
C(4)	6346(1)	10694(2)	9351(1)	25(1)
C(5)	1366(1)	524(2)	9243(1)	26(1)
C(6)	544(1)	-259(2)	8096(1)	28(1)
C(7)	-110(1)	164(2)	6609(1)	28(1)
C(8)	-147(1)	1500(2)	5606(1)	30(1)
C(9)	3436(1)	10717(2)	7940(1)	36(1)
C(10)	2765(1)	11221(2)	8135(1)	38(1)
C(11)	1996(1)	10960(2)	6611(1)	32(1)
C(12)	2672(1)	10458(2)	6424(1)	33(1)
C(13)	2022(1)	6558(2)	6999(1)	35(1)
C(14)	1550(1)	6279(2)	7557(1)	34(1)
C(15)	2523(1)	4970(2)	8541(1)	35(1)
C(16)	2989(1)	5200(2)	7972(1)	38(1)

Table S9. Bond lengths [A] and angles [deg] for **2**·DIOX.

Na(1)-O(13)	2.3627(12)
Na(1)-O(15)	2.3649(13)
Na(1)-N(4)#1	2.4520(13)
Na(1)-N(2)#1	2.5384(13)
Na(1)-N(3)	2.5950(14)
Na(1)-O(5)#1	2.7841(14)
Na(1)-O(4)#1	3.0164(15)
Na(2)-O(16)	2.3611(12)
Na(2)-N(9)	2.4734(14)
Na(2)-N(11)	2.5005(14)
Na(2)-O(14)#2	2.5085(12)
Na(2)-N(10)#3	2.5998(14)
Na(2)-O(11)	2.9199(16)
Na(2)-O(10)	2.9209(14)
O(1)-C(2)	1.3629(17)
O(1)-N(1)	1.4164(17)
O(2)-C(3)	1.3684(17)
O(2)-N(5)	1.4145(17)
O(3)-N(6)	1.2221(17)
O(4)-N(6)	1.2202(18)
O(4)-Na(1)#4	3.0163(15)
O(5)-N(7)	1.2209(16)
O(5)-Na(1)#4	2.7842(14)
O(6)-N(7)	1.2207(16)
O(7)-C(6)	1.3681(19)

O(7)-N(8)	1.4080(18)
O(8)-C(7)	1.3641(18)
O(8)-N(12)	1.417(2)
O(9)-N(13)	1.2220(17)
O(10)-N(13)	1.2217(17)
O(11)-N(14)	1.223(2)
O(12)-N(14)	1.2220(19)
O(13)-C(12)	1.4289(18)
O(13)-C(9)	1.4298(18)
O(14)-C(10)	1.4256(18)
O(14)-C(11)	1.4305(18)
O(14)-Na(2)#5	2.5085(12)
O(16)-C(15)	1.4320(18)
O(16)-C(14)	1.4338(19)
O(15)-C(13)	1.4273(18)
O(15)-C(16)	1.4359(19)
N(1)-C(1)	1.2990(19)
N(2)-C(2)	1.3295(18)
N(2)-C(1)	1.3407(18)
N(2)-Na(1)#4	2.5384(13)
N(3)-C(3)	1.3241(18)
N(3)-C(2)	1.3310(19)
N(4)-C(3)	1.3244(18)
N(4)-C(4)	1.3403(18)
N(4)-Na(1)#4	2.4521(14)
N(5)-C(4)	1.2925(19)
N(6)-C(1)	1.4629(19)
N(7)-C(4)	1.4590(19)
N(8)-C(5)	1.289(2)
N(9)-C(6)	1.3299(19)
N(9)-C(5)	1.3435(19)
N(10)-C(7)	1.327(2)
N(10)-C(6)	1.329(2)
N(10)-Na(2)#6	2.5997(15)
N(11)-C(7)	1.326(2)
N(11)-C(8)	1.3434(19)
N(12)-C(8)	1.291(2)
N(13)-C(5)	1.461(2)
N(14)-C(8)	1.462(2)
C(9)-C(10)	1.504(2)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.506(2)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900

C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.504(2)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.500(2)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900

O(13)-Na(1)-O(15)	93.72(5)
O(13)-Na(1)-N(4)#1	139.09(5)
O(15)-Na(1)-N(4)#1	89.76(5)
O(13)-Na(1)-N(2)#1	151.42(5)
O(15)-Na(1)-N(2)#1	93.08(4)
N(4)#1-Na(1)-N(2)#1	68.61(4)
O(13)-Na(1)-N(3)	78.66(5)
O(15)-Na(1)-N(3)	167.85(5)
N(4)#1-Na(1)-N(3)	102.20(4)
N(2)#1-Na(1)-N(3)	89.40(4)
O(13)-Na(1)-O(5)#1	78.81(4)
O(15)-Na(1)-O(5)#1	81.75(4)
N(4)#1-Na(1)-O(5)#1	61.38(4)
N(2)#1-Na(1)-O(5)#1	129.68(4)
N(3)-Na(1)-O(5)#1	105.71(4)
O(13)-Na(1)-O(4)#1	96.13(4)
O(15)-Na(1)-O(4)#1	83.05(4)
N(4)#1-Na(1)-O(4)#1	124.73(4)
N(2)#1-Na(1)-O(4)#1	57.27(4)
N(3)-Na(1)-O(4)#1	88.32(4)
O(5)#1-Na(1)-O(4)#1	163.61(4)
O(16)-Na(2)-N(9)	137.03(5)
O(16)-Na(2)-N(11)	153.63(5)
N(9)-Na(2)-N(11)	69.32(5)
O(16)-Na(2)-O(14)#2	91.54(4)
N(9)-Na(2)-O(14)#2	88.64(4)
N(11)-Na(2)-O(14)#2	89.79(4)
O(16)-Na(2)-N(10)#3	80.19(4)
N(9)-Na(2)-N(10)#3	101.77(5)
N(11)-Na(2)-N(10)#3	94.80(5)
O(14)#2-Na(2)-N(10)#3	169.54(5)
O(16)-Na(2)-O(11)	95.25(4)
N(9)-Na(2)-O(11)	127.20(5)
N(11)-Na(2)-O(11)	58.88(4)

O(14)#2-Na(2)-O(11)	81.97(4)
N(10)#3-Na(2)-O(11)	92.35(4)
O(16)-Na(2)-O(10)	77.91(4)
N(9)-Na(2)-O(10)	59.21(4)
N(11)-Na(2)-O(10)	128.45(4)
O(14)#2-Na(2)-O(10)	86.44(4)
N(10)#3-Na(2)-O(10)	97.96(5)
O(11)-Na(2)-O(10)	166.41(4)
C(2)-O(1)-N(1)	107.38(11)
C(3)-O(2)-N(5)	107.47(11)
N(6)-O(4)-Na(1)#4	115.00(9)
N(7)-O(5)-Na(1)#4	117.84(9)
C(6)-O(7)-N(8)	107.87(11)
C(7)-O(8)-N(12)	107.52(12)
N(13)-O(10)-Na(2)	116.38(9)
N(14)-O(11)-Na(2)	116.12(10)
C(12)-O(13)-C(9)	108.55(12)
C(12)-O(13)-Na(1)	133.78(9)
C(9)-O(13)-Na(1)	116.82(9)
C(10)-O(14)-C(11)	109.54(12)
C(10)-O(14)-Na(2)#5	116.50(9)
C(11)-O(14)-Na(2)#5	112.04(8)
C(15)-O(16)-C(14)	108.37(11)
C(15)-O(16)-Na(2)	117.89(9)
C(14)-O(16)-Na(2)	130.81(9)
C(13)-O(15)-C(16)	109.54(12)
C(13)-O(15)-Na(1)	129.70(9)
C(16)-O(15)-Na(1)	116.55(9)
C(1)-N(1)-O(1)	100.45(11)
C(2)-N(2)-C(1)	100.95(12)
C(2)-N(2)-Na(1)#4	131.65(10)
C(1)-N(2)-Na(1)#4	126.46(10)
C(3)-N(3)-C(2)	116.81(12)
C(3)-N(3)-Na(1)	128.40(10)
C(2)-N(3)-Na(1)	113.51(9)
C(3)-N(4)-C(4)	101.19(12)
C(3)-N(4)-Na(1)#4	134.96(10)
C(4)-N(4)-Na(1)#4	123.51(10)
C(4)-N(5)-O(2)	100.40(12)
O(4)-N(6)-O(3)	125.87(14)
O(4)-N(6)-C(1)	116.61(13)
O(3)-N(6)-C(1)	117.51(14)
O(6)-N(7)-O(5)	125.57(13)
O(6)-N(7)-C(4)	117.74(13)
O(5)-N(7)-C(4)	116.69(12)
C(5)-N(8)-O(7)	100.40(13)
C(6)-N(9)-C(5)	100.86(13)

C(6)-N(9)-Na(2)	132.60(10)
C(5)-N(9)-Na(2)	126.47(10)
C(7)-N(10)-C(6)	117.12(13)
C(7)-N(10)-Na(2)#6	120.34(10)
C(6)-N(10)-Na(2)#6	117.06(10)
C(7)-N(11)-C(8)	101.10(13)
C(7)-N(11)-Na(2)	131.97(11)
C(8)-N(11)-Na(2)	124.80(11)
C(8)-N(12)-O(8)	100.44(13)
O(10)-N(13)-O(9)	125.69(14)
O(10)-N(13)-C(5)	116.57(13)
O(9)-N(13)-C(5)	117.74(13)
O(12)-N(14)-O(11)	125.60(17)
O(12)-N(14)-C(8)	117.67(16)
O(11)-N(14)-C(8)	116.72(14)
N(1)-C(1)-N(2)	119.51(14)
N(1)-C(1)-N(6)	119.77(13)
N(2)-C(1)-N(6)	120.61(13)
N(2)-C(2)-N(3)	133.11(13)
N(2)-C(2)-O(1)	111.68(13)
N(3)-C(2)-O(1)	115.18(12)
N(3)-C(3)-N(4)	133.51(14)
N(3)-C(3)-O(2)	115.22(13)
N(4)-C(3)-O(2)	111.27(12)
N(5)-C(4)-N(4)	119.67(14)
N(5)-C(4)-N(7)	119.94(13)
N(4)-C(4)-N(7)	120.39(13)
N(8)-C(5)-N(9)	119.87(15)
N(8)-C(5)-N(13)	119.55(14)
N(9)-C(5)-N(13)	120.58(13)
N(10)-C(6)-N(9)	133.93(15)
N(10)-C(6)-O(7)	115.07(13)
N(9)-C(6)-O(7)	110.99(13)
N(11)-C(7)-N(10)	132.70(14)
N(11)-C(7)-O(8)	111.37(14)
N(10)-C(7)-O(8)	115.90(14)
N(12)-C(8)-N(11)	119.57(16)
N(12)-C(8)-N(14)	120.17(15)
N(11)-C(8)-N(14)	120.22(14)
O(13)-C(9)-C(10)	110.50(13)
O(13)-C(9)-H(9A)	109.6
C(10)-C(9)-H(9A)	109.6
O(13)-C(9)-H(9B)	109.6
C(10)-C(9)-H(9B)	109.6
H(9A)-C(9)-H(9B)	108.1
O(14)-C(10)-C(9)	111.61(13)
O(14)-C(10)-H(10A)	109.3

C(9)-C(10)-H(10A)	109.3
O(14)-C(10)-H(10B)	109.3
C(9)-C(10)-H(10B)	109.3
H(10A)-C(10)-H(10B)	108.0
O(14)-C(11)-C(12)	111.54(12)
O(14)-C(11)-H(11A)	109.3
C(12)-C(11)-H(11A)	109.3
O(14)-C(11)-H(11B)	109.3
C(12)-C(11)-H(11B)	109.3
H(11A)-C(11)-H(11B)	108.0
O(13)-C(12)-C(11)	110.35(13)
O(13)-C(12)-H(12A)	109.6
C(11)-C(12)-H(12A)	109.6
O(13)-C(12)-H(12B)	109.6
C(11)-C(12)-H(12B)	109.6
H(12A)-C(12)-H(12B)	108.1
O(15)-C(13)-C(14)	110.72(13)
O(15)-C(13)-H(13A)	109.5
C(14)-C(13)-H(13A)	109.5
O(15)-C(13)-H(13B)	109.5
C(14)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	108.1
O(16)-C(14)-C(13)	110.61(13)
O(16)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14A)	109.5
O(16)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	108.1
O(16)-C(15)-C(16)	109.72(13)
O(16)-C(15)-H(15A)	109.7
C(16)-C(15)-H(15A)	109.7
O(16)-C(15)-H(15B)	109.7
C(16)-C(15)-H(15B)	109.7
H(15A)-C(15)-H(15B)	108.2
O(15)-C(16)-C(15)	109.83(14)
O(15)-C(16)-H(16A)	109.7
C(15)-C(16)-H(16A)	109.7
O(15)-C(16)-H(16B)	109.7
C(15)-C(16)-H(16B)	109.7
H(16A)-C(16)-H(16B)	108.2

Symmetry transformations used to generate equivalent atoms:

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

#4 -x+1,y+1/2,-z+3/2 #5 x,y+1,z #6 -x,y-1/2,-z+3/2

Table S10. Anisotropic displacement parameters (A^2 x 10^3) for **2**·DIOX.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Na(1)	21(1)	20(1)	30(1)	0(1)	9(1)	1(1)
Na(2)	22(1)	23(1)	29(1)	-1(1)	8(1)	-1(1)
O(1)	26(1)	36(1)	28(1)	-6(1)	8(1)	-9(1)
O(2)	40(1)	30(1)	27(1)	6(1)	8(1)	-10(1)
O(3)	53(1)	53(1)	24(1)	10(1)	11(1)	12(1)
O(4)	40(1)	38(1)	42(1)	4(1)	19(1)	-6(1)
O(5)	37(1)	27(1)	35(1)	4(1)	8(1)	-6(1)
O(6)	42(1)	45(1)	25(1)	1(1)	3(1)	-5(1)
O(7)	41(1)	28(1)	47(1)	8(1)	16(1)	-7(1)
O(8)	29(1)	42(1)	44(1)	-15(1)	6(1)	-6(1)
O(9)	44(1)	51(1)	27(1)	7(1)	6(1)	1(1)
O(10)	48(1)	28(1)	33(1)	1(1)	13(1)	-6(1)
O(11)	34(1)	58(1)	50(1)	20(1)	14(1)	3(1)
O(12)	61(1)	91(1)	29(1)	17(1)	14(1)	27(1)
O(13)	32(1)	31(1)	25(1)	-2(1)	6(1)	13(1)
O(14)	29(1)	29(1)	26(1)	0(1)	9(1)	9(1)
O(16)	22(1)	32(1)	38(1)	6(1)	8(1)	-4(1)
O(15)	26(1)	38(1)	48(1)	16(1)	13(1)	-2(1)
N(1)	27(1)	39(1)	25(1)	-3(1)	8(1)	-2(1)
N(2)	21(1)	22(1)	22(1)	0(1)	7(1)	0(1)
N(3)	25(1)	27(1)	28(1)	1(1)	10(1)	-5(1)
N(4)	22(1)	23(1)	22(1)	1(1)	7(1)	-1(1)
N(5)	38(1)	32(1)	26(1)	4(1)	7(1)	-6(1)
N(6)	34(1)	30(1)	27(1)	3(1)	14(1)	7(1)
N(7)	28(1)	27(1)	25(1)	0(1)	7(1)	2(1)
N(8)	42(1)	32(1)	39(1)	7(1)	16(1)	-2(1)
N(9)	24(1)	24(1)	29(1)	1(1)	10(1)	-1(1)
N(10)	24(1)	26(1)	45(1)	-3(1)	12(1)	-3(1)
N(11)	21(1)	27(1)	28(1)	-3(1)	7(1)	3(1)
N(12)	30(1)	51(1)	34(1)	-10(1)	4(1)	5(1)
N(13)	31(1)	33(1)	27(1)	1(1)	14(1)	2(1)
N(14)	34(1)	56(1)	31(1)	10(1)	14(1)	17(1)
C(1)	22(1)	26(1)	22(1)	-1(1)	9(1)	4(1)
C(2)	17(1)	25(1)	26(1)	-4(1)	8(1)	-2(1)
C(3)	25(1)	23(1)	26(1)	2(1)	11(1)	-1(1)
C(4)	26(1)	24(1)	24(1)	2(1)	10(1)	2(1)
C(5)	28(1)	24(1)	31(1)	4(1)	15(1)	3(1)

C(6)	24(1)	24(1)	39(1)	2(1)	16(1)	0(1)
C(7)	19(1)	27(1)	36(1)	-8(1)	8(1)	0(1)
C(8)	23(1)	38(1)	27(1)	-6(1)	8(1)	7(1)
C(9)	31(1)	44(1)	26(1)	-6(1)	4(1)	13(1)
C(10)	42(1)	46(1)	26(1)	3(1)	13(1)	20(1)
C(11)	27(1)	33(1)	31(1)	-5(1)	5(1)	6(1)
C(12)	32(1)	40(1)	24(1)	-1(1)	6(1)	15(1)
C(13)	29(1)	38(1)	35(1)	10(1)	9(1)	0(1)
C(14)	27(1)	32(1)	42(1)	6(1)	13(1)	3(1)
C(15)	27(1)	38(1)	32(1)	8(1)	4(1)	-7(1)
C(16)	27(1)	38(1)	49(1)	13(1)	13(1)	2(1)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **2**·DIOX.

x	y	z	U(eq)	
H(9A)	3699	11483	7789	43
H(9B)	3799	10269	8484	43
H(10A)	2521	10459	8321	46
H(10B)	2943	11867	8644	46
H(11A)	1642	11426	6069	38
H(11B)	1723	10186	6739	38
H(12A)	2499	9829	5905	40
H(12B)	2929	11223	6261	40
H(13A)	1900	5891	6504	42
H(13B)	1897	7461	6724	42
H(14A)	1646	6980	8027	40
H(14B)	1004	6309	7165	40
H(15A)	2658	4092	8852	41
H(15B)	2632	5680	9007	41
H(16A)	3536	5156	8357	45
H(16B)	2878	4491	7505	45

Table S12. Torsion angles [deg] for **2**·DIOX.

C(2)-O(1)-N(1)-C(1)	-0.69(14)
C(3)-O(2)-N(5)-C(4)	-0.32(16)
Na(1)#4-O(4)-N(6)-O(3)	163.95(12)
Na(1)#4-O(4)-N(6)-C(1)	-17.46(16)
Na(1)#4-O(5)-N(7)-O(6)	-177.53(12)

Na(1)#4-O(5)-N(7)-C(4)	2.40(16)
C(6)-O(7)-N(8)-C(5)	-0.61(16)
C(7)-O(8)-N(12)-C(8)	0.18(15)
Na(2)-O(10)-N(13)-O(9)	170.53(12)
Na(2)-O(10)-N(13)-C(5)	-9.29(16)
Na(2)-O(11)-N(14)-O(12)	169.83(13)
Na(2)-O(11)-N(14)-C(8)	-11.57(17)
O(1)-N(1)-C(1)-N(2)	-0.13(17)
O(1)-N(1)-C(1)-N(6)	176.23(12)
C(2)-N(2)-C(1)-N(1)	0.88(17)
Na(1)#4-N(2)-C(1)-N(1)	-169.00(10)
C(2)-N(2)-C(1)-N(6)	-175.44(12)
Na(1)#4-N(2)-C(1)-N(6)	14.68(18)
O(4)-N(6)-C(1)-N(1)	-171.26(14)
O(3)-N(6)-C(1)-N(1)	7.5(2)
O(4)-N(6)-C(1)-N(2)	5.1(2)
O(3)-N(6)-C(1)-N(2)	-176.23(13)
C(1)-N(2)-C(2)-N(3)	176.51(16)
Na(1)#4-N(2)-C(2)-N(3)	-14.4(2)
C(1)-N(2)-C(2)-O(1)	-1.28(15)
Na(1)#4-N(2)-C(2)-O(1)	167.82(9)
C(3)-N(3)-C(2)-N(2)	4.0(2)
Na(1)-N(3)-C(2)-N(2)	172.20(13)
C(3)-N(3)-C(2)-O(1)	-178.23(12)
Na(1)-N(3)-C(2)-O(1)	-10.07(15)
N(1)-O(1)-C(2)-N(2)	1.31(16)
N(1)-O(1)-C(2)-N(3)	-176.91(12)
C(2)-N(3)-C(3)-N(4)	7.9(2)
Na(1)-N(3)-C(3)-N(4)	-158.22(13)
C(2)-N(3)-C(3)-O(2)	-172.99(13)
Na(1)-N(3)-C(3)-O(2)	20.90(19)
C(4)-N(4)-C(3)-N(3)	178.81(16)
Na(1)#4-N(4)-C(3)-N(3)	-8.0(3)
C(4)-N(4)-C(3)-O(2)	-0.33(15)
Na(1)#4-N(4)-C(3)-O(2)	172.83(10)
N(5)-O(2)-C(3)-N(3)	-178.88(12)
N(5)-O(2)-C(3)-N(4)	0.43(16)
O(2)-N(5)-C(4)-N(4)	0.13(18)
O(2)-N(5)-C(4)-N(7)	-179.10(12)
C(3)-N(4)-C(4)-N(5)	0.12(18)
Na(1)#4-N(4)-C(4)-N(5)	-174.08(11)
C(3)-N(4)-C(4)-N(7)	179.34(13)
Na(1)#4-N(4)-C(4)-N(7)	5.14(18)
O(6)-N(7)-C(4)-N(5)	-5.7(2)
O(5)-N(7)-C(4)-N(5)	174.33(14)
O(6)-N(7)-C(4)-N(4)	175.05(13)
O(5)-N(7)-C(4)-N(4)	-4.9(2)

O(7)-N(8)-C(5)-N(9)	-0.04(18)
O(7)-N(8)-C(5)-N(13)	179.83(12)
C(6)-N(9)-C(5)-N(8)	0.67(18)
Na(2)-N(9)-C(5)-N(8)	-176.64(11)
C(6)-N(9)-C(5)-N(13)	-179.20(13)
Na(2)-N(9)-C(5)-N(13)	3.48(19)
O(10)-N(13)-C(5)-N(8)	-174.82(14)
O(9)-N(13)-C(5)-N(8)	5.3(2)
O(10)-N(13)-C(5)-N(9)	5.1(2)
O(9)-N(13)-C(5)-N(9)	-174.78(13)
C(7)-N(10)-C(6)-N(9)	9.2(3)
Na(2)#6-N(10)-C(6)-N(9)	-144.87(15)
C(7)-N(10)-C(6)-O(7)	-172.23(13)
Na(2)#6-N(10)-C(6)-O(7)	33.73(16)
C(5)-N(9)-C(6)-N(10)	177.62(17)
Na(2)-N(9)-C(6)-N(10)	-5.3(3)
C(5)-N(9)-C(6)-O(7)	-1.02(16)
Na(2)-N(9)-C(6)-O(7)	176.05(10)
N(8)-O(7)-C(6)-N(10)	-177.83(13)
N(8)-O(7)-C(6)-N(9)	1.08(17)
C(8)-N(11)-C(7)-N(10)	177.50(17)
Na(2)-N(11)-C(7)-N(10)	-19.0(3)
C(8)-N(11)-C(7)-O(8)	-0.38(16)
Na(2)-N(11)-C(7)-O(8)	163.08(9)
C(6)-N(10)-C(7)-N(11)	3.8(3)
Na(2)#6-N(10)-C(7)-N(11)	156.97(14)
C(6)-N(10)-C(7)-O(8)	-178.38(13)
Na(2)#6-N(10)-C(7)-O(8)	-25.23(17)
N(12)-O(8)-C(7)-N(11)	0.14(16)
N(12)-O(8)-C(7)-N(10)	-178.13(13)
O(8)-N(12)-C(8)-N(11)	-0.48(18)
O(8)-N(12)-C(8)-N(14)	177.27(13)
C(7)-N(11)-C(8)-N(12)	0.56(18)
Na(2)-N(11)-C(8)-N(12)	-164.49(11)
C(7)-N(11)-C(8)-N(14)	-177.18(13)
Na(2)-N(11)-C(8)-N(14)	17.76(19)
O(12)-N(14)-C(8)-N(12)	-0.7(2)
O(11)-N(14)-C(8)-N(12)	-179.44(15)
O(12)-N(14)-C(8)-N(11)	177.01(15)
O(11)-N(14)-C(8)-N(11)	-1.7(2)
C(12)-O(13)-C(9)-C(10)	59.31(18)
Na(1)-O(13)-C(9)-C(10)	-129.77(12)
C(11)-O(14)-C(10)-C(9)	55.39(19)
Na(2)#5-O(14)-C(10)-C(9)	-176.16(11)
O(13)-C(9)-C(10)-O(14)	-58.5(2)
C(10)-O(14)-C(11)-C(12)	-55.45(18)
Na(2)#5-O(14)-C(11)-C(12)	173.67(11)

C(9)-O(13)-C(12)-C(11)	-59.32(17)
Na(1)-O(13)-C(12)-C(11)	131.93(12)
O(14)-C(11)-C(12)-O(13)	58.52(18)
C(16)-O(15)-C(13)-C(14)	56.95(18)
Na(1)-O(15)-C(13)-C(14)	-147.40(12)
C(15)-O(16)-C(14)-C(13)	59.12(17)
Na(2)-O(16)-C(14)-C(13)	-100.60(14)
O(15)-C(13)-C(14)-O(16)	-57.95(18)
C(14)-O(16)-C(15)-C(16)	-60.85(17)
Na(2)-O(16)-C(15)-C(16)	101.88(13)
C(13)-O(15)-C(16)-C(15)	-58.68(18)
Na(1)-O(15)-C(16)-C(15)	142.10(11)
O(16)-C(15)-C(16)-O(15)	61.38(18)

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

Table S13. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **2'**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Na(01)	5000	5000	5000	36(1)
Na(02)	5874(1)	4677(1)	3375(1)	60(1)
O	4940(1)	4586(1)	4173(1)	67(1)
N(004)	5392(1)	4697(1)	3802(1)	51(1)
N(005)	6126(1)	5120(1)	2972(1)	55(1)
N(006)	5420(1)	4240(1)	3208(1)	53(1)
O(007)	7113(1)	4735(1)	3368(1)	82(1)
N(008)	6525(1)	4648(1)	3411(1)	58(1)
O(009)	4941(1)	3892(1)	3163(1)	82(1)
O(0AA)	5885(1)	5205(1)	3891(1)	83(1)
O(1)	5932(1)	4293(1)	2701(1)	88(1)
O(00C)	6478(1)	5436(1)	2606(1)	86(1)
N(00D)	5648(1)	5202(1)	4115(1)	66(1)
N(00E)	4966(1)	4222(1)	3678(1)	65(1)
O(2)	6208(1)	4171(1)	3849(1)	93(1)
N(00G)	5125(1)	4884(1)	4315(1)	65(1)
N(00H)	5682(1)	4096(1)	2626(1)	67(1)
O(00I)	5646(1)	3933(1)	2345(1)	90(1)
O(3)	5402(1)	5140(1)	2951(1)	94(1)
O(00K)	5411(1)	5580(1)	2570(1)	97(1)
N(00L)	6779(1)	5083(1)	2996(1)	71(1)

N(00M)	6533(1)	4186(1)	3869(1)	79(1)
O(00N)	5624(1)	5408(1)	4366(1)	104(1)
N(00O)	5555(1)	5352(1)	2756(1)	71(1)
C(00P)	5376(1)	4923(1)	4081(1)	54(1)
C(00Q)	5112(1)	4491(1)	3863(1)	55(1)
N(00R)	5138(1)	3844(1)	2841(1)	77(1)
C(00S)	5405(1)	4055(1)	2898(1)	56(1)
O(00T)	6717(1)	4006(1)	4071(1)	113(1)
C(00U)	5946(1)	5332(1)	2745(1)	59(1)
N(00V)	6121(1)	5528(1)	2520(1)	82(1)
C(00W)	6463(1)	5192(1)	2881(1)	60(1)
N(00X)	7062(1)	4465(1)	3628(1)	83(1)
C(00Y)	5124(1)	4135(1)	3369(1)	57(1)
C(00Z)	6782(1)	4836(1)	3247(1)	64(1)
C(010)	6716(1)	4438(1)	3629(1)	64(1)

Table S14. Bond lengths [A] and angles [deg] for **2'**.

Na(01)-N(00G)#1	2.627(2)
Na(01)-N(00G)#2	2.627(2)
Na(01)-N(00G)#3	2.627(2)
Na(01)-N(00G)#4	2.627(2)
Na(01)-N(00G)#5	2.627(2)
Na(01)-N(00G)	2.627(2)
Na(02)-N(004)	2.392(2)
Na(02)-N(005)	2.420(2)
Na(02)-N(006)	2.423(2)
Na(02)-N(008)	2.428(2)
Na(02)-O(0AA)	2.748(2)
Na(02)-O(1)	2.895(2)
Na(02)-O(2)	2.862(3)
Na(02)-O(3)	2.921(3)
O-N(00G)	1.408(3)
O-C(00Q)	1.366(3)
N(004)-C(00P)	1.336(3)
N(004)-C(00Q)	1.315(3)
N(005)-C(00U)	1.335(3)
N(005)-C(00W)	1.326(3)
N(006)-C(00S)	1.344(3)
N(006)-C(00Y)	1.315(3)
O(007)-N(00X)	1.405(3)
O(007)-C(00Z)	1.366(3)
N(008)-C(00Z)	1.332(3)
N(008)-C(010)	1.332(3)

O(009)-N(00R)	1.414(3)
O(009)-C(00Y)	1.367(3)
O(0AA)-N(00D)	1.211(3)
O(1)-N(00H)	1.217(3)
O(00C)-N(00V)	1.408(3)
O(00C)-C(00W)	1.368(3)
N(00D)-O(00N)	1.210(3)
N(00D)-C(00P)	1.454(3)
N(00E)-C(00Q)	1.329(3)
N(00E)-C(00Y)	1.332(3)
O(2)-N(00M)	1.211(3)
N(00G)-C(00P)	1.287(3)
N(00H)-O(00I)	1.214(3)
N(00H)-C(00S)	1.454(3)
O(3)-N(00O)	1.214(3)
O(00K)-N(00O)	1.218(3)
N(00L)-C(00W)	1.317(3)
N(00L)-C(00Z)	1.309(4)
N(00M)-O(00T)	1.217(3)
N(00M)-C(010)	1.463(4)
N(00O)-C(00U)	1.455(4)
N(00R)-C(00S)	1.285(3)
C(00U)-N(00V)	1.286(4)
N(00X)-C(010)	1.293(4)

N(00G)#1-Na(01)-N(00G)#3	180.0
N(00G)#5-Na(01)-N(00G)#4	180.00(10)
N(00G)#1-Na(01)-N(00G)#4	92.35(8)
N(00G)#2-Na(01)-N(00G)#4	92.35(8)
N(00G)#3-Na(01)-N(00G)	92.34(8)
N(00G)#5-Na(01)-N(00G)	92.35(8)
N(00G)#1-Na(01)-N(00G)#5	87.65(8)
N(00G)#1-Na(01)-N(00G)#2	92.35(8)
N(00G)#3-Na(01)-N(00G)#5	92.35(8)
N(00G)#1-Na(01)-N(00G)	87.66(8)
N(00G)#2-Na(01)-N(00G)#5	87.65(8)
N(00G)#3-Na(01)-N(00G)#2	87.65(8)
N(00G)#2-Na(01)-N(00G)	180.0
N(00G)#3-Na(01)-N(00G)#4	87.65(8)
N(00G)#4-Na(01)-N(00G)	87.65(8)
N(004)-Na(02)-N(005)	132.82(8)
N(004)-Na(02)-N(006)	70.80(7)
N(004)-Na(02)-N(008)	135.38(8)
N(004)-Na(02)-O(0AA)	61.66(7)
N(004)-Na(02)-O(1)	130.28(7)
N(004)-Na(02)-O(2)	86.47(7)
N(004)-Na(02)-O(3)	83.71(7)

N(005)-Na(02)-N(006)	124.57(8)
N(005)-Na(02)-N(008)	71.18(7)
N(005)-Na(02)-O(0AA)	86.59(7)
N(005)-Na(02)-O(1)	76.63(7)
N(005)-Na(02)-O(2)	131.39(8)
N(005)-Na(02)-O(3)	59.68(7)
N(006)-Na(02)-N(008)	132.69(8)
N(006)-Na(02)-O(0AA)	132.05(7)
N(006)-Na(02)-O(1)	59.94(7)
N(006)-Na(02)-O(2)	91.15(7)
N(006)-Na(02)-O(3)	80.77(7)
N(008)-Na(02)-O(0AA)	88.79(7)
N(008)-Na(02)-O(1)	87.13(7)
N(008)-Na(02)-O(2)	60.22(7)
N(008)-Na(02)-O(3)	130.85(8)
O(0AA)-Na(02)-O(1)	163.17(8)
O(0AA)-Na(02)-O(2)	91.89(7)
O(0AA)-Na(02)-O(3)	87.98(7)
O(1)-Na(02)-O(3)	82.40(7)
O(2)-Na(02)-O(1)	100.19(8)
O(2)-Na(02)-O(3)	168.91(8)
C(00Q)-O-N(00G)	106.89(19)
C(00P)-N(004)-Na(02)	124.62(16)
C(00Q)-N(004)-Na(02)	133.60(16)
C(00Q)-N(004)-C(00P)	101.4(2)
C(00U)-N(005)-Na(02)	126.90(17)
C(00W)-N(005)-Na(02)	131.46(17)
C(00W)-N(005)-C(00U)	101.2(2)
C(00S)-N(006)-Na(02)	126.41(17)
C(00Y)-N(006)-Na(02)	131.73(16)
C(00Y)-N(006)-C(00S)	101.7(2)
C(00Z)-O(007)-N(00X)	107.6(2)
C(00Z)-N(008)-Na(02)	131.90(17)
C(010)-N(008)-Na(02)	126.26(19)
C(010)-N(008)-C(00Z)	101.7(2)
C(00Y)-O(009)-N(00R)	107.66(19)
N(00D)-O(0AA)-Na(02)	117.51(17)
N(00H)-O(1)-Na(02)	116.03(16)
C(00W)-O(00C)-N(00V)	107.0(2)
O(0AA)-N(00D)-C(00P)	116.9(2)
O(00N)-N(00D)-O(0AA)	125.2(3)
O(00N)-N(00D)-C(00P)	117.9(2)
C(00Q)-N(00E)-C(00Y)	116.6(2)
N(00M)-O(2)-Na(02)	116.29(19)
O-N(00G)-Na(01)	113.98(14)
C(00P)-N(00G)-Na(01)	140.03(18)
C(00P)-N(00G)-O	101.01(19)

O(1)-N(00H)-C(00S)	116.4(2)
O(00I)-N(00H)-O(1)	125.6(3)
O(00I)-N(00H)-C(00S)	118.0(2)
N(00O)-O(3)-Na(02)	115.23(17)
C(00Z)-N(00L)-C(00W)	117.1(2)
O(2)-N(00M)-O(00T)	125.0(3)
O(2)-N(00M)-C(010)	117.0(2)
O(00T)-N(00M)-C(010)	117.9(3)
O(3)-N(00O)-O(00K)	126.0(3)
O(3)-N(00O)-C(00U)	116.8(2)
O(00K)-N(00O)-C(00U)	117.2(3)
N(004)-C(00P)-N(00D)	119.1(2)
N(00G)-C(00P)-N(004)	119.2(2)
N(00G)-C(00P)-N(00D)	121.8(2)
N(004)-C(00Q)-O	111.6(2)
N(004)-C(00Q)-N(00E)	132.4(2)
N(00E)-C(00Q)-O	116.0(2)
C(00S)-N(00R)-O(009)	100.5(2)
N(006)-C(00S)-N(00H)	120.9(2)
N(00R)-C(00S)-N(006)	119.2(2)
N(00R)-C(00S)-N(00H)	119.9(2)
N(005)-C(00U)-N(00O)	120.9(2)
N(00V)-C(00U)-N(005)	119.4(3)
N(00V)-C(00U)-N(00O)	119.7(3)
C(00U)-N(00V)-O(00C)	101.1(2)
N(005)-C(00W)-O(00C)	111.2(2)
N(00L)-C(00W)-N(005)	134.4(3)
N(00L)-C(00W)-O(00C)	114.4(2)
C(010)-N(00X)-O(007)	101.1(2)
N(006)-C(00Y)-O(009)	110.9(2)
N(006)-C(00Y)-N(00E)	133.8(2)
N(00E)-C(00Y)-O(009)	115.2(2)
N(008)-C(00Z)-O(007)	110.6(3)
N(00L)-C(00Z)-O(007)	115.8(3)
N(00L)-C(00Z)-N(008)	133.6(2)
N(008)-C(010)-N(00M)	120.0(3)
N(00X)-C(010)-N(008)	119.0(3)
N(00X)-C(010)-N(00M)	121.0(3)

Symmetry transformations used to generate equivalent atoms:

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

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

Table S15. Anisotropic displacement parameters (A^2 x 10^3) for **2'**.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Na(01)	36(1)	36(1)	36(1)	-1(1)	-1(1)	-1(1)
Na(02)	54(1)	72(1)	56(1)	-7(1)	4(1)	-7(1)
O	61(1)	96(1)	45(1)	12(1)	10(1)	13(1)
N(004)	51(1)	60(1)	42(1)	-1(1)	2(1)	6(1)
N(005)	60(1)	53(1)	51(1)	-5(1)	-3(1)	-1(1)
N(006)	55(1)	53(1)	51(1)	-7(1)	-1(1)	-2(1)
O(007)	58(1)	96(2)	91(2)	-4(1)	-13(1)	5(1)
N(008)	60(1)	59(1)	55(1)	-10(1)	-13(1)	4(1)
O(009)	82(1)	85(1)	77(1)	-7(1)	-2(1)	-33(1)
O(0AA)	80(1)	86(1)	82(1)	-24(1)	13(1)	-8(1)
O(1)	85(1)	99(2)	79(1)	-28(1)	19(1)	-16(1)
O(00C)	86(2)	87(1)	85(1)	23(1)	-2(1)	-18(1)
N(00D)	66(1)	74(2)	58(1)	-16(1)	-9(1)	19(1)
N(00E)	64(1)	76(2)	56(1)	9(1)	7(1)	-9(1)
O(2)	97(2)	90(2)	92(2)	14(1)	-12(1)	-10(1)
N(00G)	65(1)	86(2)	44(1)	-3(1)	-2(1)	20(1)
N(00H)	76(2)	68(1)	57(1)	-16(1)	0(1)	9(1)
O(00I)	106(2)	105(2)	59(1)	-33(1)	-2(1)	13(1)
O(3)	71(1)	123(2)	90(2)	12(1)	3(1)	6(1)
O(00K)	101(2)	84(2)	105(2)	-1(1)	-38(1)	22(1)
N(00L)	62(1)	74(2)	76(2)	2(1)	-5(1)	-6(1)
N(00M)	97(2)	73(2)	66(2)	-8(1)	-27(1)	11(2)
O(00N)	101(2)	118(2)	93(2)	-60(2)	-4(1)	13(1)
N(00O)	79(2)	72(2)	63(1)	-11(1)	-16(1)	10(1)
C(00P)	53(1)	73(2)	36(1)	-2(1)	-2(1)	20(1)
C(00Q)	57(1)	68(2)	40(1)	7(1)	4(1)	10(1)
N(00R)	92(2)	75(2)	65(2)	-17(1)	-5(1)	-18(1)
C(00S)	65(2)	50(1)	53(1)	-7(1)	-6(1)	2(1)
O(00T)	147(2)	101(2)	93(2)	15(1)	-49(2)	18(2)
C(00U)	72(2)	53(1)	51(1)	-9(1)	-9(1)	1(1)
N(00V)	92(2)	77(2)	77(2)	18(1)	-10(1)	-5(1)
C(00W)	70(2)	54(2)	58(2)	-5(1)	-4(1)	-8(1)
N(00X)	68(2)	95(2)	85(2)	-13(2)	-22(1)	15(1)
C(00Y)	60(2)	57(1)	55(2)	5(1)	-7(1)	-9(1)
C(00Z)	49(2)	71(2)	71(2)	-18(2)	-10(1)	-1(1)
C(010)	72(2)	61(2)	60(2)	-13(1)	-15(1)	8(1)

Table S16. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3**·DIOX.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

x	y	z	U(eq)	
C(1)	4781(3)	654(1)	7165(3)	47(1)
C(2)	4558(3)	1902(1)	7338(3)	49(1)
C(3)	3684(4)	229(1)	6161(3)	48(1)
C(4)	3421(3)	2323(1)	6332(4)	50(1)
C(5)	4476(4)	1015(1)	1305(4)	76(1)
C(6)	4094(4)	912(1)	2777(4)	64(1)
C(7)	5287(4)	1449(1)	3592(4)	84(2)
C(8)	5683(5)	1550(1)	2128(5)	74(1)
N(1)	4700(3)	1278(1)	7328(3)	46(1)
N(2)	5390(3)	972(1)	7732(3)	51(1)
N(3)	5247(3)	1590(1)	7854(3)	52(1)
N(4)	3606(3)	1939(1)	6344(3)	45(1)
N(5)	4167(4)	2530(1)	7221(4)	72(1)
N(6)	3673(3)	612(1)	6324(3)	45(1)
N(7)	4646(4)	26(1)	6780(3)	68(1)
N(8)	2634(4)	36(1)	5262(4)	66(1)
N(9)	2472(3)	2516(1)	5349(4)	66(1)
O(1)	2657(4)	-312(1)	5243(4)	104(1)
O(2)	1862(4)	236(1)	4574(3)	87(1)
O(3)	1848(4)	2314(1)	4536(4)	93(1)
O(4)	2399(4)	2864(1)	5391(4)	107(1)
O(5)	4948(3)	2240(1)	7921(3)	68(1)
O(6)	5415(3)	320(1)	7470(3)	64(1)
O(7)	4004(2)	1241(1)	3657(2)	54(1)
O(8)	5769(2)	1222(1)	1251(2)	53(1)
Na(1)	2400(1)	1256(1)	5628(1)	41(1)

Table S17. Bond lengths [A] and angles [deg] for **3**·DIOX.

C(1)-N(6)	1.320(4)
C(1)-O(6)	1.343(4)
C(1)-N(2)	1.360(4)
C(2)-N(4)	1.304(4)

C(2)-O(5)	1.356(4)
C(2)-N(3)	1.359(4)
C(3)-N(7)	1.291(4)
C(3)-N(6)	1.349(4)
C(3)-N(8)	1.468(5)
C(4)-N(5)	1.310(4)
C(4)-N(4)	1.355(4)
C(4)-N(9)	1.452(5)
C(5)-O(8)	1.420(4)
C(5)-C(6)	1.476(5)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(6)-O(7)	1.420(4)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(7)-O(7)	1.413(4)
C(7)-C(8)	1.471(6)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(8)-O(8)	1.414(4)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
N(1)-N(3)	1.304(3)
N(1)-N(2)	1.312(4)
N(2)-Na(1)#1	2.640(3)
N(3)-Na(1)#1	2.744(3)
N(5)-O(5)	1.415(4)
N(7)-O(6)	1.416(4)
N(8)-O(2)	1.201(5)
N(8)-O(1)	1.219(4)
N(9)-O(3)	1.194(4)
N(9)-O(4)	1.221(4)
O(8)-Na(1)#2	2.348(2)
Na(1)-O(8)#3	2.348(2)
Na(1)-N(2)#4	2.640(3)
Na(1)-N(3)#4	2.744(3)

N(6)-C(1)-O(6)	112.6(3)
N(6)-C(1)-N(2)	131.4(3)
O(6)-C(1)-N(2)	116.0(3)
N(4)-C(2)-O(5)	112.9(3)
N(4)-C(2)-N(3)	131.8(3)
O(5)-C(2)-N(3)	115.2(3)
N(7)-C(3)-N(6)	120.0(3)
N(7)-C(3)-N(8)	118.8(3)
N(6)-C(3)-N(8)	121.2(3)
N(5)-C(4)-N(4)	118.1(3)

N(5)-C(4)-N(9)	118.9(3)
N(4)-C(4)-N(9)	122.9(3)
O(8)-C(5)-C(6)	111.6(3)
O(8)-C(5)-H(5A)	109.3
C(6)-C(5)-H(5A)	109.3
O(8)-C(5)-H(5B)	109.3
C(6)-C(5)-H(5B)	109.3
H(5A)-C(5)-H(5B)	108.0
O(7)-C(6)-C(5)	111.4(3)
O(7)-C(6)-H(6A)	109.4
C(5)-C(6)-H(6A)	109.4
O(7)-C(6)-H(6B)	109.4
C(5)-C(6)-H(6B)	109.4
H(6A)-C(6)-H(6B)	108.0
O(7)-C(7)-C(8)	112.4(3)
O(7)-C(7)-H(7A)	109.1
C(8)-C(7)-H(7A)	109.1
O(7)-C(7)-H(7B)	109.1
C(8)-C(7)-H(7B)	109.1
H(7A)-C(7)-H(7B)	107.8
O(8)-C(8)-C(7)	111.5(3)
O(8)-C(8)-H(8A)	109.3
C(7)-C(8)-H(8A)	109.3
O(8)-C(8)-H(8B)	109.3
C(7)-C(8)-H(8B)	109.3
H(8A)-C(8)-H(8B)	108.0
N(3)-N(1)-N(2)	112.1(3)
N(1)-N(2)-C(1)	110.2(3)
N(1)-N(2)-Na(1)#1	102.58(19)
C(1)-N(2)-Na(1)#1	147.3(2)
N(1)-N(3)-C(2)	110.2(3)
N(1)-N(3)-Na(1)#1	97.77(19)
C(2)-N(3)-Na(1)#1	151.8(2)
C(2)-N(4)-C(4)	101.3(3)
C(4)-N(5)-O(5)	100.6(3)
C(1)-N(6)-C(3)	99.9(3)
C(3)-N(7)-O(6)	99.7(3)
O(2)-N(8)-O(1)	126.0(4)
O(2)-N(8)-C(3)	116.8(3)
O(1)-N(8)-C(3)	117.2(4)
O(3)-N(9)-O(4)	125.5(4)
O(3)-N(9)-C(4)	116.1(3)
O(4)-N(9)-C(4)	118.4(4)
C(2)-O(5)-N(5)	107.2(3)
C(1)-O(6)-N(7)	107.8(3)
C(7)-O(7)-C(6)	109.9(3)
C(8)-O(8)-C(5)	110.1(3)

C(8)-O(8)-Na(1)#2	115.89(19)
C(5)-O(8)-Na(1)#2	128.0(2)
O(8)#3-Na(1)-N(2)#4	87.12(9)
O(8)#3-Na(1)-N(3)#4	85.85(9)
N(2)#4-Na(1)-N(3)#4	47.49(9)

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

Table S18. Anisotropic displacement parameters (A^2 x 10^3) for **3**·DIOX.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	51(2)	56(2)	34(2)	5(1)	5(1)	12(2)
C(2)	46(2)	55(2)	45(2)	-13(2)	8(1)	-16(2)
C(3)	58(2)	47(2)	40(2)	2(1)	16(1)	-3(2)
C(4)	44(2)	49(2)	55(2)	-6(2)	18(2)	-6(1)
C(5)	55(2)	113(4)	59(2)	-27(2)	16(2)	-31(2)
C(6)	65(2)	49(2)	77(3)	-7(2)	29(2)	-15(2)
C(7)	65(2)	111(3)	76(3)	-48(3)	36(2)	-38(2)
C(8)	74(3)	50(2)	98(3)	-10(2)	43(2)	-14(2)
N(1)	44(1)	58(2)	36(1)	-5(1)	0(1)	-4(1)
N(2)	52(2)	57(2)	43(1)	0(1)	-9(1)	7(1)
N(3)	48(2)	61(2)	47(2)	-5(1)	-9(1)	-8(1)
N(4)	44(1)	48(2)	45(2)	-9(1)	4(1)	-2(1)
N(5)	74(2)	54(2)	88(2)	-15(2)	12(2)	-14(2)
N(6)	48(1)	47(2)	41(1)	2(1)	4(1)	2(1)
N(7)	89(2)	54(2)	60(2)	5(2)	7(2)	15(2)
N(8)	79(2)	61(2)	57(2)	-4(2)	21(2)	-20(2)
N(9)	61(2)	63(2)	74(2)	4(2)	22(2)	11(2)
O(1)	130(3)	57(2)	125(3)	-10(2)	17(2)	-30(2)
O(2)	93(2)	92(2)	76(2)	-7(2)	-16(2)	-21(2)
O(3)	107(3)	91(2)	82(2)	3(2)	-18(2)	10(2)
O(4)	112(3)	60(2)	149(3)	1(2)	3(2)	31(2)
O(5)	72(2)	58(2)	74(2)	-14(1)	-7(1)	-19(1)
O(6)	74(2)	60(2)	60(1)	4(1)	-9(1)	22(1)
O(7)	50(1)	62(2)	52(1)	-11(1)	22(1)	-11(1)
O(8)	49(1)	61(1)	50(1)	-8(1)	19(1)	-12(1)
Na(1)	32(1)	58(1)	32(1)	0(1)	-2(1)	-2(1)

Table S19. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **3**·DIOX.

x	y	z	U(eq)	
H(5A)	4566	784	742	91
H(5B)	3725	1169	894	91
H(6A)	3189	781	2778	76
H(6B)	4801	739	3158	76
H(7A)	6038	1297	4011	101
H(7B)	5193	1681	4148	101
H(8A)	4985	1725	1741	89
H(8B)	6592	1679	2135	89

Table S20. Torsion angles [deg] for **3**·DIOX.

O(8)-C(5)-C(6)-O(7)	56.7(5)
O(7)-C(7)-C(8)-O(8)	-56.0(5)
N(3)-N(1)-N(2)-C(1)	179.8(3)
N(3)-N(1)-N(2)-Na(1)#1	0.4(3)
N(6)-C(1)-N(2)-N(1)	-0.1(5)
O(6)-C(1)-N(2)-N(1)	178.3(3)
N(6)-C(1)-N(2)-Na(1)#1	178.8(3)
O(6)-C(1)-N(2)-Na(1)#1	-2.9(5)
N(2)-N(1)-N(3)-C(2)	176.2(3)
N(2)-N(1)-N(3)-Na(1)#1	-0.4(3)
N(4)-C(2)-N(3)-N(1)	-8.5(5)
O(5)-C(2)-N(3)-N(1)	173.8(3)
N(4)-C(2)-N(3)-Na(1)#1	164.3(3)
O(5)-C(2)-N(3)-Na(1)#1	-13.5(6)
O(5)-C(2)-N(4)-C(4)	0.2(3)
N(3)-C(2)-N(4)-C(4)	-177.6(3)
N(5)-C(4)-N(4)-C(2)	0.1(4)
N(9)-C(4)-N(4)-C(2)	178.0(3)
N(4)-C(4)-N(5)-O(5)	-0.3(4)
N(9)-C(4)-N(5)-O(5)	-178.2(3)
O(6)-C(1)-N(6)-C(3)	0.6(3)
N(2)-C(1)-N(6)-C(3)	178.9(3)
N(7)-C(3)-N(6)-C(1)	-0.2(4)
N(8)-C(3)-N(6)-C(1)	-178.8(3)

N(6)-C(3)-N(7)-O(6)	-0.2(4)
N(8)-C(3)-N(7)-O(6)	178.4(3)
N(7)-C(3)-N(8)-O(2)	-171.5(3)
N(6)-C(3)-N(8)-O(2)	7.1(5)
N(7)-C(3)-N(8)-O(1)	6.1(5)
N(6)-C(3)-N(8)-O(1)	-175.3(3)
N(5)-C(4)-N(9)-O(3)	178.0(3)
N(4)-C(4)-N(9)-O(3)	0.1(5)
N(5)-C(4)-N(9)-O(4)	-0.3(5)
N(4)-C(4)-N(9)-O(4)	-178.2(3)
N(4)-C(2)-O(5)-N(5)	-0.4(4)
N(3)-C(2)-O(5)-N(5)	177.8(3)
C(4)-N(5)-O(5)-C(2)	0.4(3)
N(6)-C(1)-O(6)-N(7)	-0.7(4)
N(2)-C(1)-O(6)-N(7)	-179.4(3)
C(3)-N(7)-O(6)-C(1)	0.6(3)
C(8)-C(7)-O(7)-C(6)	55.2(5)
C(5)-C(6)-O(7)-C(7)	-55.3(5)
C(7)-C(8)-O(8)-C(5)	55.0(5)
C(7)-C(8)-O(8)-Na(1)#2	-149.9(3)
C(6)-C(5)-O(8)-C(8)	-55.8(5)
C(6)-C(5)-O(8)-Na(1)#2	153.0(3)

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

Table S21. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **4**·EtOAc.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

x	y	z	U(eq)	
C(1)	6324(2)	461(1)	7500	43(1)
C(2)	5006(2)	970(1)	7500	45(1)
C(3)	7557(2)	767(1)	7500	48(1)
C(4)	3975(2)	1709(2)	7500	69(1)
C(5)	6317(1)	3756(1)	7500	38(1)
C(6)	9015(2)	5282(2)	7500	91(1)
C(7)	9066(2)	4401(2)	7500	59(1)
C(8)	9960(2)	3279(2)	7500	97(1)

C(9)	10860(2)	3112(2)	7500	108(1)
N(1)	5504(1)	351(1)	7500	46(1)
N(2)	6798(1)	1104(1)	7500	42(1)
N(3)	7616(1)	-2(1)	7500	69(1)
N(4)	8308(1)	1254(2)	7500	64(1)
N(5)	4185(1)	936(1)	7500	60(1)
N(6)	4556(1)	2243(1)	7500	75(1)
N(7)	3107(2)	1974(2)	7500	119(2)
N(8)	6704(1)	3054(1)	7500	51(1)
N(9)	6761(1)	4422(1)	7500	46(1)
N(10)	5502(1)	3796(1)	7500	49(1)
O(1)	6776(1)	-225(1)	7500	64(1)
O(2)	8970(1)	909(2)	7500	94(1)
O(3)	8231(1)	1964(1)	7500	107(1)
O(4)	5272(1)	1748(1)	7500	56(1)
O(5)	2986(2)	2686(2)	7500	182(2)
O(6)	2587(2)	1458(2)	7500	150(2)
O(7)	8470(1)	3961(1)	7500	79(1)
O(8)	9838(1)	4136(1)	7500	71(1)

Table S22. Bond lengths [A] and angles [deg] for **4**·EtOAc.

C(1)-N(2)	1.319(3)
C(1)-N(1)	1.336(3)
C(1)-O(1)	1.358(3)
C(2)-N(1)	1.310(3)
C(2)-N(5)	1.326(3)
C(2)-O(4)	1.370(2)
C(3)-N(3)	1.288(3)
C(3)-N(2)	1.348(3)
C(3)-N(4)	1.460(3)
C(4)-N(6)	1.294(3)
C(4)-N(5)	1.335(3)
C(4)-N(7)	1.469(4)
C(5)-N(10)	1.317(3)
C(5)-N(9)	1.324(3)
C(5)-N(8)	1.328(3)
C(6)-C(7)	1.475(4)
C(6)-H(6A)	0.9600
C(6)-H(6B)	0.9600
C(6)-H(6C)	0.9600
C(7)-O(7)	1.210(3)
C(7)-O(8)	1.322(3)
C(8)-O(8)	1.446(4)
C(8)-C(9)	1.480(5)

C(8)-H(8C)	0.9700
C(8)-H(8D)	0.9700
C(9)-H(9C)	0.9600
C(9)-H(9D)	0.9600
C(9)-H(9E)	0.9600
N(3)-O(1)	1.407(3)
N(4)-O(3)	1.193(3)
N(4)-O(2)	1.215(3)
N(6)-O(4)	1.421(3)
N(7)-O(6)	1.203(4)
N(7)-O(5)	1.205(4)
N(8)-H(8A)	0.8600
N(8)-H(8B)	0.8600
N(9)-H(9A)	0.8600
N(9)-H(9B)	0.8600
N(10)-H(10A)	0.8600
N(10)-H(10B)	0.8600

N(2)-C(1)-N(1)	133.32(19)
N(2)-C(1)-O(1)	112.1(2)
N(1)-C(1)-O(1)	114.58(18)
N(1)-C(2)-N(5)	125.48(19)
N(1)-C(2)-O(4)	123.8(2)
N(5)-C(2)-O(4)	110.74(19)
N(3)-C(3)-N(2)	118.9(2)
N(3)-C(3)-N(4)	119.6(2)
N(2)-C(3)-N(4)	121.4(2)
N(6)-C(4)-N(5)	118.9(2)
N(6)-C(4)-N(7)	118.9(2)
N(5)-C(4)-N(7)	122.2(2)
N(10)-C(5)-N(9)	119.87(18)
N(10)-C(5)-N(8)	120.97(19)
N(9)-C(5)-N(8)	119.2(2)
C(7)-C(6)-H(6A)	109.5
C(7)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(7)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
O(7)-C(7)-O(8)	123.1(3)
O(7)-C(7)-C(6)	124.2(3)
O(8)-C(7)-C(6)	112.7(2)
O(8)-C(8)-C(9)	108.7(3)
O(8)-C(8)-H(8C)	110.0
C(9)-C(8)-H(8C)	110.0
O(8)-C(8)-H(8D)	110.0
C(9)-C(8)-H(8D)	110.0

H(8C)-C(8)-H(8D)	108.3
C(8)-C(9)-H(9C)	109.5
C(8)-C(9)-H(9D)	109.5
H(9C)-C(9)-H(9D)	109.5
C(8)-C(9)-H(9E)	109.5
H(9C)-C(9)-H(9E)	109.5
H(9D)-C(9)-H(9E)	109.5
C(2)-N(1)-C(1)	120.03(18)
C(1)-N(2)-C(3)	100.77(18)
C(3)-N(3)-O(1)	101.12(19)
O(3)-N(4)-O(2)	124.3(3)
O(3)-N(4)-C(3)	117.9(2)
O(2)-N(4)-C(3)	117.8(2)
C(2)-N(5)-C(4)	102.27(19)
C(4)-N(6)-O(4)	100.89(19)
O(6)-N(7)-O(5)	126.4(3)
O(6)-N(7)-C(4)	116.8(3)
O(5)-N(7)-C(4)	116.8(3)
C(5)-N(8)-H(8A)	120.0
C(5)-N(8)-H(8B)	120.0
H(8A)-N(8)-H(8B)	120.0
C(5)-N(9)-H(9A)	120.0
C(5)-N(9)-H(9B)	120.0
H(9A)-N(9)-H(9B)	120.0
C(5)-N(10)-H(10A)	120.0
C(5)-N(10)-H(10B)	120.0
H(10A)-N(10)-H(10B)	120.0
C(1)-O(1)-N(3)	107.07(17)
C(2)-O(4)-N(6)	107.23(17)
C(7)-O(8)-C(8)	117.4(2)

Symmetry transformations used to generate equivalent atoms:

Table S23. Anisotropic displacement parameters (A^2 x 10^3) for **4**·EtOAc.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	56(1)	32(1)	40(1)	0	0	4(1)
C(2)	52(1)	28(1)	56(1)	0	0	-10(1)
C(3)	48(1)	46(1)	50(1)	0	0	8(1)

C(4)	49(1)	37(1)	121(3)	0	0	-4(1)
C(5)	49(1)	28(1)	35(1)	0	0	1(1)
C(6)	59(2)	55(2)	160(4)	0	0	-1(1)
C(7)	42(1)	58(2)	76(2)	0	0	-4(1)
C(8)	68(2)	60(2)	162(4)	0	0	10(2)
C(9)	80(3)	96(3)	148(4)	0	0	32(2)
N(1)	53(1)	31(1)	56(1)	0	0	-4(1)
N(2)	44(1)	37(1)	44(1)	0	0	1(1)
N(3)	59(1)	50(1)	97(2)	0	0	14(1)
N(4)	43(1)	67(2)	84(2)	0	0	8(1)
N(5)	48(1)	36(1)	97(2)	0	0	-7(1)
N(6)	50(1)	32(1)	142(2)	0	0	0(1)
N(7)	50(2)	57(2)	250(5)	0	0	-1(1)
N(8)	57(1)	30(1)	65(1)	0	0	7(1)
N(9)	45(1)	30(1)	64(1)	0	0	0(1)
N(10)	47(1)	28(1)	71(1)	0	0	-1(1)
O(1)	68(1)	35(1)	90(1)	0	0	9(1)
O(2)	48(1)	101(2)	132(2)	0	0	21(1)
O(3)	51(1)	57(1)	213(3)	0	0	-2(1)
O(4)	48(1)	29(1)	91(1)	0	0	-5(1)
O(5)	70(2)	59(2)	418(7)	0	0	15(1)
O(6)	54(1)	80(2)	316(5)	0	0	-14(1)
O(7)	45(1)	62(1)	129(2)	0	0	-8(1)
O(8)	43(1)	57(1)	114(2)	0	0	1(1)

Table S24. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **4**·EtOAc.

x	y	z	U(eq)	
H(6A)	9495	5500	6826	137
H(6B)	8990	5473	8907	137
H(6C)	8526	5448	6767	137
H(8C)	9704	3045	6277	116
H(8D)	9704	3045	8723	116
H(9C)	11130	3456	8487	162
H(9D)	11081	3210	6137	162
H(9E)	10953	2564	7875	162
H(8A)	6422	2618	7500	61
H(8B)	7236	3037	7500	61
H(9A)	6518	4880	7500	55
H(9B)	7293	4397	7500	55

H(10A)	5260	4255	7500	59
H(10B)	5212	3364	7500	59

Table S25. Torsion angles [deg] for **4**·EtOAc.

N(5)-C(2)-N(1)-C(1)	180.0
O(4)-C(2)-N(1)-C(1)	0.0
N(2)-C(1)-N(1)-C(2)	0.0
O(1)-C(1)-N(1)-C(2)	180.0
N(1)-C(1)-N(2)-C(3)	180.0
O(1)-C(1)-N(2)-C(3)	0.0
N(3)-C(3)-N(2)-C(1)	0.0
N(4)-C(3)-N(2)-C(1)	180.0
N(2)-C(3)-N(3)-O(1)	0.0
N(4)-C(3)-N(3)-O(1)	180.0
N(3)-C(3)-N(4)-O(3)	180.0
N(2)-C(3)-N(4)-O(3)	0.0
N(3)-C(3)-N(4)-O(2)	0.0
N(2)-C(3)-N(4)-O(2)	180.0
N(1)-C(2)-N(5)-C(4)	180.0
O(4)-C(2)-N(5)-C(4)	0.0
N(6)-C(4)-N(5)-C(2)	0.0
N(7)-C(4)-N(5)-C(2)	180.0
N(5)-C(4)-N(6)-O(4)	0.0
N(7)-C(4)-N(6)-O(4)	180.0
N(6)-C(4)-N(7)-O(6)	180.0
N(5)-C(4)-N(7)-O(6)	0.0
N(6)-C(4)-N(7)-O(5)	0.0
N(5)-C(4)-N(7)-O(5)	180.0
N(2)-C(1)-O(1)-N(3)	0.0
N(1)-C(1)-O(1)-N(3)	180.0
C(3)-N(3)-O(1)-C(1)	0.0
N(1)-C(2)-O(4)-N(6)	180.0
N(5)-C(2)-O(4)-N(6)	0.0
C(4)-N(6)-O(4)-C(2)	0.0
O(7)-C(7)-O(8)-C(8)	0.0
C(6)-C(7)-O(8)-C(8)	180.0
C(9)-C(8)-O(8)-C(7)	180.0

Symmetry transformations used to generate equivalent atoms:

Table S26. Hydrogen bonds for **4**·EtOAc [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(6)-H(6C)...O(6)#1	0.96	2.51	3.247(4)	133.6
C(6)-H(6A)...O(2)#2	0.96	2.61	3.416(4)	142.4
N(9)-H(9B)...O(7)	0.86	2.03	2.864(3)	161.8
N(9)-H(9A)...N(5)#1	0.86	2.10	2.955(3)	174.5
N(8)-H(8B)...O(7)	0.86	2.52	3.229(3)	140.2
N(8)-H(8B)...O(3)	0.86	2.41	3.064(3)	133.8
N(8)-H(8A)...N(2)	0.86	2.60	3.262(3)	134.5
N(8)-H(8A)...O(4)	0.86	2.36	3.177(3)	160.0
N(10)-H(10B)...N(6)	0.86	2.15	3.010(3)	176.6
N(10)-H(10A)...N(1)#1	0.86	2.21	3.064(3)	173.1
C(6)-H(6C)...O(6)#1	0.96	2.51	3.247(4)	133.6
C(6)-H(6A)...O(2)#2	0.96	2.61	3.416(4)	142.4
N(9)-H(9B)...O(7)	0.86	2.03	2.864(3)	161.8
N(9)-H(9A)...N(5)#1	0.86	2.10	2.955(3)	174.5
N(8)-H(8B)...O(7)	0.86	2.52	3.229(3)	140.2
N(8)-H(8B)...O(3)	0.86	2.41	3.064(3)	133.8
N(8)-H(8A)...N(2)	0.86	2.60	3.262(3)	134.5
N(8)-H(8A)...O(4)	0.86	2.36	3.177(3)	160.0
N(10)-H(10B)...N(6)	0.86	2.15	3.010(3)	176.6
N(10)-H(10A)...N(1)#1	0.86	2.21	3.064(3)	173.1
N(10)-H(10A)...N(1)#1	0.86	2.21	3.064(3)	173.1
N(10)-H(10B)...N(6)	0.86	2.15	3.010(3)	176.6
N(8)-H(8A)...O(4)	0.86	2.36	3.177(3)	160.0
N(8)-H(8A)...N(2)	0.86	2.60	3.262(3)	134.5
N(8)-H(8B)...O(3)	0.86	2.41	3.064(3)	133.8
N(8)-H(8B)...O(7)	0.86	2.52	3.229(3)	140.2
N(9)-H(9A)...N(5)#1	0.86	2.10	2.955(3)	174.5
N(9)-H(9B)...O(7)	0.86	2.03	2.864(3)	161.8
C(6)-H(6A)...O(2)#2	0.96	2.61	3.416(4)	142.4
C(6)-H(6C)...O(6)#1	0.96	2.51	3.247(4)	133.6

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

Table S27. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

x	y	z	U(eq)	
C(1)	4882(2)	4166(2)	2630(4)	35(1)
C(2)	4420(2)	5647(1)	2673(4)	35(1)
C(3)	4314(2)	2893(2)	3032(4)	38(1)
C(4)	3169(2)	6496(2)	3097(4)	42(1)
C(5)	1957(2)	4417(1)	7812(3)	32(1)
N(1)	5157(1)	5022(1)	2432(3)	41(1)
N(2)	5272(2)	2707(1)	2550(4)	54(1)
N(3)	3910(2)	7079(1)	2877(4)	56(1)
N(4)	4006(1)	3753(1)	3136(3)	37(1)
N(5)	3397(1)	5616(1)	2986(3)	36(1)
N(6)	3602(2)	2152(2)	3477(4)	54(1)
N(7)	2092(2)	6800(2)	3467(4)	58(1)
N(8)	2687(2)	4639(2)	9069(4)	47(1)
N(9)	967(1)	4269(1)	8360(3)	36(1)
N(10)	740(2)	4259(2)	10338(3)	57(1)
N(11)	2192(2)	4352(2)	5953(3)	50(1)
N(12)	1394(2)	4140(2)	4650(3)	58(1)
O(1)	5677(1)	3575(1)	2254(3)	55(1)
O(2)	4780(1)	6509(1)	2564(4)	56(1)
O(3)	3899(2)	1404(1)	3078(6)	96(1)
O(4)	2765(2)	2333(2)	4229(5)	74(1)
O(5)	1977(2)	7553(2)	4093(6)	97(1)
O(6)	1386(2)	6274(2)	3100(6)	87(1)

Table S28. Bond lengths [A] and angles [deg] for **5**.

C(1)-N(4)	1.317(3)
C(1)-N(1)	1.329(3)
C(1)-O(1)	1.364(3)
C(2)-N(5)	1.317(3)
C(2)-N(1)	1.329(3)
C(2)-O(2)	1.364(3)
C(3)-N(2)	1.290(3)
C(3)-N(4)	1.340(3)
C(3)-N(6)	1.459(3)
C(4)-N(3)	1.288(3)
C(4)-N(5)	1.343(3)
C(4)-N(7)	1.462(3)
C(5)-N(8)	1.312(3)
C(5)-N(11)	1.322(3)
C(5)-N(9)	1.330(3)

N(2)-O(1)	1.405(3)
N(3)-O(2)	1.409(3)
N(6)-O(3)	1.207(3)
N(6)-O(4)	1.212(3)
N(7)-O(5)	1.211(4)
N(7)-O(6)	1.215(3)
N(8)-H(8A)	0.8600
N(8)-H(8B)	0.8600
N(9)-N(10)	1.396(3)
N(9)-H(9)	0.8600
N(10)-H(10A)	0.8875
N(10)-H(10B)	0.8878
N(11)-N(12)	1.391(3)
N(11)-H(11)	0.8600
N(12)-H(12A)	0.8887
N(12)-H(12B)	0.8887

N(4)-C(1)-N(1)	134.2(2)
N(4)-C(1)-O(1)	111.9(2)
N(1)-C(1)-O(1)	113.91(19)
N(5)-C(2)-N(1)	133.6(2)
N(5)-C(2)-O(2)	111.8(2)
N(1)-C(2)-O(2)	114.57(19)
N(2)-C(3)-N(4)	119.6(2)
N(2)-C(3)-N(6)	118.4(2)
N(4)-C(3)-N(6)	122.0(2)
N(3)-C(4)-N(5)	119.5(2)
N(3)-C(4)-N(7)	119.6(2)
N(5)-C(4)-N(7)	120.8(2)
N(8)-C(5)-N(11)	120.1(2)
N(8)-C(5)-N(9)	121.3(2)
N(11)-C(5)-N(9)	118.6(2)
C(2)-N(1)-C(1)	118.25(19)
C(3)-N(2)-O(1)	100.65(18)
C(4)-N(3)-O(2)	100.57(19)
C(1)-N(4)-C(3)	100.75(18)
C(2)-N(5)-C(4)	100.82(18)
O(3)-N(6)-O(4)	125.2(2)
O(3)-N(6)-C(3)	117.1(2)
O(4)-N(6)-C(3)	117.7(2)
O(5)-N(7)-O(6)	125.6(3)
O(5)-N(7)-C(4)	117.5(2)
O(6)-N(7)-C(4)	116.9(2)
C(5)-N(8)-H(8A)	120.0
C(5)-N(8)-H(8B)	120.0
H(8A)-N(8)-H(8B)	120.0
C(5)-N(9)-N(10)	118.4(2)

C(5)-N(9)-H(9)	120.8
N(10)-N(9)-H(9)	120.8
N(9)-N(10)-H(10A)	109.5
N(9)-N(10)-H(10B)	109.3
H(10A)-N(10)-H(10B)	109.4
C(5)-N(11)-N(12)	118.7(2)
C(5)-N(11)-H(11)	120.6
N(12)-N(11)-H(11)	120.7
N(11)-N(12)-H(12A)	109.2
N(11)-N(12)-H(12B)	109.2
H(12A)-N(12)-H(12B)	109.4
C(1)-O(1)-N(2)	107.18(18)
C(2)-O(2)-N(3)	107.24(18)

Symmetry transformations used to generate equivalent atoms:

Table S29. Anisotropic displacement parameters (A^2 x 10^3) for **5**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	29(1)	41(1)	36(1)	-2(1)	2(1)	2(1)
C(2)	34(1)	35(1)	37(1)	2(1)	-2(1)	-7(1)
C(3)	40(1)	36(1)	40(1)	-2(1)	6(1)	2(1)
C(4)	41(1)	37(1)	46(1)	1(1)	1(1)	0(1)
C(5)	32(1)	26(1)	39(1)	2(1)	3(1)	0(1)
N(1)	28(1)	41(1)	53(1)	1(1)	4(1)	-4(1)
N(2)	48(1)	39(1)	74(2)	2(1)	17(1)	6(1)
N(3)	48(1)	36(1)	85(2)	0(1)	-1(1)	-2(1)
N(4)	32(1)	35(1)	46(1)	-1(1)	6(1)	-1(1)
N(5)	33(1)	34(1)	42(1)	-1(1)	2(1)	-2(1)
N(6)	55(1)	38(1)	69(2)	1(1)	16(1)	-1(1)
N(7)	50(1)	47(1)	78(2)	9(1)	12(1)	10(1)
N(8)	31(1)	58(1)	51(1)	-3(1)	-1(1)	-10(1)
N(9)	30(1)	44(1)	34(1)	-1(1)	0(1)	-8(1)
N(10)	47(1)	86(2)	37(1)	3(1)	7(1)	-17(1)
N(11)	40(1)	70(2)	40(1)	-1(1)	10(1)	0(1)
N(12)	67(2)	73(2)	35(1)	-5(1)	-2(1)	10(1)
O(1)	37(1)	45(1)	83(2)	4(1)	18(1)	5(1)
O(2)	39(1)	37(1)	91(2)	1(1)	1(1)	-8(1)
O(3)	99(2)	36(1)	153(3)	-3(2)	54(2)	0(1)

O(4)	53(1)	56(1)	114(2)	7(1)	30(1)	-4(1)
O(5)	91(2)	53(1)	147(3)	-5(2)	33(2)	24(1)
O(6)	41(1)	75(2)	144(3)	5(2)	16(2)	0(1)

Table S30. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **5**.

x	y	z	U(eq)
H(8A)	3321	4743	8684	56
H(8B)	2533	4682	10277	56
H(9)	479	4181	7517	43
H(10A)	639	3697	10724	68
H(10B)	158	4576	10553	68
H(11)	2828	4437	5557	60
H(12A)	1518	3601	4144	70
H(12B)	1382	4548	3711	70

Table S31. Torsion angles [deg] for **5**.

N(5)-C(2)-N(1)-C(1)	-4.5(4)
O(2)-C(2)-N(1)-C(1)	176.1(2)
N(4)-C(1)-N(1)-C(2)	-4.3(4)
O(1)-C(1)-N(1)-C(2)	176.7(2)
N(4)-C(3)-N(2)-O(1)	-0.9(3)
N(6)-C(3)-N(2)-O(1)	-179.9(2)
N(5)-C(4)-N(3)-O(2)	0.1(4)
N(7)-C(4)-N(3)-O(2)	-180.0(2)
N(1)-C(1)-N(4)-C(3)	-179.4(3)
O(1)-C(1)-N(4)-C(3)	-0.4(3)
N(2)-C(3)-N(4)-C(1)	0.9(3)
N(6)-C(3)-N(4)-C(1)	179.9(2)
N(1)-C(2)-N(5)-C(4)	179.4(3)
O(2)-C(2)-N(5)-C(4)	-1.2(3)
N(3)-C(4)-N(5)-C(2)	0.7(3)
N(7)-C(4)-N(5)-C(2)	-179.2(3)
N(2)-C(3)-N(6)-O(3)	-11.3(4)
N(4)-C(3)-N(6)-O(3)	169.7(4)
N(2)-C(3)-N(6)-O(4)	168.1(3)
N(4)-C(3)-N(6)-O(4)	-10.9(4)

N(3)-C(4)-N(7)-O(5)	-20.6(5)
N(5)-C(4)-N(7)-O(5)	159.3(3)
N(3)-C(4)-N(7)-O(6)	158.8(3)
N(5)-C(4)-N(7)-O(6)	-21.3(4)
N(8)-C(5)-N(9)-N(10)	-6.9(4)
N(11)-C(5)-N(9)-N(10)	174.3(2)
N(8)-C(5)-N(11)-N(12)	-178.2(2)
N(9)-C(5)-N(11)-N(12)	0.6(4)
N(4)-C(1)-O(1)-N(2)	-0.1(3)
N(1)-C(1)-O(1)-N(2)	179.2(2)
C(3)-N(2)-O(1)-C(1)	0.5(3)
N(5)-C(2)-O(2)-N(3)	1.4(3)
N(1)-C(2)-O(2)-N(3)	-179.1(2)
C(4)-N(3)-O(2)-C(2)	-0.8(3)

Symmetry transformations used to generate equivalent atoms:

Table S32. Hydrogen bonds for **5** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(12)-H(12B)...O(6)	0.89	2.60	3.352(4)	142.4
N(12)-H(12B)...N(10)#1	0.89	2.51	3.097(3)	124.5
N(12)-H(12A)...O(4)	0.89	2.46	3.217(3)	142.7
N(11)-H(11)...N(5)	0.86	2.60	3.174(3)	125.3
N(11)-H(11)...N(4)	0.86	2.46	3.142(3)	136.3
N(10)-H(10A)...N(2)#2	0.89	2.48	3.354(4)	166.5
N(9)-H(9)...O(6)#3	0.86	2.49	3.097(3)	127.9
N(8)-H(8B)...N(5)#4	0.86	2.58	3.201(3)	130.4
N(8)-H(8A)...N(1)#5	0.86	2.14	3.001(3)	174.2
N(8)-H(8A)...N(1)#5	0.86	2.14	3.001(3)	174.2
N(8)-H(8B)...N(5)#4	0.86	2.58	3.201(3)	130.4
N(9)-H(9)...O(6)#3	0.86	2.49	3.097(3)	127.9
N(10)-H(10A)...N(2)#2	0.89	2.48	3.354(4)	166.5
N(11)-H(11)...N(4)	0.86	2.46	3.142(3)	136.3
N(11)-H(11)...N(5)	0.86	2.60	3.174(3)	125.3
N(12)-H(12A)...O(4)	0.89	2.46	3.217(3)	142.7
N(12)-H(12B)...N(10)#1	0.89	2.51	3.097(3)	124.5
N(12)-H(12B)...O(6)	0.89	2.60	3.352(4)	142.4

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

Table S33. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **7**·2DIOX.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

x	y	z	U(eq)	
C(1)	7304(2)	6721(2)	7460(2)	51(1)
C(2)	5102(2)	5225(2)	6590(2)	45(1)
C(3)	3131(2)	1046(2)	4152(2)	44(1)
C(4)	3949(2)	-432(2)	3359(2)	48(1)
C(5)	9141(2)	3215(2)	5389(2)	51(1)
C(6)	2419(6)	4867(3)	10444(3)	121(1)
C(7)	2509(6)	5275(3)	9401(3)	119(1)
C(8)	1906(5)	3066(3)	8222(3)	103(1)
C(9)	1856(6)	2655(3)	9272(3)	118(1)
C(11)	3445(3)	9448(3)	10186(2)	73(1)
C(13)	3829(3)	9221(4)	8993(3)	95(1)
N(1)	9069(2)	7448(2)	7859(2)	66(1)
N(2)	6345(2)	7359(2)	7750(2)	64(1)
N(3)	6653(2)	5420(2)	6754(1)	47(1)
N(4)	3730(2)	4153(2)	5943(1)	48(1)
N(5)	4080(2)	3137(2)	5372(1)	43(1)
N(6)	2760(2)	2106(2)	4744(1)	48(1)
N(7)	4506(2)	858(2)	4090(1)	44(1)
N(8)	2402(2)	-1072(2)	2962(2)	64(1)
N(9)	5056(2)	-1133(2)	3038(2)	56(1)
N(10)	10384(2)	4274(2)	6090(2)	69(1)
N(11)	9382(2)	2145(2)	4751(2)	67(1)
N(12)	7661(2)	3224(2)	5309(2)	62(1)
O(1)	9544(3)	8638(2)	8444(2)	100(1)
O(2)	9919(2)	6808(2)	7558(2)	83(1)
O(3)	4825(2)	6338(2)	7161(1)	60(1)
O(4)	1824(2)	-57(2)	3496(1)	62(1)
O(5)	6504(2)	-465(2)	3376(2)	67(1)
O(6)	4450(2)	-2331(2)	2481(2)	83(1)
O(7)	2925(3)	4433(2)	8478(2)	99(1)
O(8)	1459(3)	3527(2)	10230(2)	102(1)
O(10)	4810(2)	9687(2)	11047(2)	92(1)

Table S34. Bond lengths [A] and angles [deg] for **7**·2DIOX.

C(1)-N(2)	1.295(3)
C(1)-N(3)	1.345(2)
C(1)-N(1)	1.466(3)
C(2)-N(3)	1.311(2)
C(2)-O(3)	1.350(2)
C(2)-N(4)	1.360(3)
C(3)-N(7)	1.314(2)
C(3)-O(4)	1.348(2)
C(3)-N(6)	1.356(2)
C(4)-N(8)	1.290(3)
C(4)-N(7)	1.346(2)
C(4)-N(9)	1.464(2)
C(5)-N(10)	1.312(3)
C(5)-N(12)	1.317(2)
C(5)-N(11)	1.319(3)
C(6)-O(8)	1.380(4)
C(6)-C(7)	1.432(5)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(7)-O(7)	1.402(4)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(8)-O(7)	1.409(4)
C(8)-C(9)	1.441(5)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(9)-O(8)	1.437(4)
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700
C(11)-O(10)	1.414(3)
C(11)-C(13)	1.467(4)
C(11)-H(11C)	0.9700
C(11)-H(11D)	0.9700
C(13)-O(10)#1	1.413(3)
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
N(1)-O(1)	1.214(3)
N(1)-O(2)	1.215(3)
N(2)-O(3)	1.404(2)
N(4)-N(5)	1.298(2)
N(5)-N(6)	1.310(2)
N(8)-O(4)	1.412(2)
N(9)-O(6)	1.210(2)

N(9)-O(5)	1.215(2)
N(10)-H(10A)	0.8600
N(10)-H(10B)	0.8600
N(11)-H(11A)	0.8600
N(11)-H(11B)	0.8600
N(12)-H(12A)	0.8600
N(12)-H(12B)	0.8600
O(10)-C(13)#1	1.413(3)

N(2)-C(1)-N(3)	118.85(18)
N(2)-C(1)-N(1)	119.37(19)
N(3)-C(1)-N(1)	121.72(18)
N(3)-C(2)-O(3)	112.74(17)
N(3)-C(2)-N(4)	133.43(17)
O(3)-C(2)-N(4)	113.80(15)
N(7)-C(3)-O(4)	112.59(16)
N(7)-C(3)-N(6)	133.48(16)
O(4)-C(3)-N(6)	113.93(15)
N(8)-C(4)-N(7)	119.08(17)
N(8)-C(4)-N(9)	119.51(18)
N(7)-C(4)-N(9)	121.38(17)
N(10)-C(5)-N(12)	120.3(2)
N(10)-C(5)-N(11)	119.73(17)
N(12)-C(5)-N(11)	120.0(2)
O(8)-C(6)-C(7)	114.6(3)
O(8)-C(6)-H(6A)	108.6
C(7)-C(6)-H(6A)	108.6
O(8)-C(6)-H(6B)	108.6
C(7)-C(6)-H(6B)	108.6
H(6A)-C(6)-H(6B)	107.6
O(7)-C(7)-C(6)	113.9(3)
O(7)-C(7)-H(7A)	108.8
C(6)-C(7)-H(7A)	108.8
O(7)-C(7)-H(7B)	108.8
C(6)-C(7)-H(7B)	108.8
H(7A)-C(7)-H(7B)	107.7
O(7)-C(8)-C(9)	112.3(3)
O(7)-C(8)-H(8A)	109.1
C(9)-C(8)-H(8A)	109.1
O(7)-C(8)-H(8B)	109.1
C(9)-C(8)-H(8B)	109.1
H(8A)-C(8)-H(8B)	107.9
O(8)-C(9)-C(8)	113.4(3)
O(8)-C(9)-H(9A)	108.9
C(8)-C(9)-H(9A)	108.9
O(8)-C(9)-H(9B)	108.9
C(8)-C(9)-H(9B)	108.9

H(9A)-C(9)-H(9B)	107.7
O(10)-C(11)-C(13)	110.7(2)
O(10)-C(11)-H(11C)	109.5
C(13)-C(11)-H(11C)	109.5
O(10)-C(11)-H(11D)	109.5
C(13)-C(11)-H(11D)	109.5
H(11C)-C(11)-H(11D)	108.1
O(10)#1-C(13)-C(11)	111.8(2)
O(10)#1-C(13)-H(13A)	109.3
C(11)-C(13)-H(13A)	109.3
O(10)#1-C(13)-H(13B)	109.3
C(11)-C(13)-H(13B)	109.3
H(13A)-C(13)-H(13B)	107.9
O(1)-N(1)-O(2)	126.1(2)
O(1)-N(1)-C(1)	116.9(2)
O(2)-N(1)-C(1)	116.96(19)
C(1)-N(2)-O(3)	100.80(16)
C(2)-N(3)-C(1)	100.53(16)
N(5)-N(4)-C(2)	110.98(14)
N(4)-N(5)-N(6)	111.05(13)
N(5)-N(6)-C(3)	110.80(14)
C(3)-N(7)-C(4)	100.57(15)
C(4)-N(8)-O(4)	100.60(15)
O(6)-N(9)-O(5)	125.72(19)
O(6)-N(9)-C(4)	117.33(19)
O(5)-N(9)-C(4)	116.93(17)
C(5)-N(10)-H(10A)	120.0
C(5)-N(10)-H(10B)	120.0
H(10A)-N(10)-H(10B)	120.0
C(5)-N(11)-H(11A)	120.0
C(5)-N(11)-H(11B)	120.0
H(11A)-N(11)-H(11B)	120.0
C(5)-N(12)-H(12A)	120.0
C(5)-N(12)-H(12B)	120.0
H(12A)-N(12)-H(12B)	120.0
C(2)-O(3)-N(2)	107.09(14)
C(3)-O(4)-N(8)	107.16(14)
C(7)-O(7)-C(8)	110.8(3)
C(6)-O(8)-C(9)	111.0(3)
C(13)#1-O(10)-C(11)	110.6(2)

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

Table S35. Anisotropic displacement parameters (A^2 x 10^3) for **7**·2DIOX.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	52(1)	52(1)	48(1)	15(1)	9(1)	18(1)
C(2)	45(1)	54(1)	44(1)	16(1)	13(1)	26(1)
C(3)	33(1)	51(1)	46(1)	16(1)	6(1)	14(1)
C(4)	49(1)	48(1)	48(1)	14(1)	10(1)	20(1)
C(5)	34(1)	65(1)	62(1)	29(1)	14(1)	22(1)
C(6)	168(4)	85(2)	72(2)	7(2)	28(2)	13(2)
C(7)	176(4)	76(2)	112(3)	39(2)	49(3)	45(2)
C(8)	121(3)	91(2)	86(2)	21(2)	33(2)	31(2)
C(9)	176(4)	73(2)	90(2)	21(2)	25(2)	31(2)
C(11)	54(1)	84(2)	75(2)	26(1)	17(1)	18(1)
C(13)	64(2)	117(2)	69(2)	19(2)	8(1)	3(2)
N(1)	54(1)	60(1)	68(1)	17(1)	6(1)	9(1)
N(2)	64(1)	56(1)	64(1)	9(1)	12(1)	22(1)
N(3)	39(1)	53(1)	49(1)	15(1)	8(1)	20(1)
N(4)	38(1)	60(1)	49(1)	13(1)	11(1)	27(1)
N(5)	34(1)	54(1)	44(1)	17(1)	10(1)	21(1)
N(6)	32(1)	57(1)	54(1)	14(1)	9(1)	20(1)
N(7)	36(1)	47(1)	47(1)	11(1)	7(1)	18(1)
N(8)	51(1)	53(1)	74(1)	8(1)	7(1)	13(1)
N(9)	62(1)	54(1)	55(1)	13(1)	13(1)	28(1)
N(10)	37(1)	70(1)	93(1)	17(1)	4(1)	23(1)
N(11)	39(1)	75(1)	86(1)	16(1)	16(1)	26(1)
N(12)	33(1)	69(1)	86(1)	21(1)	12(1)	24(1)
O(1)	78(1)	56(1)	132(2)	6(1)	0(1)	6(1)
O(2)	50(1)	84(1)	98(1)	10(1)	14(1)	20(1)
O(3)	55(1)	62(1)	65(1)	8(1)	15(1)	31(1)
O(4)	37(1)	59(1)	76(1)	10(1)	6(1)	12(1)
O(5)	55(1)	72(1)	75(1)	12(1)	11(1)	34(1)
O(6)	89(1)	52(1)	96(1)	2(1)	15(1)	31(1)
O(7)	115(2)	89(1)	87(1)	32(1)	40(1)	23(1)
O(8)	128(2)	86(1)	69(1)	24(1)	25(1)	12(1)
O(10)	64(1)	133(2)	75(1)	55(1)	12(1)	15(1)

Table S36. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **7**·2DIOX.

x	y	z	U(eq)	
H(6A)	3511	5033	10829	146
H(6B)	1998	5430	10995	146
H(7A)	1464	5290	9108	143
H(7B)	3310	6190	9620	143
H(8A)	2293	2498	7646	123
H(8B)	813	2932	7866	123
H(9A)	1056	1741	9063	142
H(9B)	2908	2639	9546	142
H(11C)	3119	10220	10387	87
H(11D)	2543	8660	10191	87
H(13A)	4049	8397	8764	114
H(13B)	2894	9102	8424	114
H(10A)	10233	4978	6500	83
H(10B)	11349	4264	6140	83
H(11A)	10351	2143	4796	81
H(11B)	8571	1449	4291	81
H(12A)	7505	3926	5718	75
H(12B)	6850	2528	4849	75

Table S37. Torsion angles [deg] for **7**·2DIOX.

O(8)-C(6)-C(7)-O(7)	-51.4(6)
O(7)-C(8)-C(9)-O(8)	52.7(5)
O(10)-C(11)-C(13)-O(10)#1	-56.3(4)
N(2)-C(1)-N(1)-O(1)	-0.7(3)
N(3)-C(1)-N(1)-O(1)	176.4(2)
N(2)-C(1)-N(1)-O(2)	-179.6(2)
N(3)-C(1)-N(1)-O(2)	-2.5(3)
N(3)-C(1)-N(2)-O(3)	0.4(2)
N(1)-C(1)-N(2)-O(3)	177.51(17)
O(3)-C(2)-N(3)-C(1)	0.0(2)
N(4)-C(2)-N(3)-C(1)	177.9(2)
N(2)-C(1)-N(3)-C(2)	-0.2(2)
N(1)-C(1)-N(3)-C(2)	-177.32(18)
N(3)-C(2)-N(4)-N(5)	-0.9(3)
O(3)-C(2)-N(4)-N(5)	176.97(15)

C(2)-N(4)-N(5)-N(6)	-179.74(15)
N(4)-N(5)-N(6)-C(3)	-179.87(15)
N(7)-C(3)-N(6)-N(5)	0.4(3)
O(4)-C(3)-N(6)-N(5)	179.39(15)
O(4)-C(3)-N(7)-C(4)	-0.2(2)
N(6)-C(3)-N(7)-C(4)	178.8(2)
N(8)-C(4)-N(7)-C(3)	-0.4(2)
N(9)-C(4)-N(7)-C(3)	-178.34(17)
N(7)-C(4)-N(8)-O(4)	0.7(2)
N(9)-C(4)-N(8)-O(4)	178.73(16)
N(8)-C(4)-N(9)-O(6)	-5.6(3)
N(7)-C(4)-N(9)-O(6)	172.32(19)
N(8)-C(4)-N(9)-O(5)	175.83(19)
N(7)-C(4)-N(9)-O(5)	-6.2(3)
N(3)-C(2)-O(3)-N(2)	0.2(2)
N(4)-C(2)-O(3)-N(2)	-178.12(16)
C(1)-N(2)-O(3)-C(2)	-0.3(2)
N(7)-C(3)-O(4)-N(8)	0.6(2)
N(6)-C(3)-O(4)-N(8)	-178.60(16)
C(4)-N(8)-O(4)-C(3)	-0.8(2)
C(6)-C(7)-O(7)-C(8)	51.7(5)
C(9)-C(8)-O(7)-C(7)	-52.5(4)
C(7)-C(6)-O(8)-C(9)	48.8(5)
C(8)-C(9)-O(8)-C(6)	-49.9(5)
C(13)-C(11)-O(10)-C(13)#1	55.6(4)

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

Table S38. Hydrogen bonds for **7**·2DIOX [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(12)-H(12B)...N(7)	0.86	2.18	3.018(2)	164.9
N(12)-H(12A)...N(3)	0.86	2.18	3.026(2)	168.8
N(11)-H(11B)...O(5)	0.86	2.20	3.047(3)	170.0
N(11)-H(11A)...N(6)#2	0.86	2.17	3.024(2)	175.0
N(10)-H(10B)...N(4)#2	0.86	2.20	3.048(2)	170.5
N(10)-H(10A)...O(2)	0.86	2.20	3.058(3)	178.5

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

5. Copies of Spectra

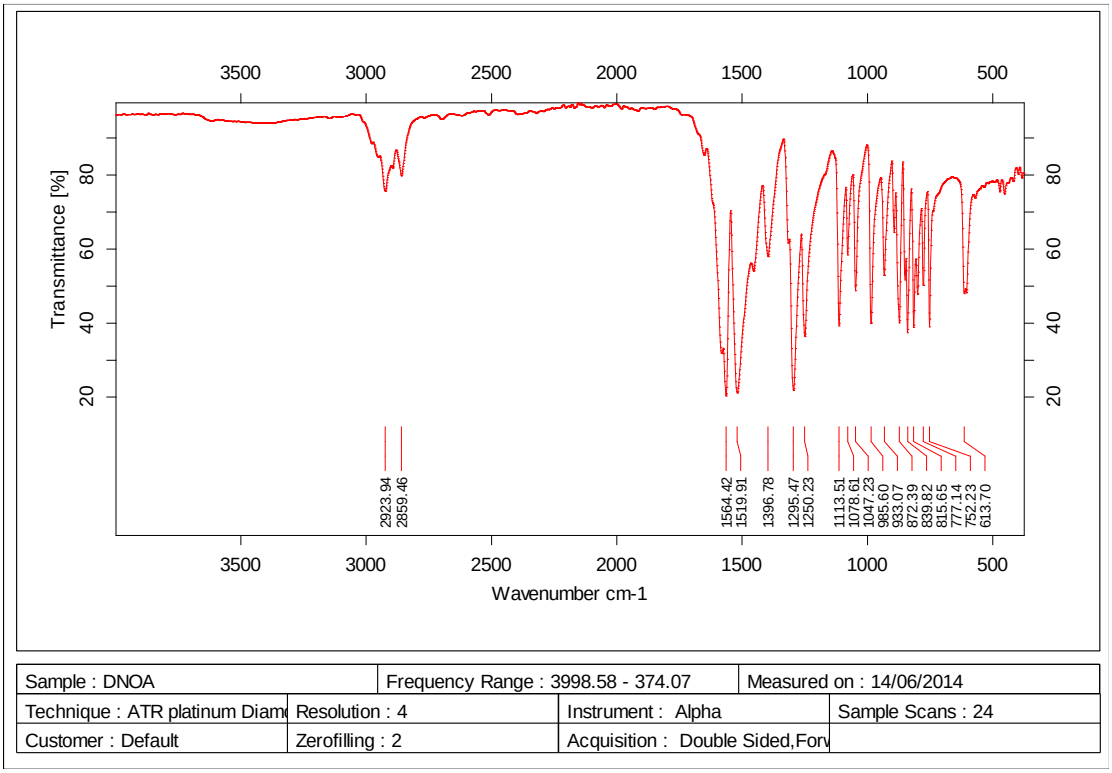

Figure S1 IR spectra of **2**.

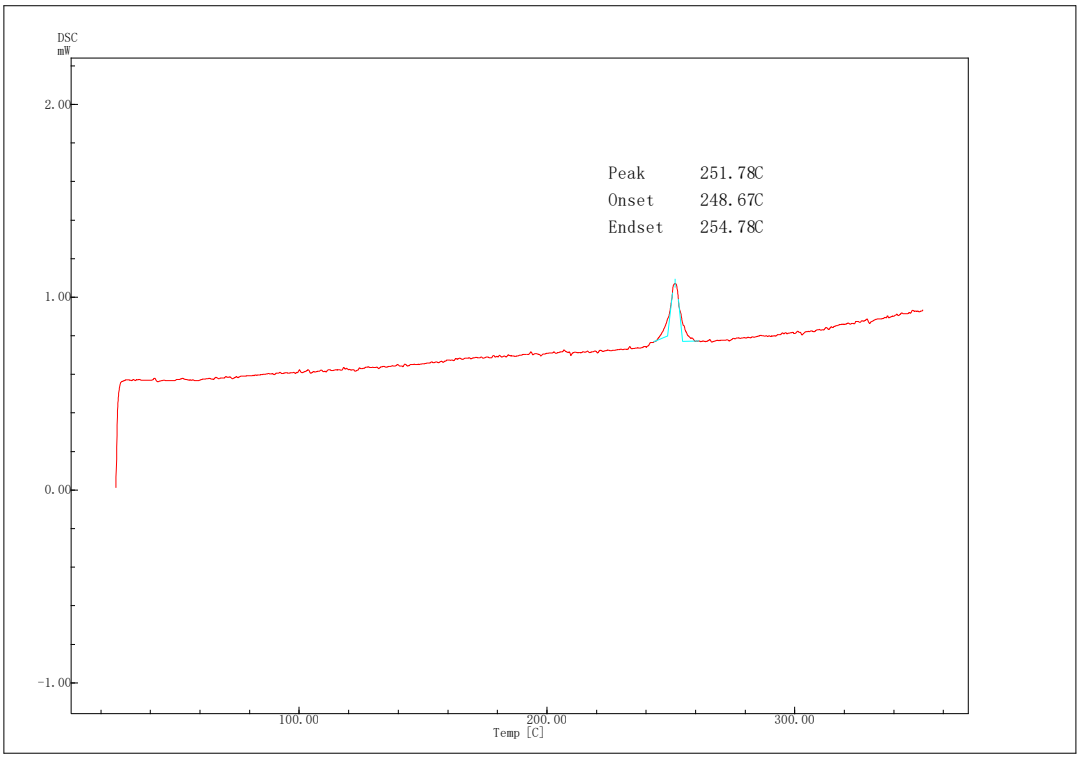

Figure S2 DSC curve of **2** (5 ºC min^{-1}).

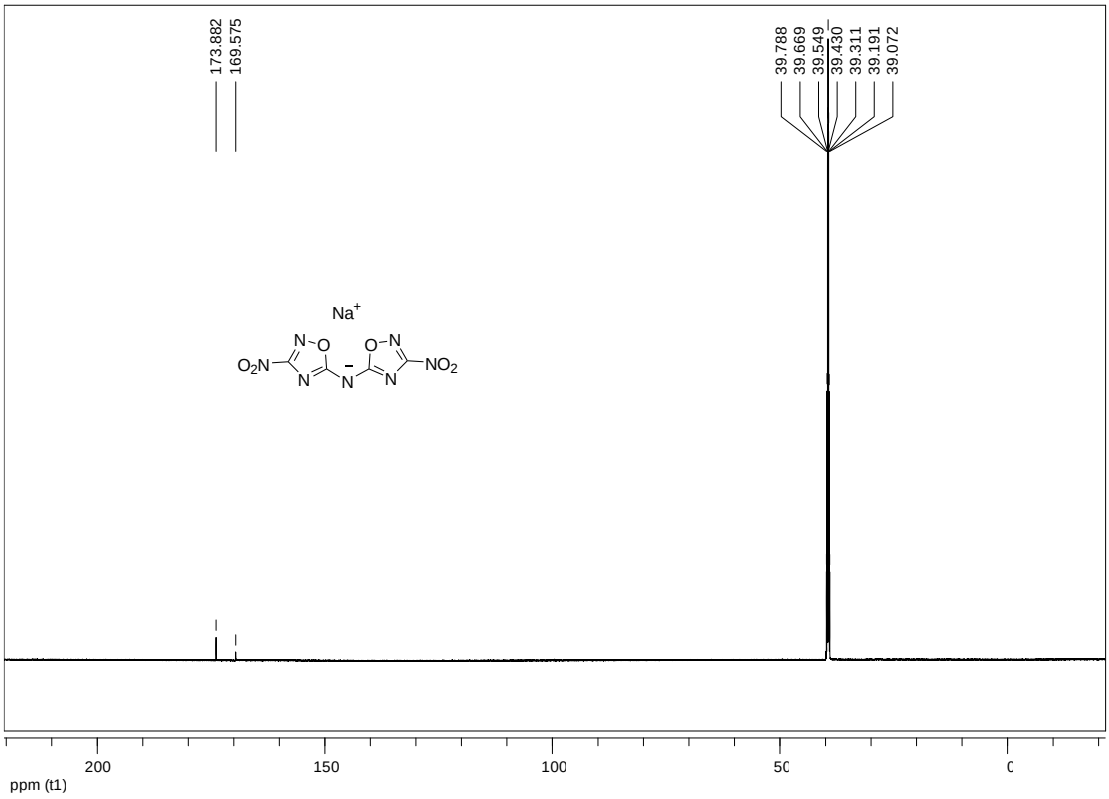

Figure S3 ^{13}C NMR spectra of **2**.

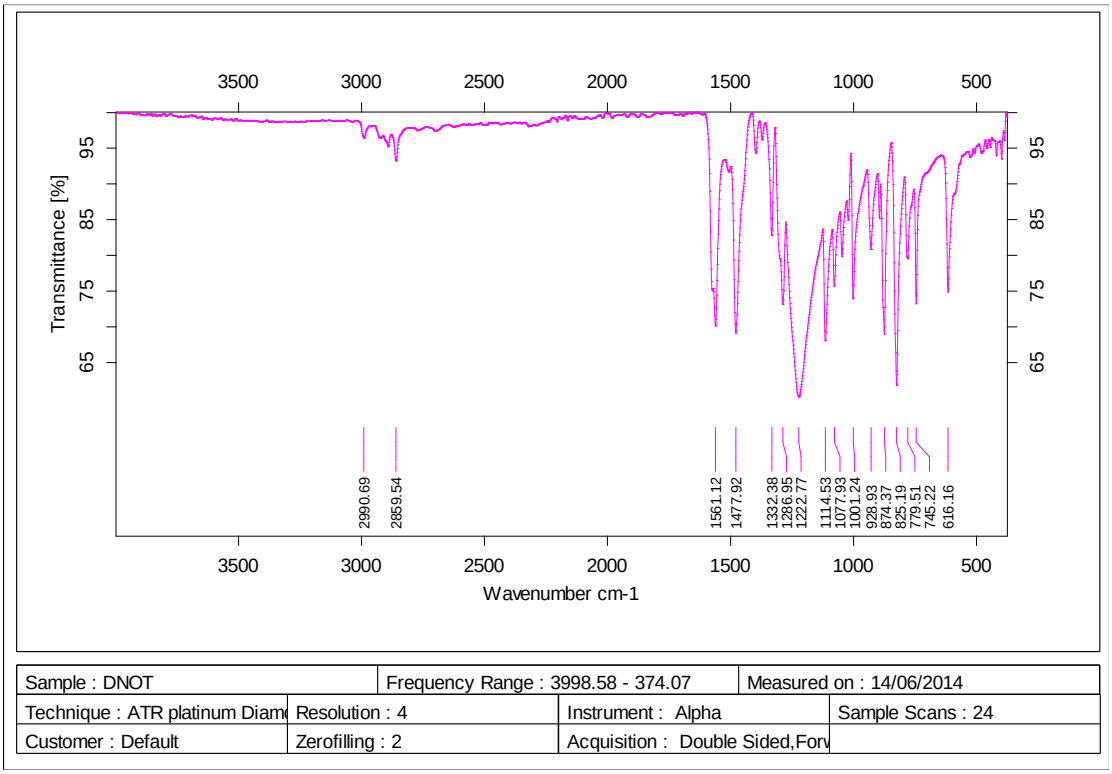

Figure S4 IR spectra of **3**.

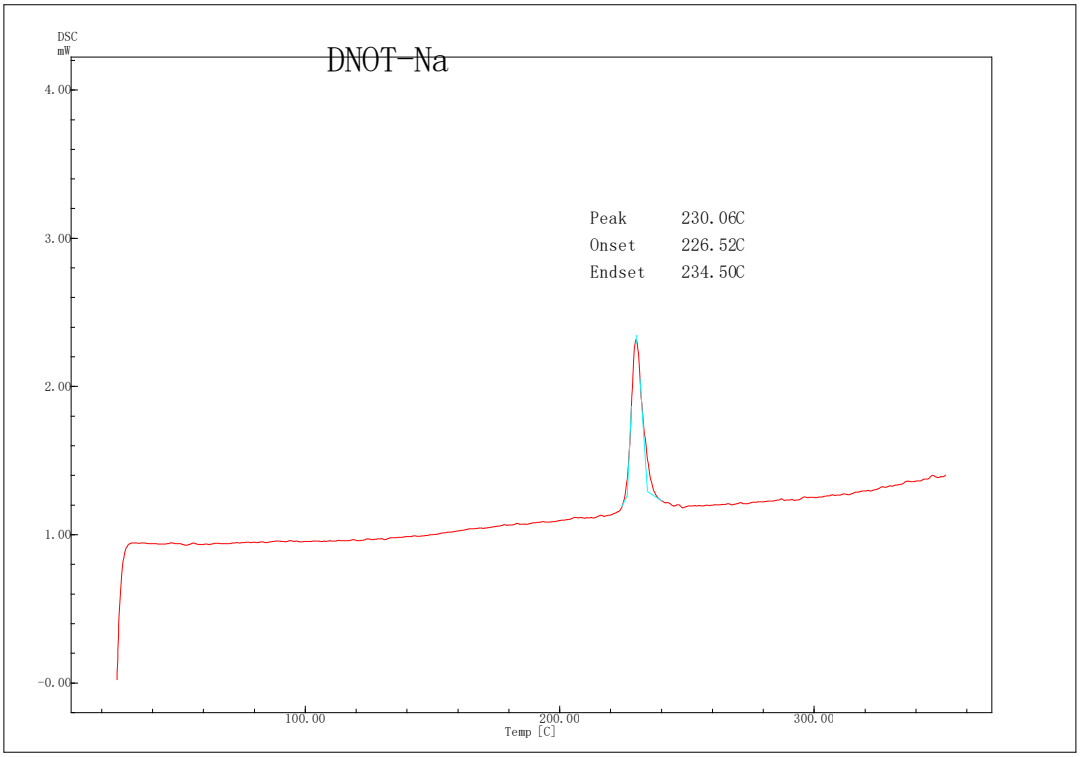

Figure S5 DSC curve of **3** (5 ºC min^{-1})

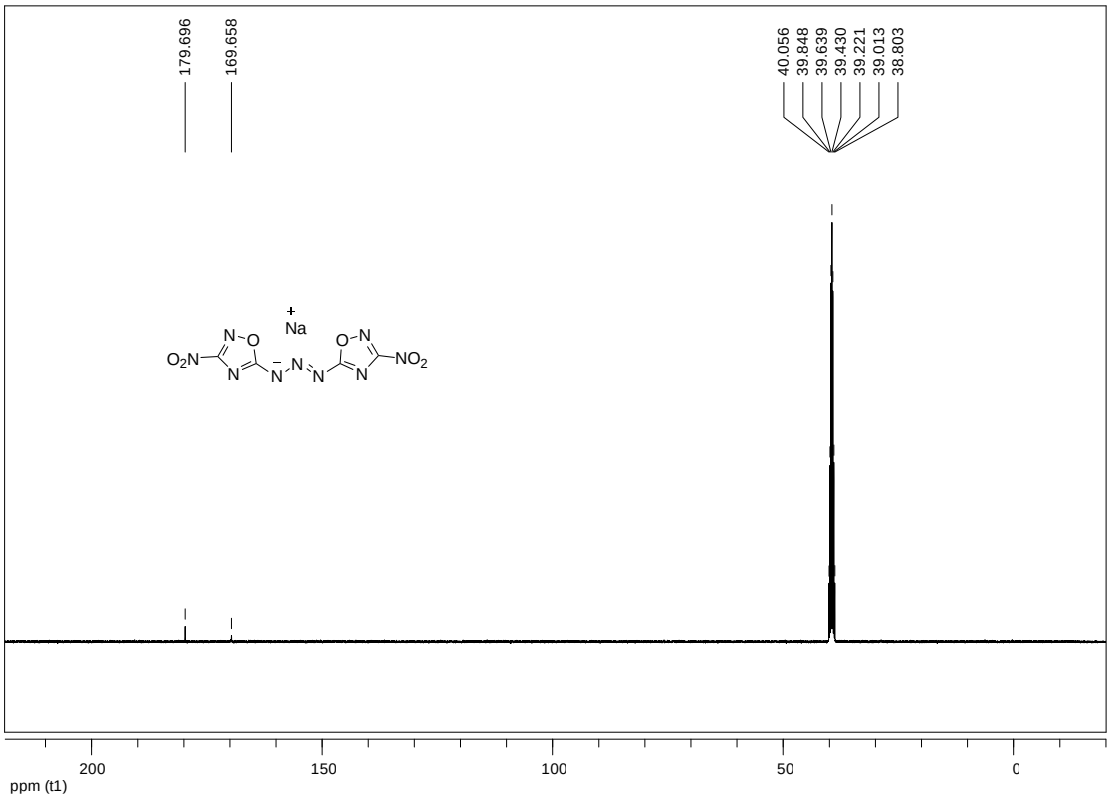

Figure S6 ^{13}C NMR spectra of **3**.

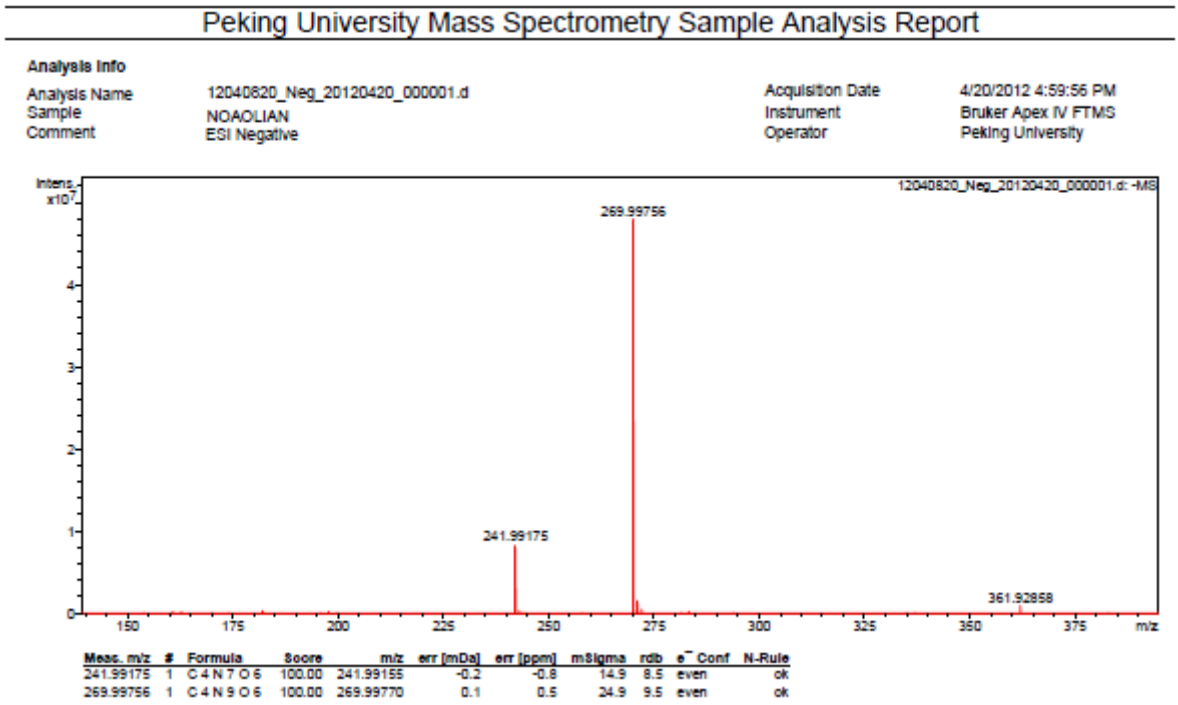

Figure S7 HRMS spectra of **2** and **3**.

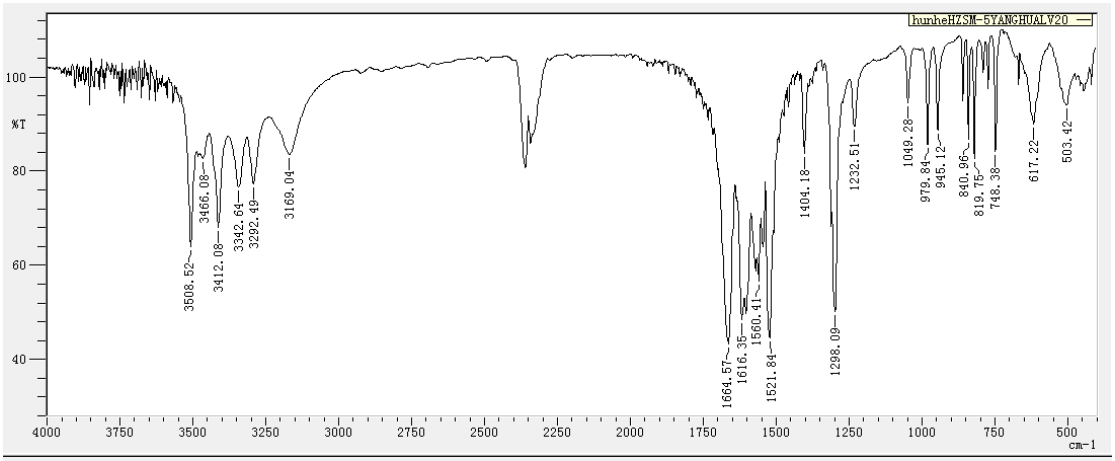

Figure S8 IR spectra of **4**.

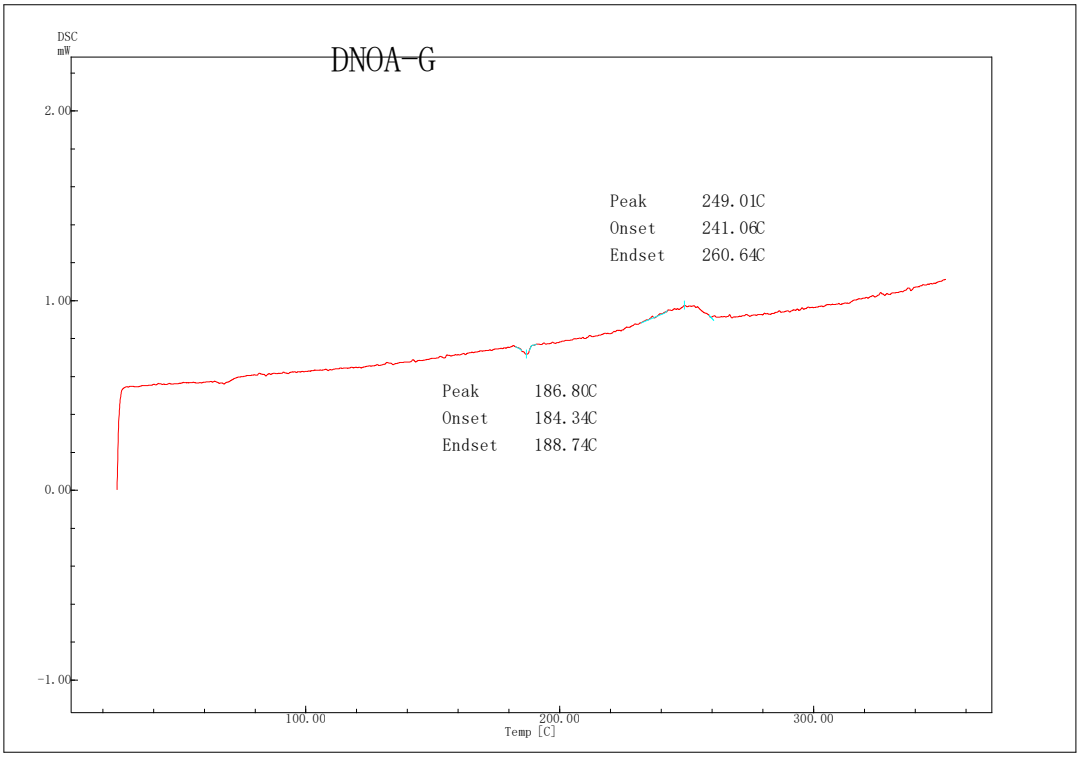

Figure S9 DSC curve of **4** (5 ºC min^{-1})

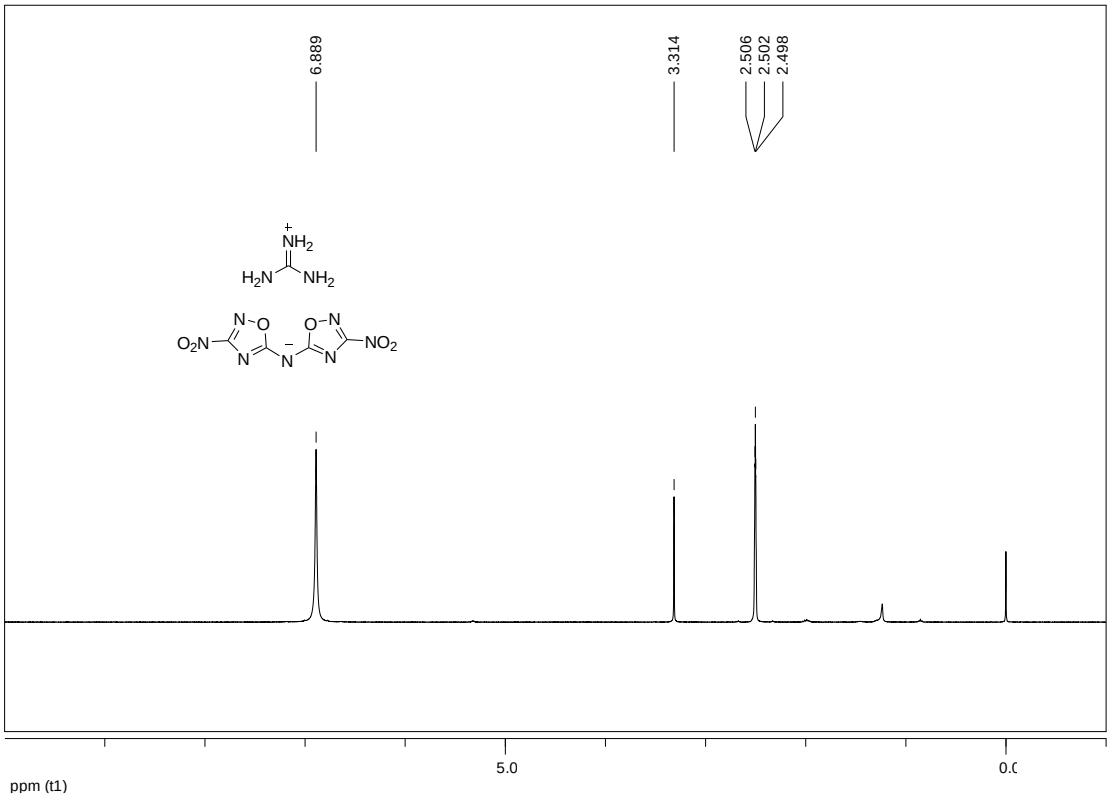

Figure S10 ^{1}H NMR spectra of **4**.

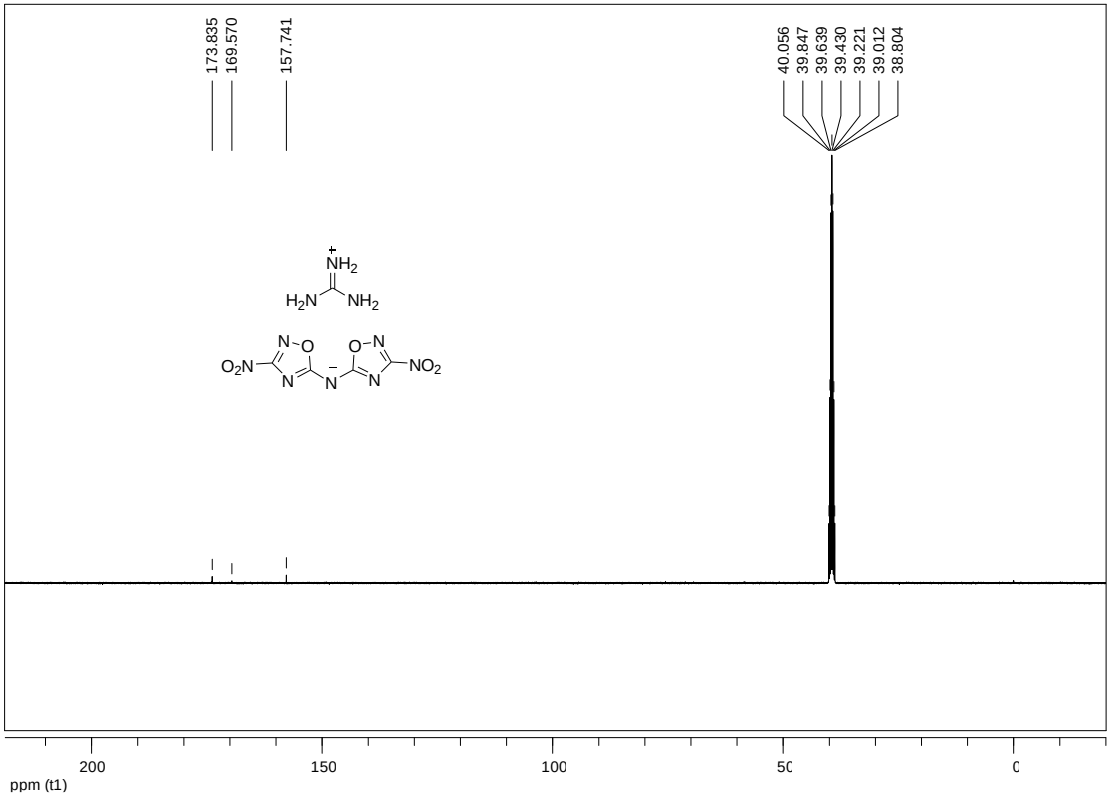

Figure S11 ^{13}C NMR spectra of **4**.

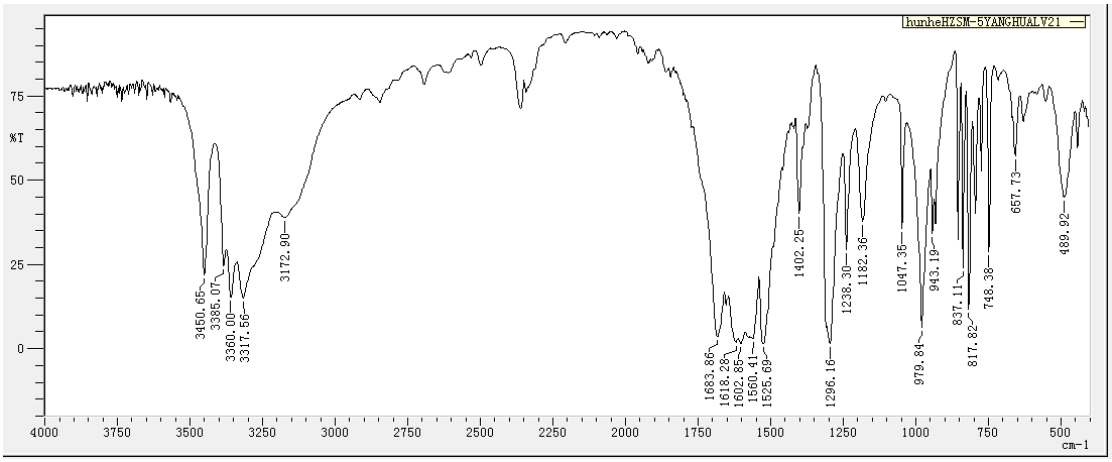

Figure S12 IR spectra of **5**.

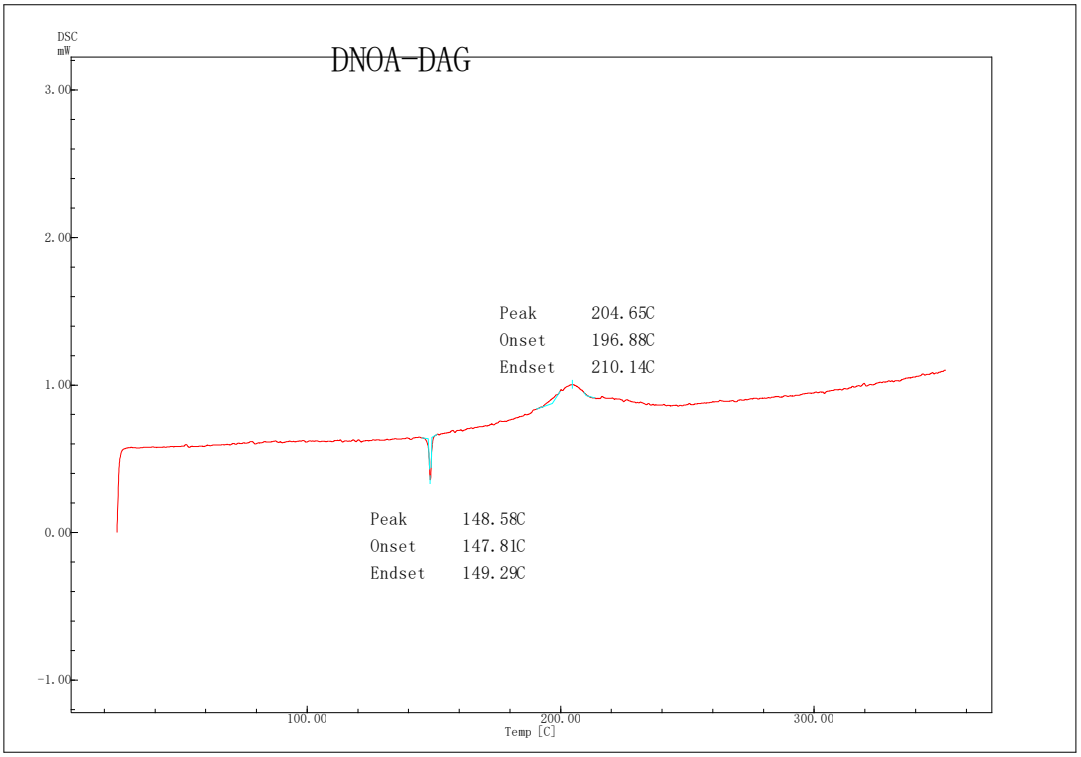

Figure S13 DSC curve of **5** (5 ºC min^{-1})

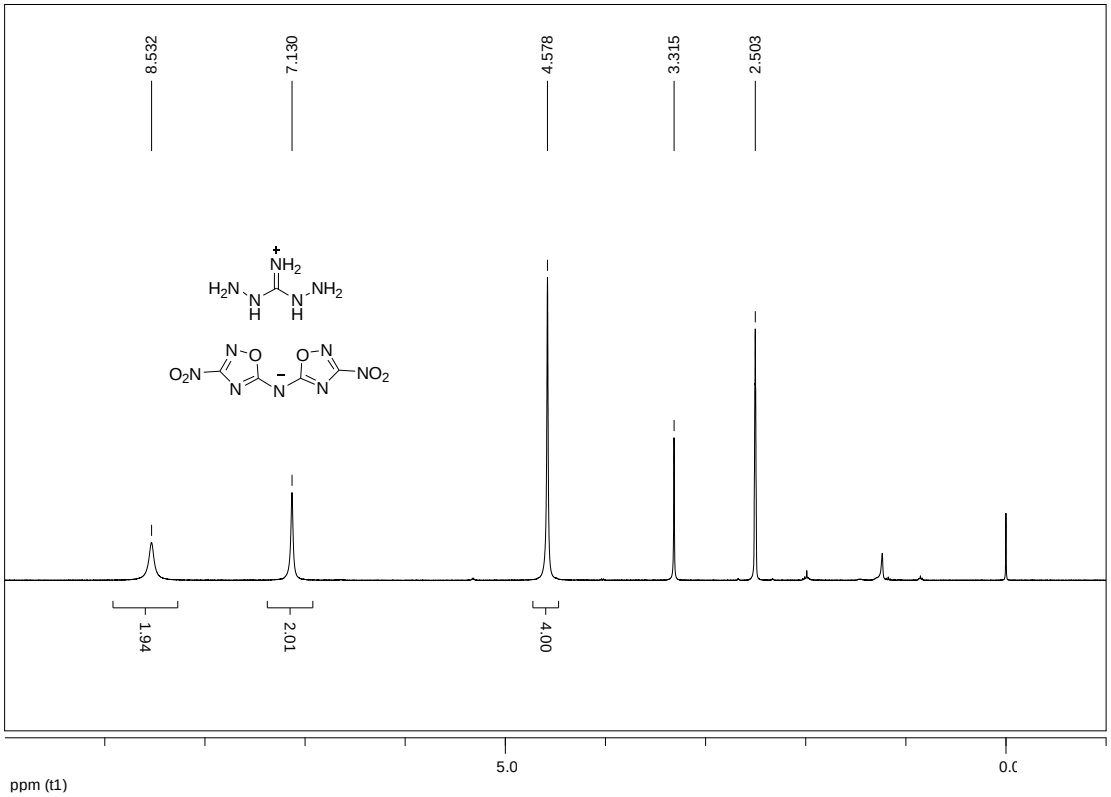

Figure S14 ^{1}H NMR spectra of **5**

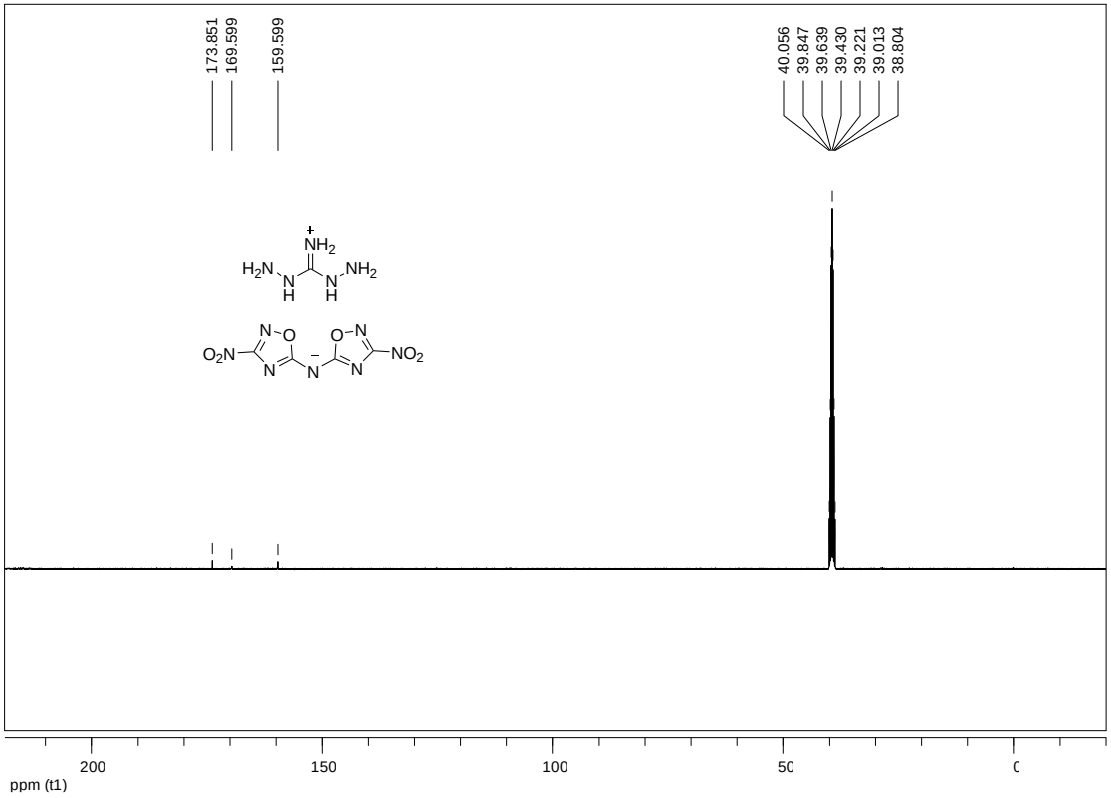

Figure S15 ^{13}C NMR spectra of **5**.

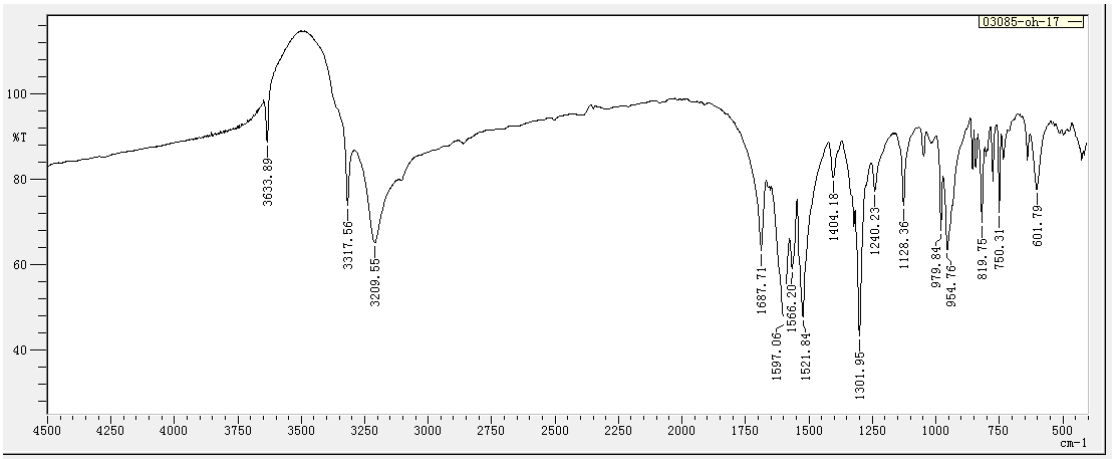

Figure S16 IR spectra of **6**.

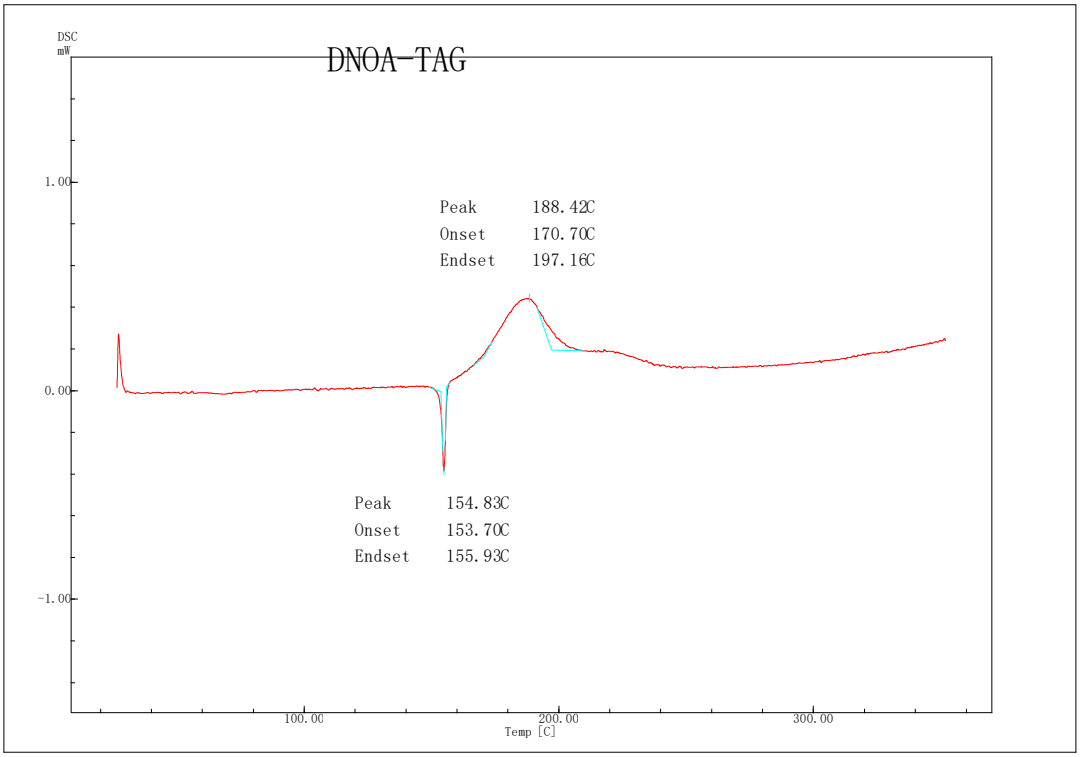

Figure S17 DSC curve of **6** (5 ºC min^{-1})

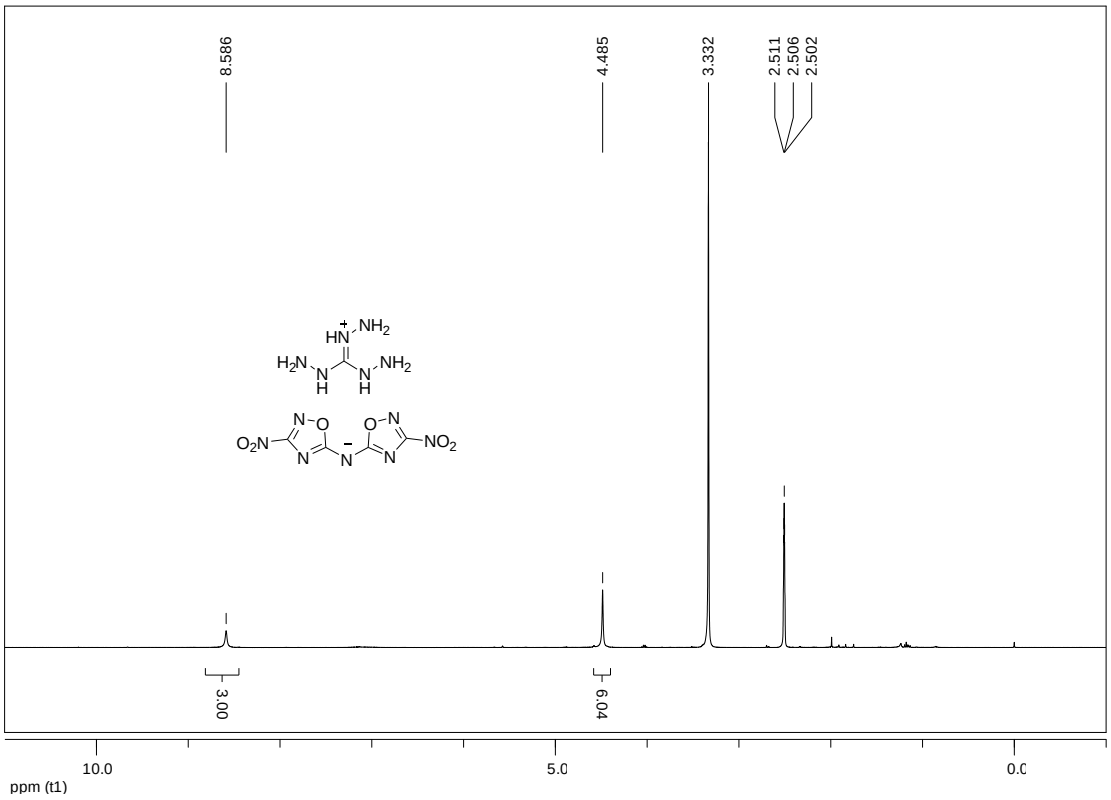

Figure S18 ^{1}H NMR spectra of **6**

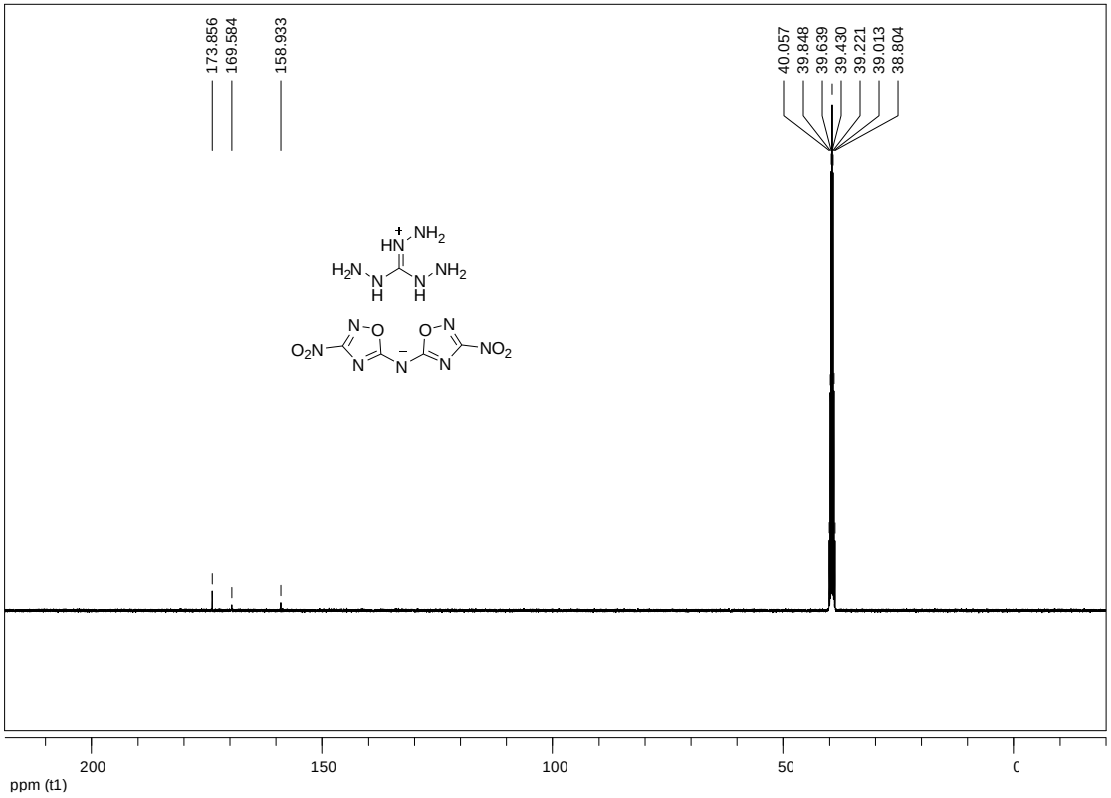

Figure S19 ^{13}C NMR spectra of **6**.

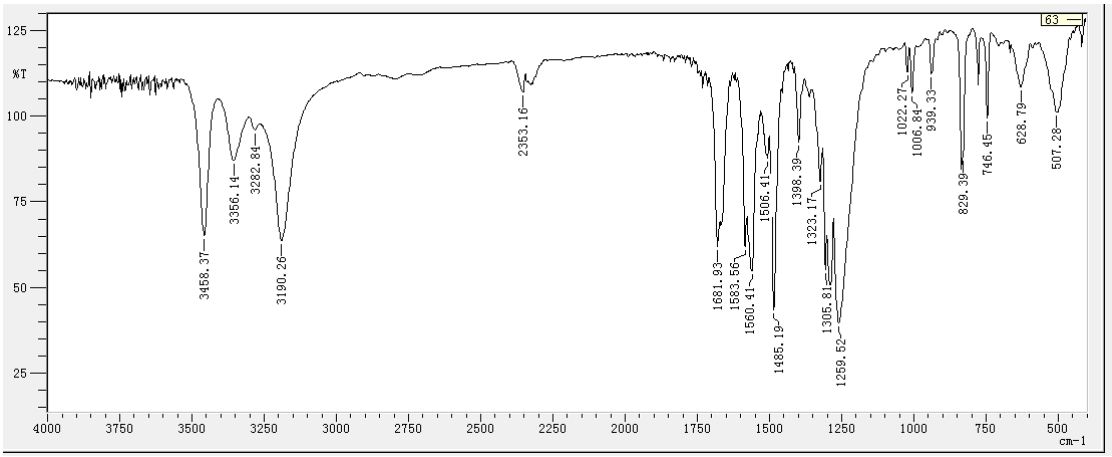

Figure S20 IR spectra of **7**.

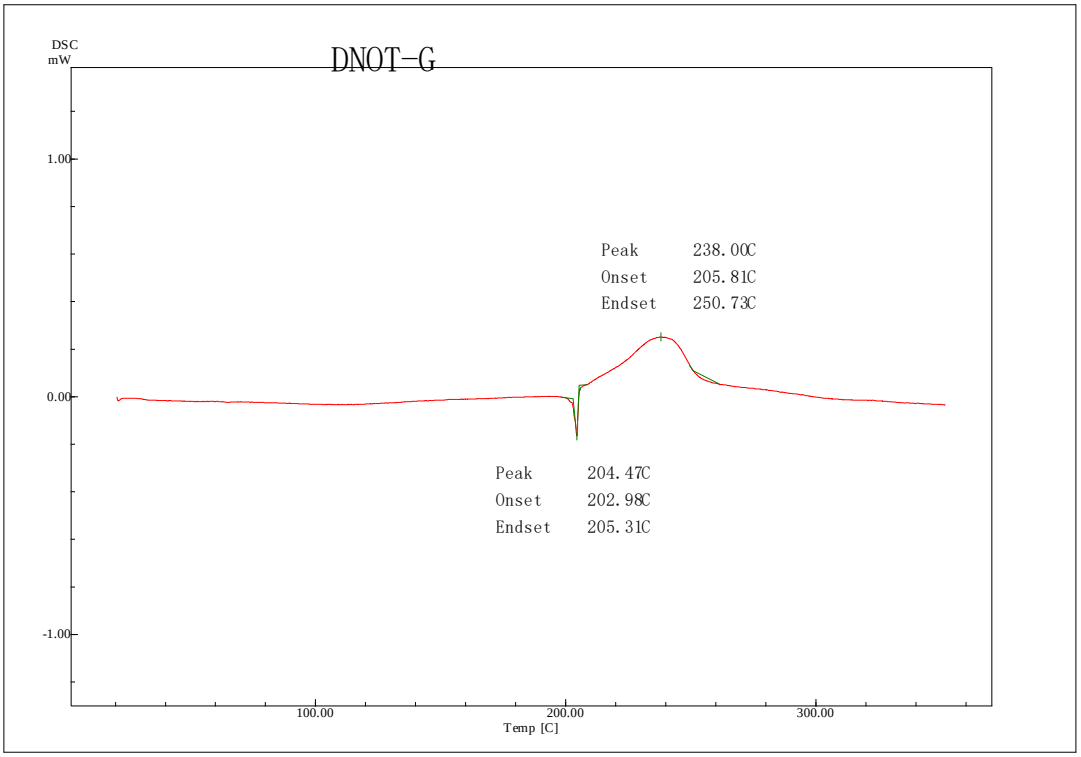

Figure S21 DSC curve of **7** (5 ºC min^{-1})

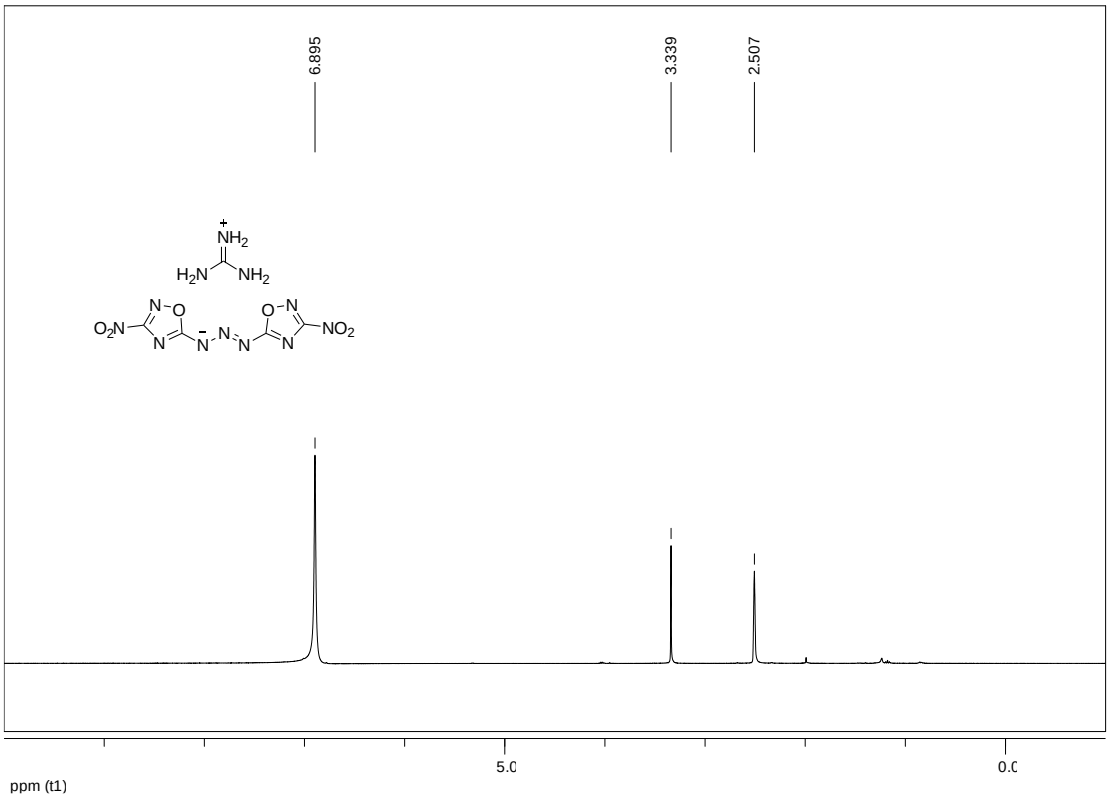

Figure S22 ^{1}H NMR spectra of **7**

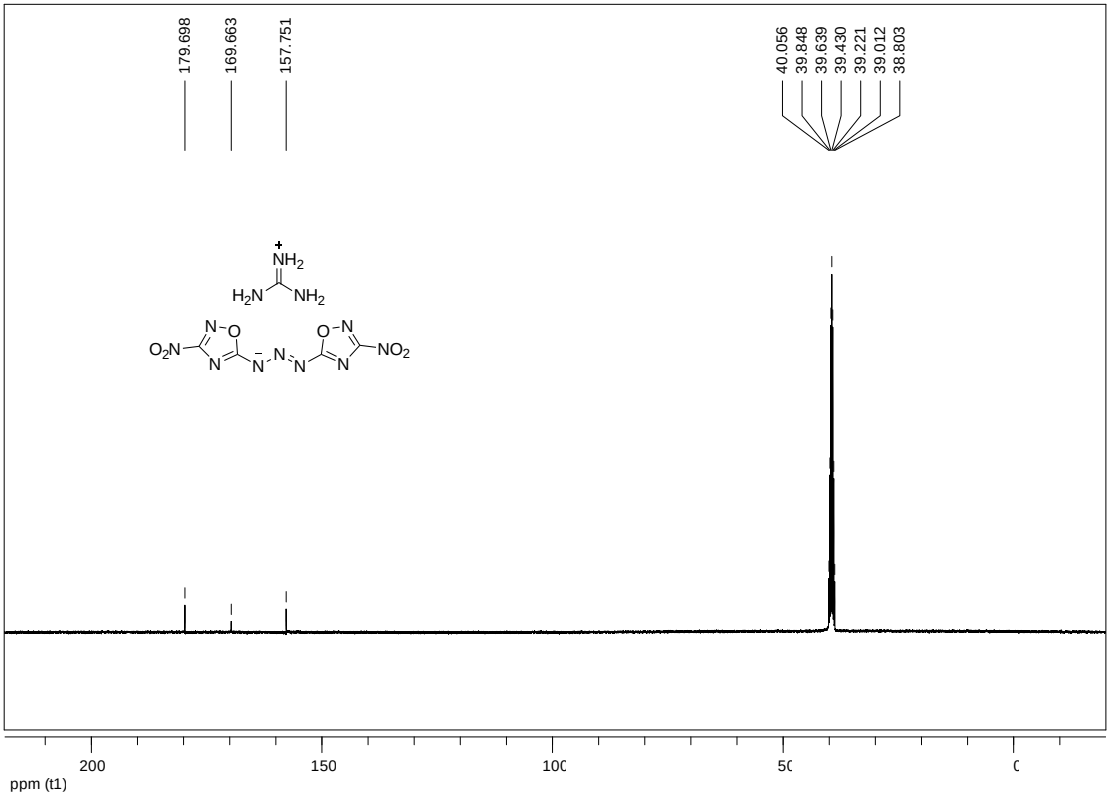

Figure S23 ^{13}C NMR spectra of **7**.

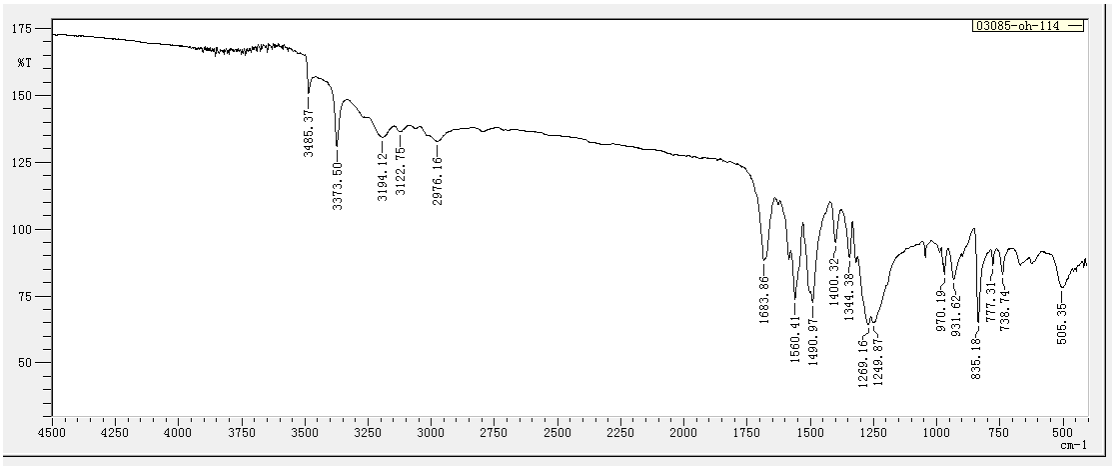

Figure S24 IR spectra of **8**.

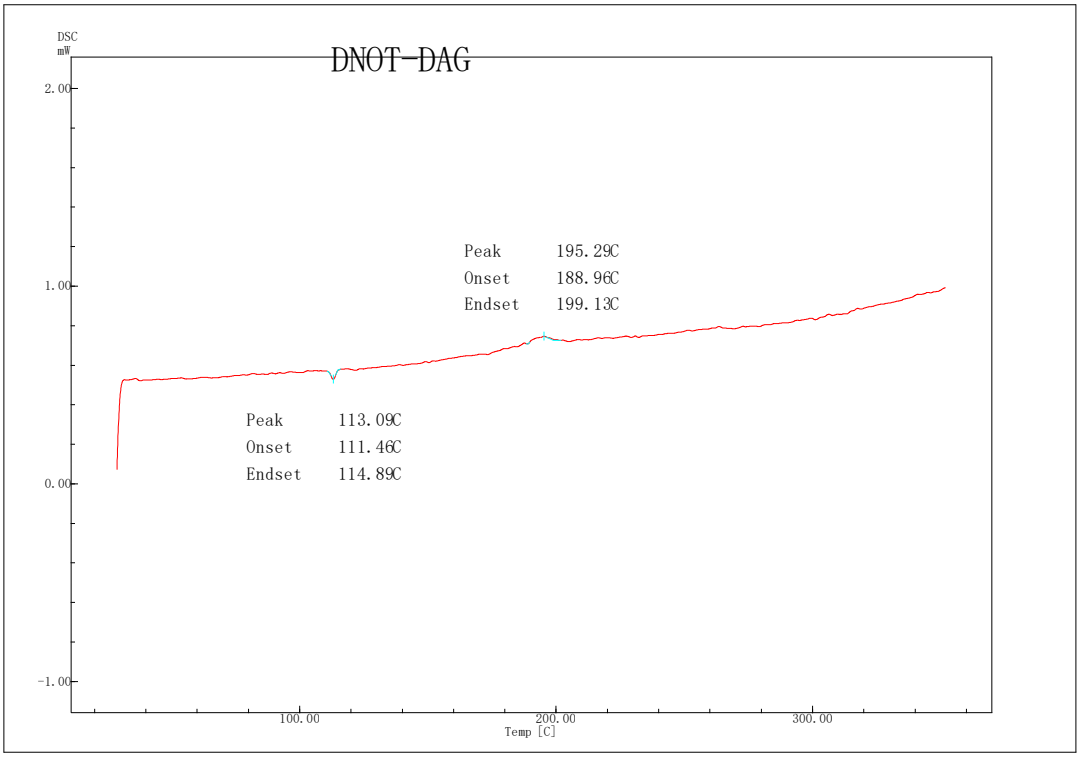

Figure S25 DSC curve of **8** (5 ºC min^{-1})

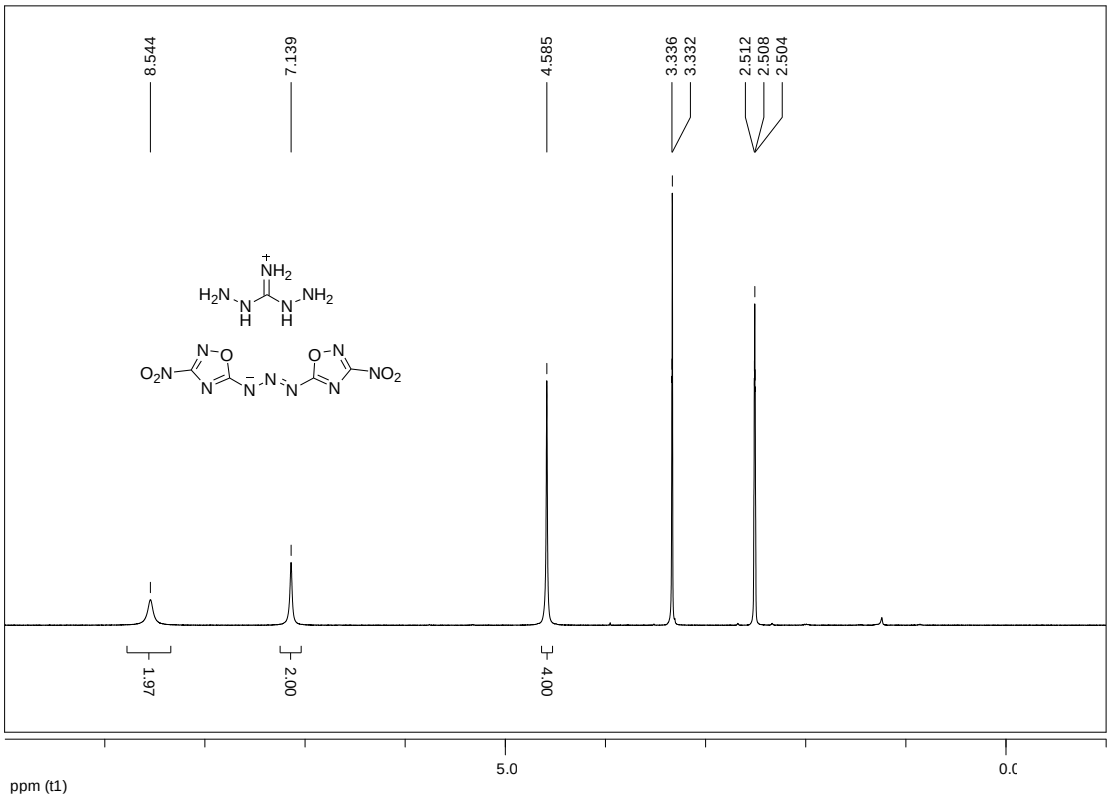

Figure S26 ^{1}H NMR spectra of **8**

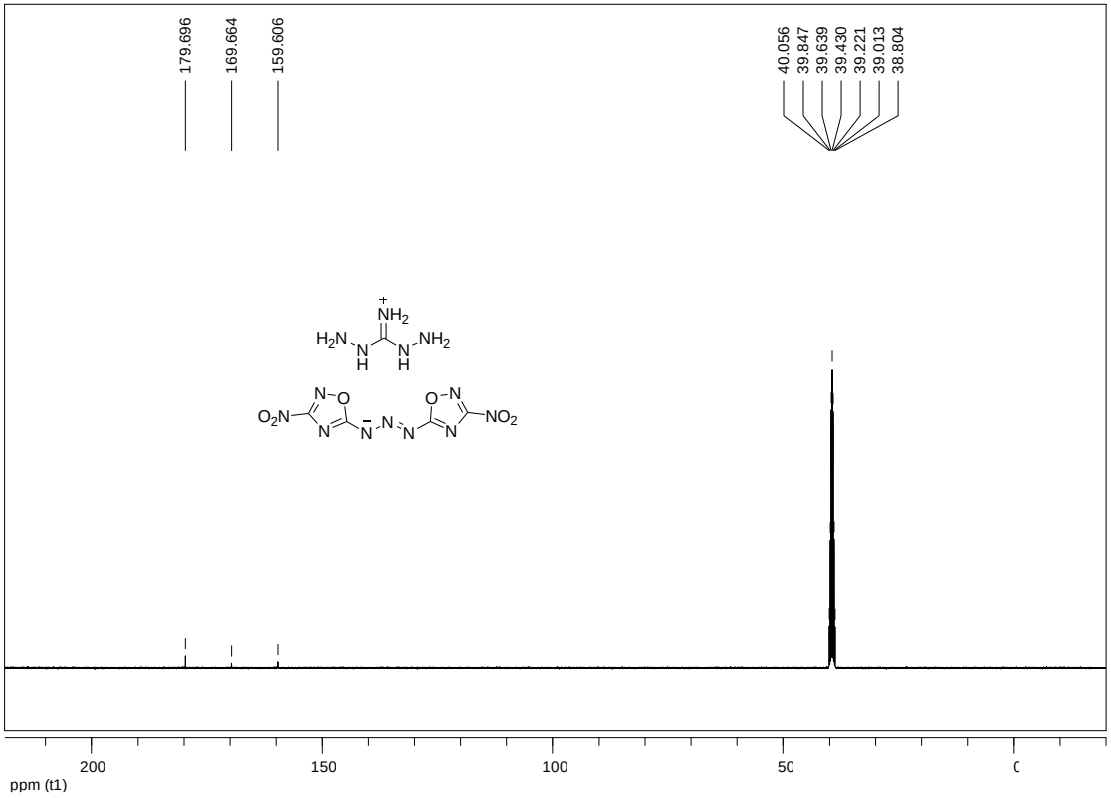

Figure S27 ^{13}C NMR spectra of **8**.

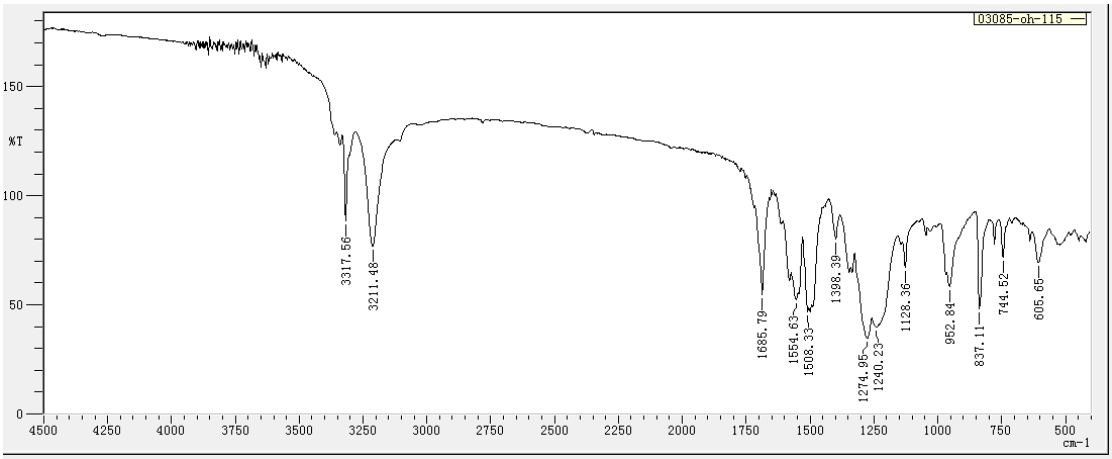

Figure S28 IR spectra of **9**.

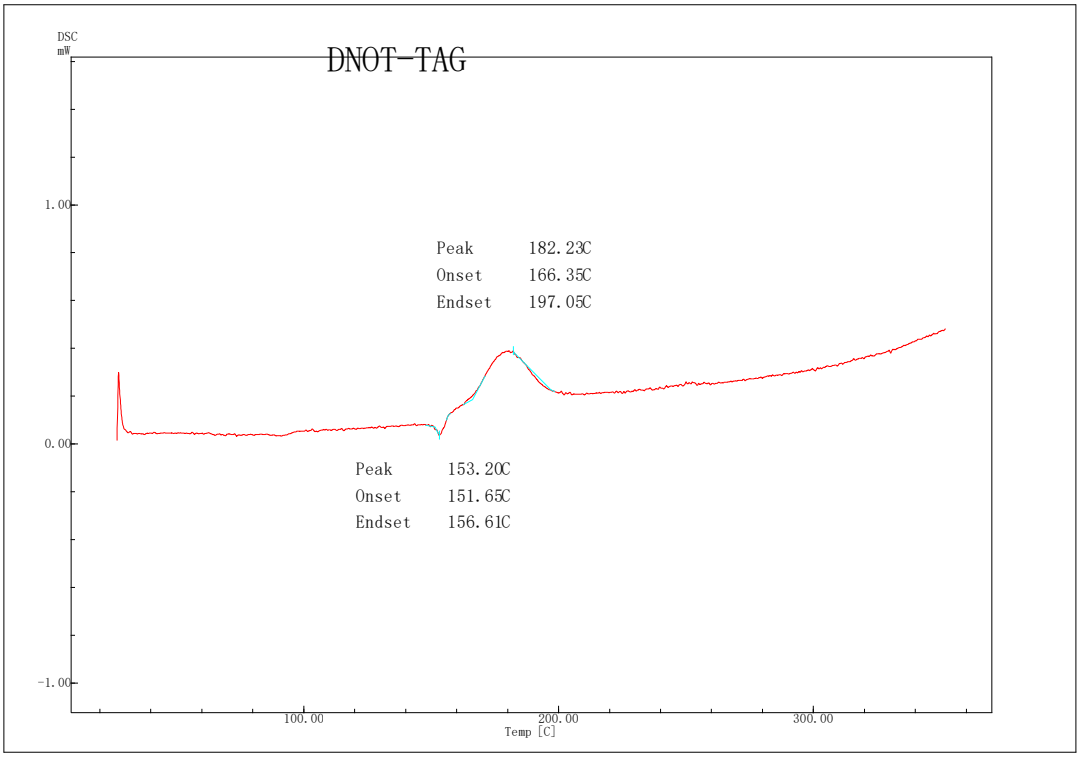

Figure S29 DSC curve of **9** (5 ºC min^{-1})

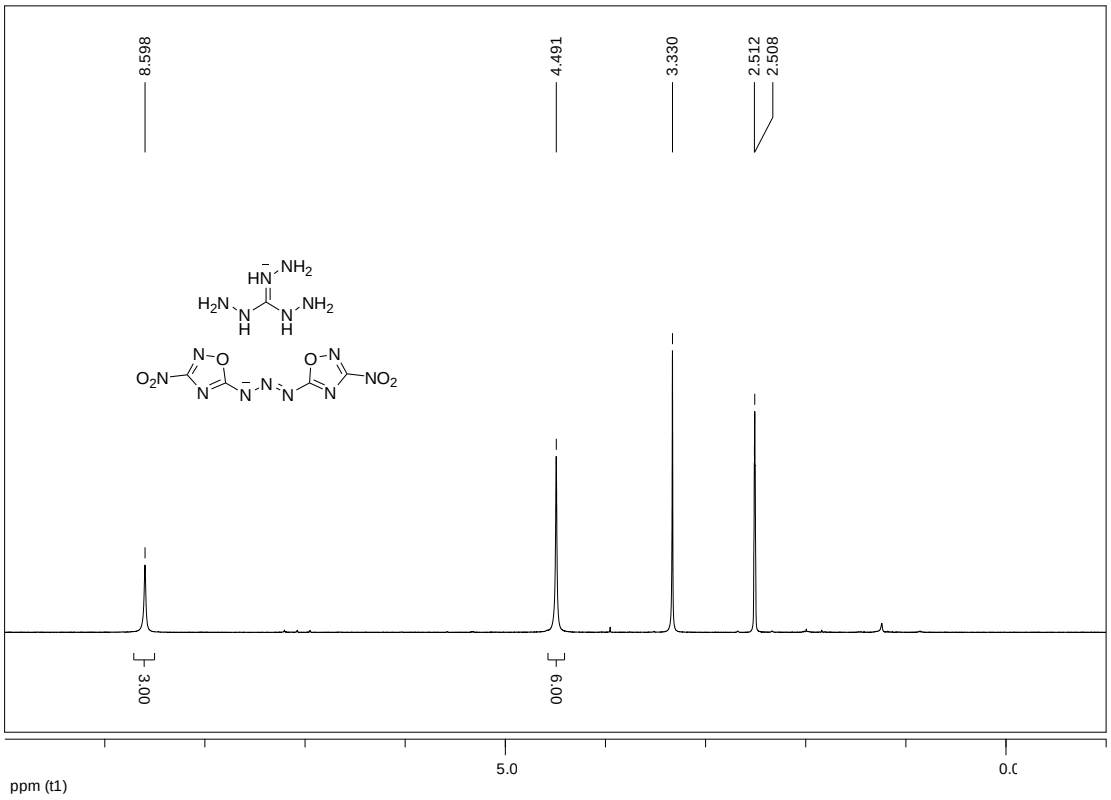

Figure S30 ^{1}H NMR spectra of **9**

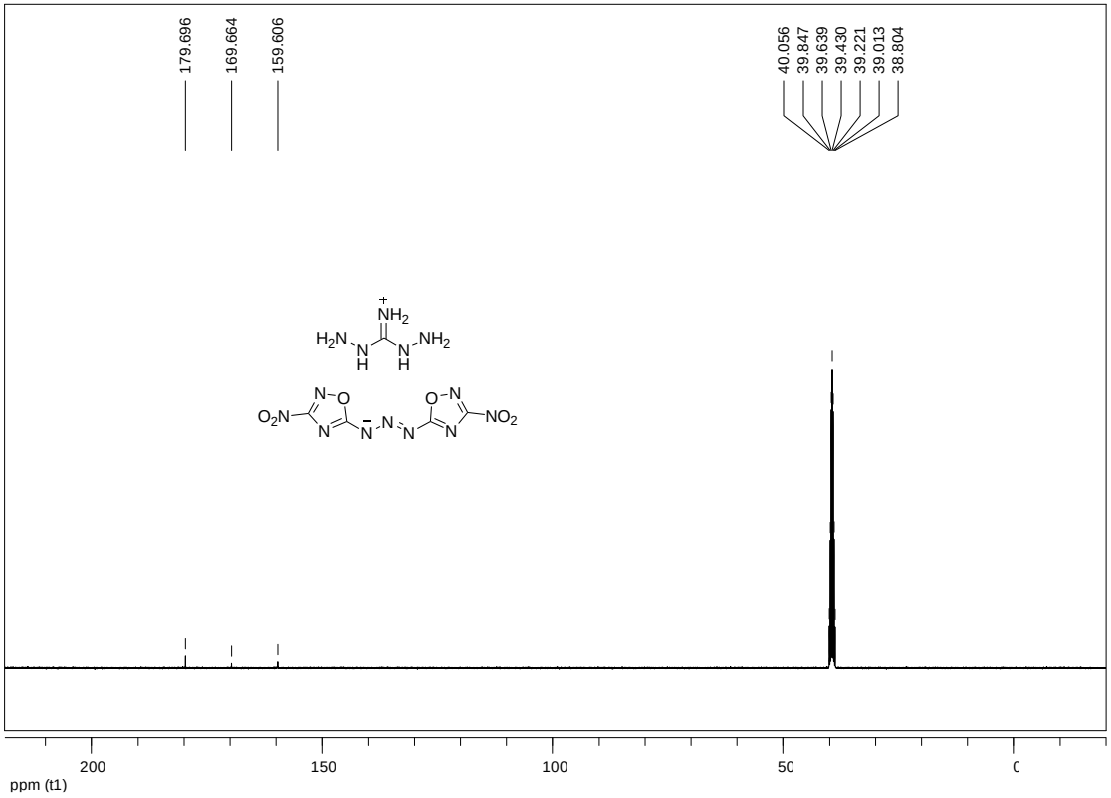

Figure S31 ^{13}C NMR spectra of **9**.