Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Electronic Supplementary Informtion

Functionalized planar aromatic rings as precursors to energetic N,N'-(4,6-dinitro-1,3-phenylene)dinitramide and its salts

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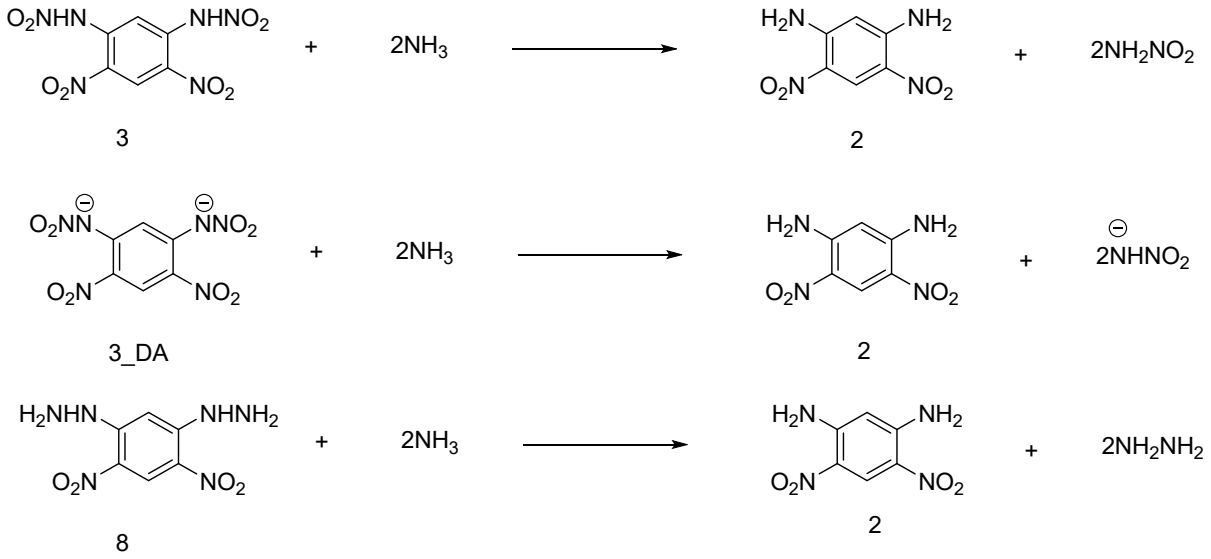
Physicochemical properties of compounds 3-8

Gaussian 03 program[1] is used to optimize the geometry of the compounds **3**-**8**. The heats of formation (gaseous) were calculated using isodesmic reactions (Scheme S1) as well as by the atomization method (equation 1).



Scheme S1: Isodesmic reactions for compounds **3**–**8.**

ΔH_f(salt, 298 K) = ΔH_f (anion, 298 K) + ΔH_f (cation, 298 K) – Lattice Energy (1)

Lattice energy of the salts (**4**–**7**) was calculated by equation 2. [2,3]

Lattice Energy (kJ/mol) = $2I[\alpha(V_m)^{-1/3} + \beta$ (2)

I is the ionic strength, α (kJmol^{-1}nm) and β (kJmol^{-1}) are appropriate fitted coefficients and V_m (nm^3) is volume of the salt. Values of I, α and β are derived from the literature[3] and V_m was obtained from crystal structure or derived from pycnometer densities.

Table S1: Physicochemical properties of compounds 3–8.

Compound	Density[a]	ΔH_f atomization(g)[b] (kJ mol^{-1})/kJg^{-1}	P (GPa)[c]	D_V (m s^{-1})[d]
3	1.87 (1.91)[e]	149.41/0.52	34.0	8682
4	1.74	283.65/0.88	31.3	8575
5	1.77* (1.74)[e]	578.33/1.64	34.3	8992
6	1.83	365.50/1.03	37.7	8980
7	1.76 (1.80)[e]	1277.35/2.14	28.3	8525
8	1.72	239.73/1.05	24.9	8121

[a]Gas pycnometer density at 25 °C. [b]Heat of formation calculated using Gaussian 03 program B3LYP/6-311++G(d,p) level of theory. [c]Detonation pressure (GPa) calculated by using EXPLO5 software. [d]Detonation velocity (m/s) calculated by using EXPLO5 software. [e]X-Ray density. *X-ray density for compound **5** is lower than the room temperature density because of solvent molecule in crystal lattice. All compounds were obtained as anhydrous powders (confirmed by elemental analysis) to determine the pycnometer density.

The solid phase heats of formation (ΔHf_s) of compounds **3**, **4** and **8** were calculated by using equation 3 (Hess's Law). [4]

$$\Delta H_f(s) = \Delta H_f(g) - \Delta H_{sub} \quad (3)$$

Where, ΔH_{sub} is the heats of sublimation, which can be obtained from equation 4.[5]

$$\Delta H_{sub} = a(SA)^2 + b(\sigma^2_{tot}\upsilon)^{0.5} + c \quad (4)$$

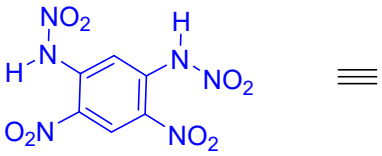
SA is surface area of the 0.001 electron/$bohr^3$ isosurface of the electron density of the title compound, *a*, *b* and *c* are constant fitted parameters, σ^2_{tot} is the electron potential on the molecule's surface and υ is the degree of balance between the positive and negative charges on the isosurface.[5]

Table S2: Physicochemical properties of the title compounds in solid state

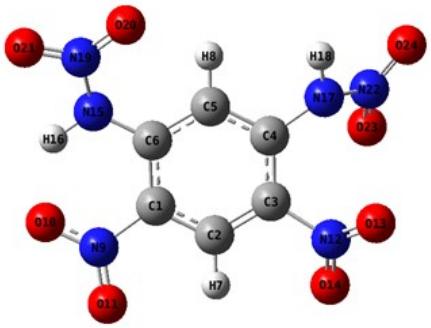
Compound	Density[a]	$HOF_{solid(s)}$[b] (kJ/mol)/kJg^{-1}	DP (GPa)[c]	DV (m/s)[d]
3	1.87 (1.91)[e]	26.61/0.09	32.8	8554
4	1.74	109.31/0.34	29.9	8433
8	1.72	118.39/0.52	23.5	7951

[a]Gas pycnometer density at 25 °C. [b]Heat of formation calculated using Gaussian 03 program B3LYP/6-311++G(d,p) level of theory. [c]Detonation pressure (GPa) calculated by using EXPLO5 software. [d]Detonation velocity (m/s) calculated by using EXPLO5 software. [e]X-Ray density.

Table S3. Atomic coordinates for optimized structure of compound **3**.



MF: $C_6H_4N_6O_8$
MW: 288.13

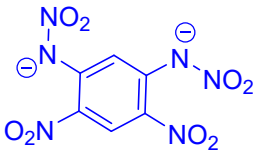


optimized structure

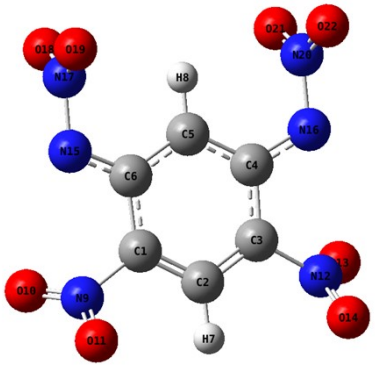
Center Number	Atomic Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	0.138199	0.893462	-0.010260
2	C	1.521399	0.999228	0.056907
3	C	2.148826	2.220017	-0.080177
4	C	1.389209	3.370849	-0.359164
5	C	0.002769	3.259447	-0.437927
6	C	-0.665943	2.044163	-0.233931
7	H	2.110708	0.113526	0.247207
8	H	-0.576730	4.135414	-0.678968
9	N	-0.415159	-0.458086	0.182671
10	O	-1.631850	-0.620555	0.033145
11	O	0.353280	-1.353899	0.476739
12	N	3.606776	2.243868	0.172280
13	O	4.067514	3.252707	0.681522
14	O	4.230815	1.231726	-0.099301
15	N	-2.045917	1.922996	-0.325533
16	H	-2.444622	0.989985	-0.227800
17	N	1.938457	4.646054	-0.543831
18	H	1.336930	5.454365	-0.446367
19	N	-2.993095	2.930110	-0.105796
20	O	-2.616267	4.086588	-0.028617
21	O	-4.137004	2.524888	-0.035134
22	N	2.913928	4.903736	-1.534639
23	O	3.468514	3.948281	-2.034579
24	O	3.095835	6.082288	-1.765042

E = -1161.080392 Hartree/particle Method: B3LYP/6-311++G(d,p)

Table S4. Atomic coordinates for optimized structure of compound **3** anion.



MF: $[C_6H_2N_6O_8]^{-2}$
MW: 286.12

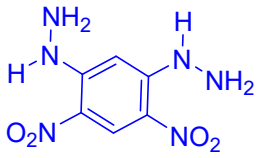


optimized structure

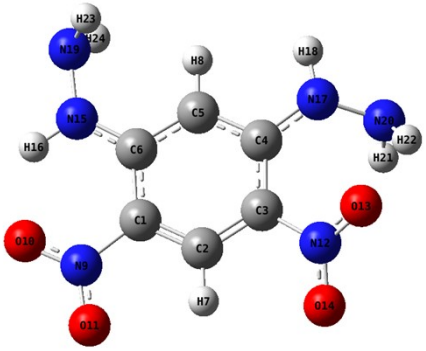
Center Number	Atomic Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	0.205798	0.741369	-0.188910
2	C	1.575687	0.691071	-0.013883
3	C	2.319878	1.844692	-0.171224
4	C	1.710890	3.119247	-0.433629
5	C	0.298154	3.148102	-0.570765
6	C	-0.487893	1.971968	-0.451597
7	H	2.061724	-0.244760	0.231668
8	H	-0.193130	4.092544	-0.767310
9	N	-0.539867	-0.529737	-0.100157
10	O	-1.241056	-0.822812	-1.049496
11	O	-0.354785	-1.193065	0.907804
12	N	3.787822	1.729974	-0.063910
13	O	4.440342	2.135716	-1.006465
14	O	4.213866	1.201715	0.950601
15	N	-1.824681	1.920257	-0.502590
16	N	2.519075	4.185926	-0.468089
17	N	-2.461971	3.174931	-0.728494
18	O	-2.554145	3.527120	-1.884828
19	O	-2.916496	3.707941	0.258945
20	N	1.858147	5.427666	-0.697897
21	O	1.642959	5.711413	-1.856629
22	O	1.662690	6.099458	0.290178

E = -1159.782944 Hartree/particle Method: B3LYP/6-311++G(d,p)

Table S5. Atomic coordinates for optimized structure of compound **8**.



MF: $C_6H_8N_6O_4$
MW: 228.17



optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-0.071388	0.925173	0.035702
2	C	1.300341	0.887607	-0.143691
3	C	2.047656	2.036918	-0.34446
4	C	1.395902	3.302227	-0.451199
5	C	0.008184	3.323262	-0.246949
6	C	-0.763861	2.185112	0.024541
7	H	1.806362	-0.065487	-0.085671
8	H	-0.497750	4.274262	-0.351797
9	N	-0.736921	-0.344068	0.266885
10	O	-1.960490	-0.337207	0.469813
11	O	-0.068973	-1.369812	0.249740
12	N	3.495365	1.868302	-0.286212
13	O	4.168287	2.799620	0.161448
14	O	3.965670	0.792444	-0.638530
15	N	-2.103115	2.283503	0.226309
16	H	-2.621755	1.435670	0.407722
17	N	2.006295	4.490786	-0.757132
18	H	1.395610	5.293556	-0.778989
19	N	-2.820696	3.480404	0.274159
20	N	3.131442	4.666338	-1.578680
21	H	3.079825	4.057662	-2.392723
22	H	3.968827	4.440439	-1.050093
23	H	-2.456480	4.097962	0.994676
24	H	-2.807529	3.952881	-0.625527

E = -862.666635 Hartree/particle Method: B3LYP/6-311++G(d,p)

References

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^{1}H NMR, ^{13}C NMR and DSC data of compounds 3-8.

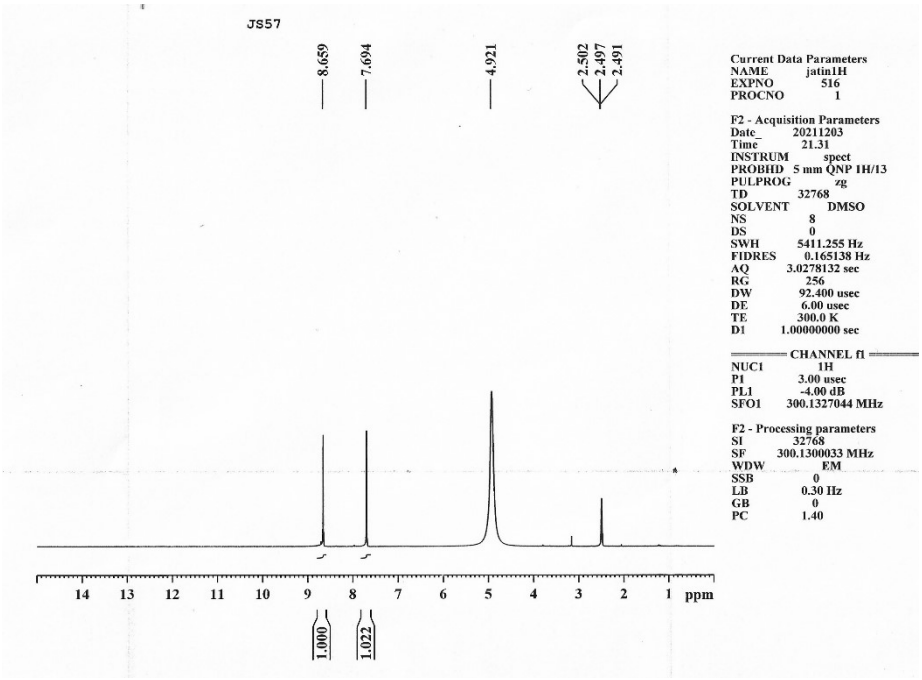

Figure S1: ^{1}H NMR of compound **3**

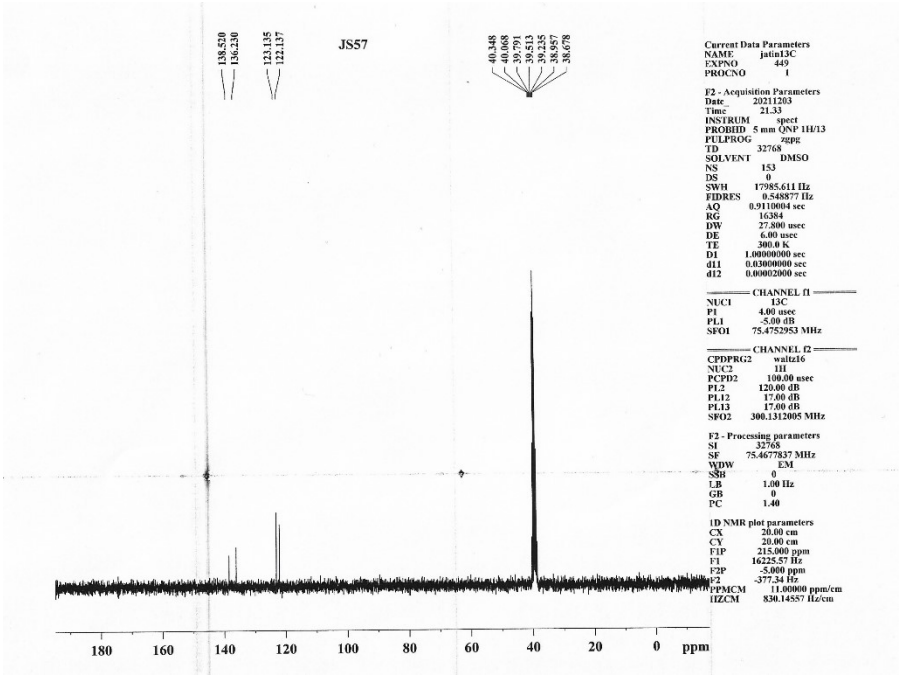

Figure S2: ^{13}C NMR of compound **3**

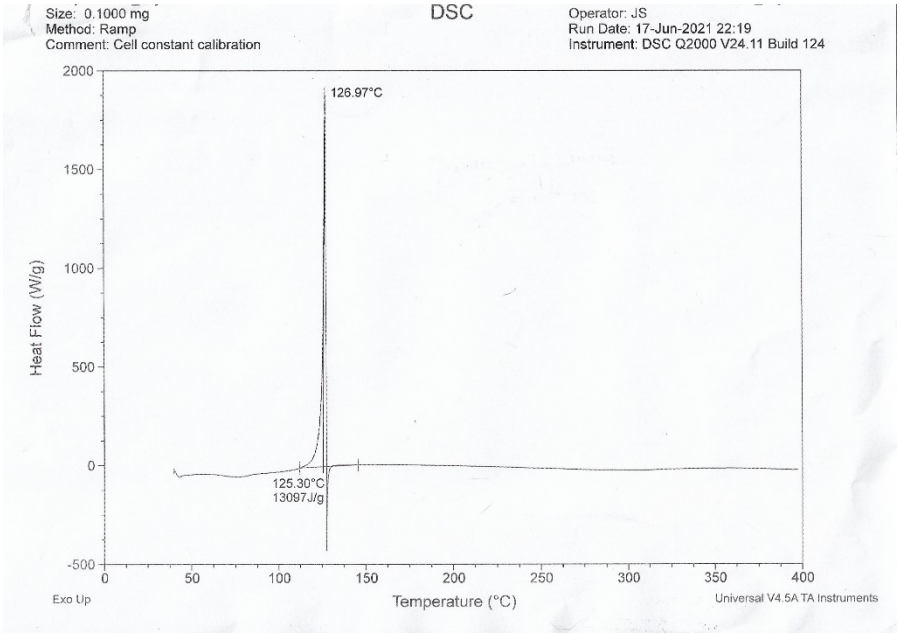

Figure S3: DSC of compound **3**

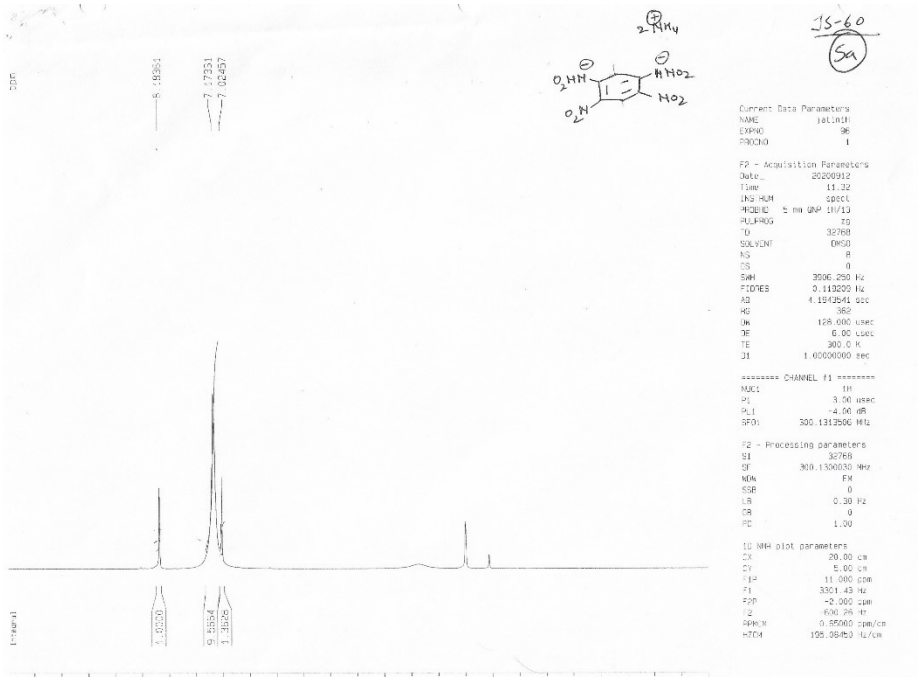

Figure S4: ^{1}H NMR of compound **4**

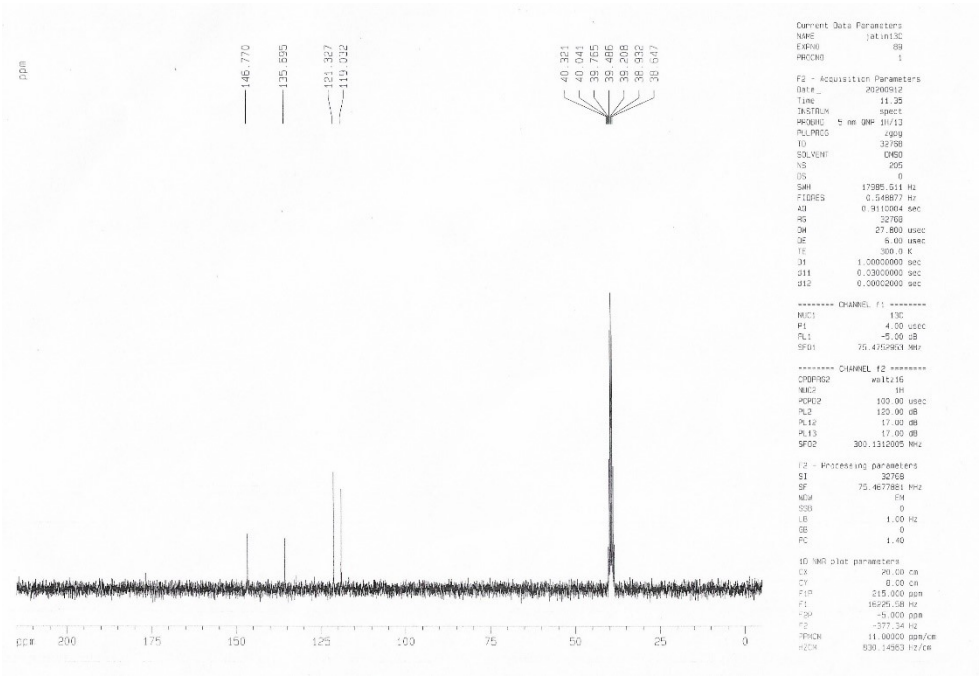

Figure S5: ^{13}C NMR of compound **4**

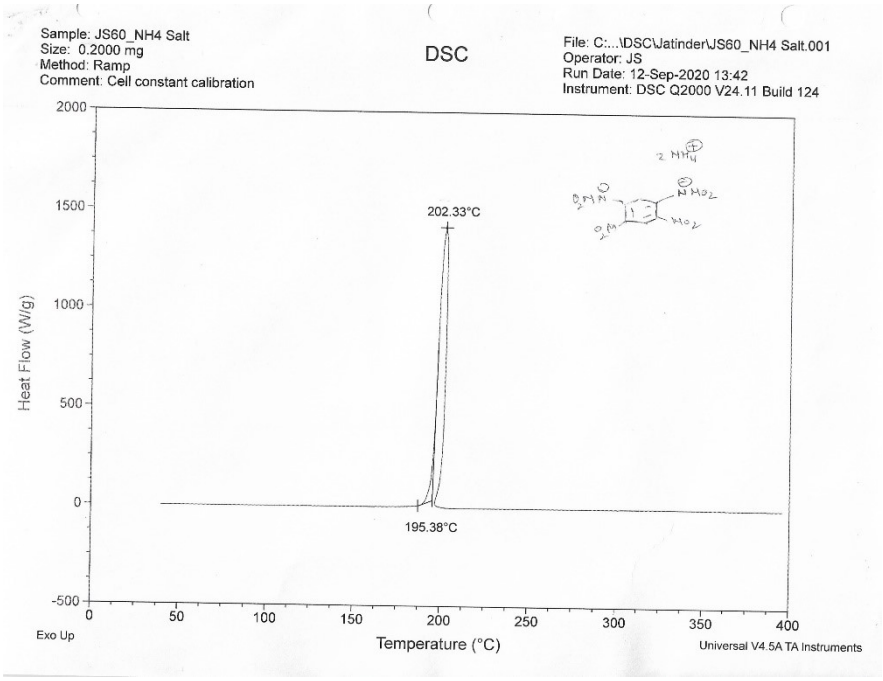

Figure S6: DSC of compound **4**

Figure S7: ^{1}H NMR of compound **5**

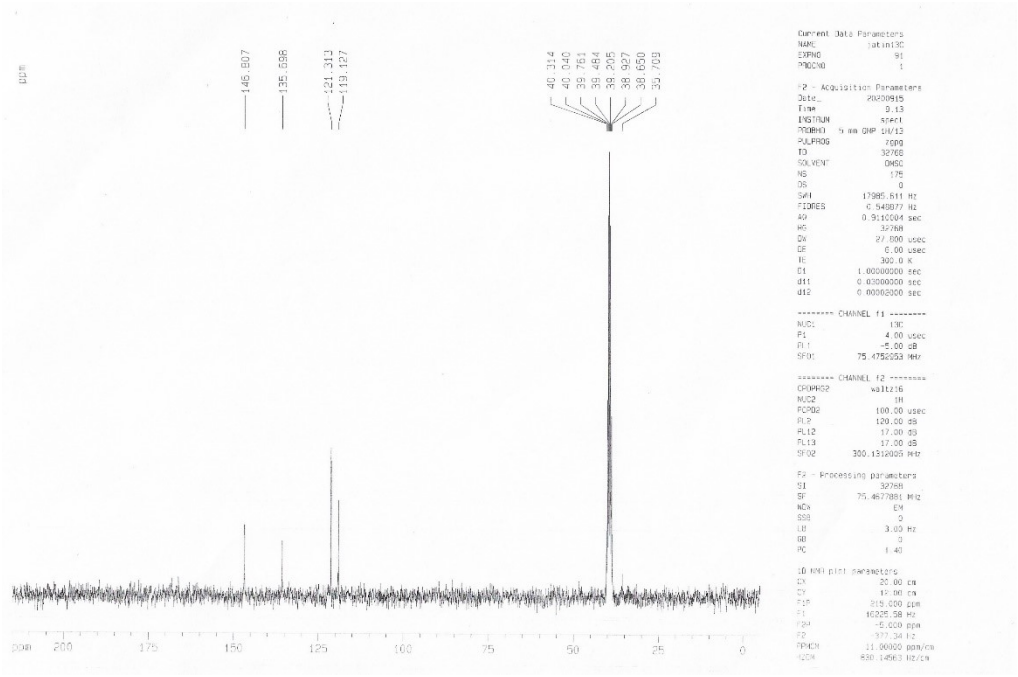

Figure S8: ^{13}C NMR of compound **5**

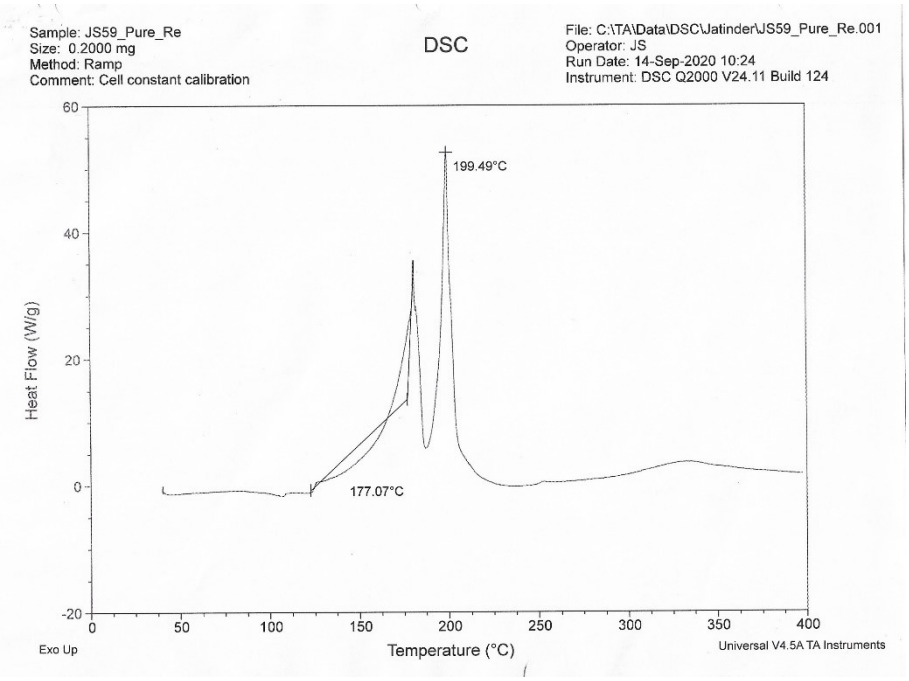

Figure S9: DSC of compound **5**

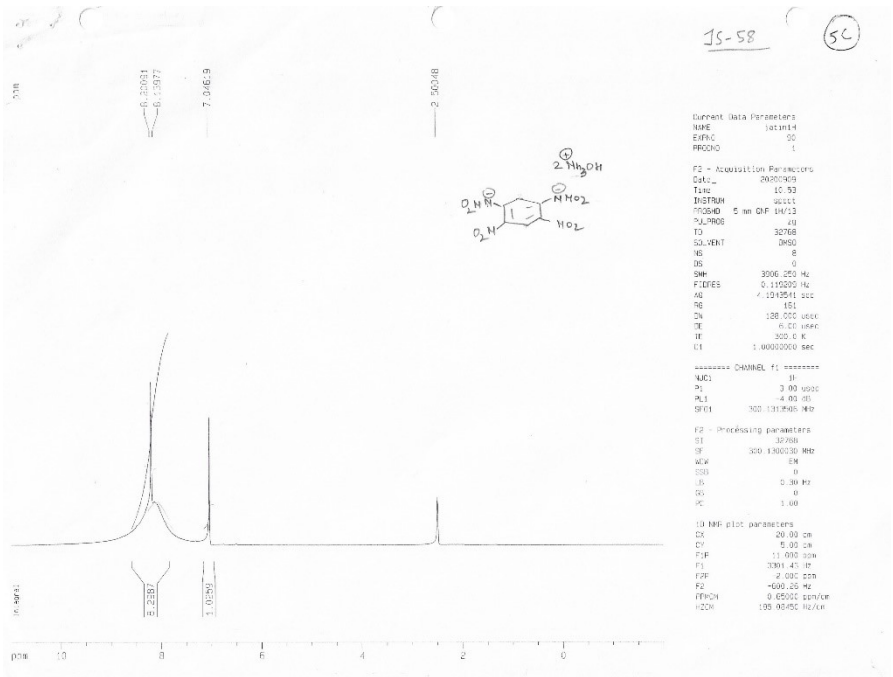

Figure S10: ^{1}H NMR of compound **6**

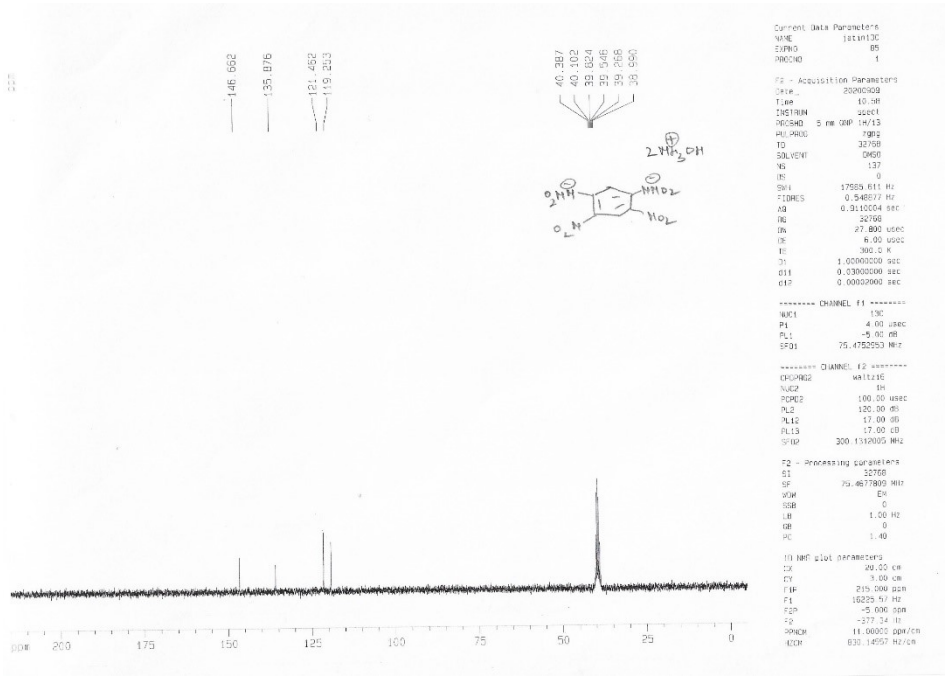

Figure S11: ^{13}C NMR of compound **6**

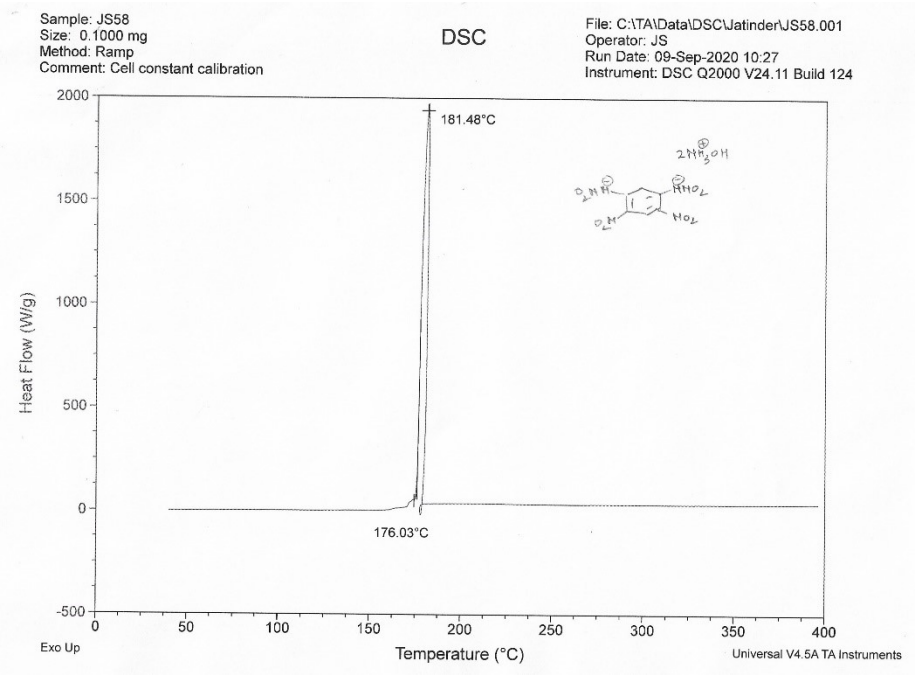

Figure S12: DSC of compound **6**

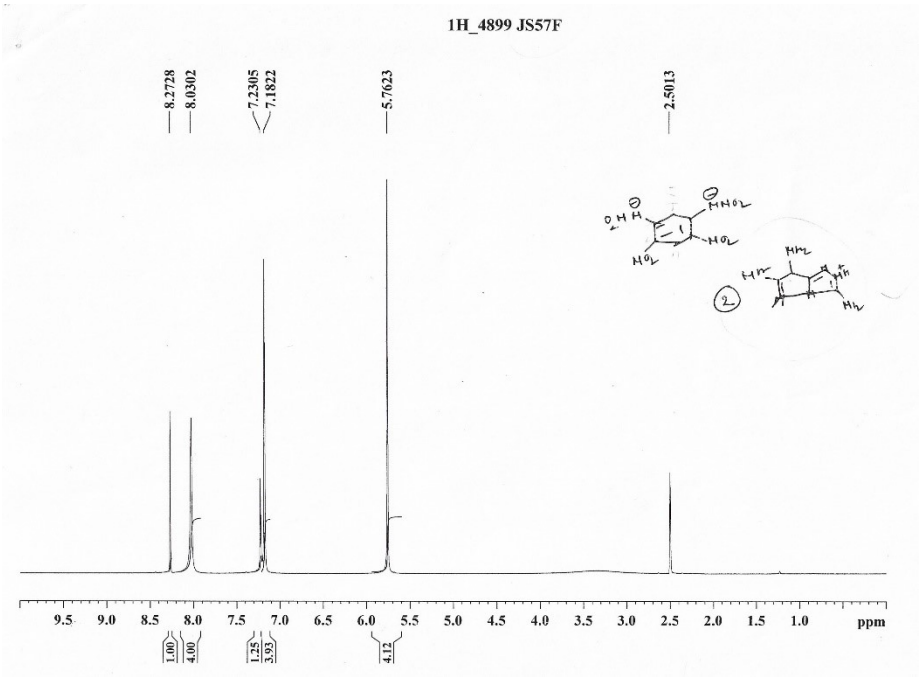

Figure S13: ^{1}H NMR of compound **7**

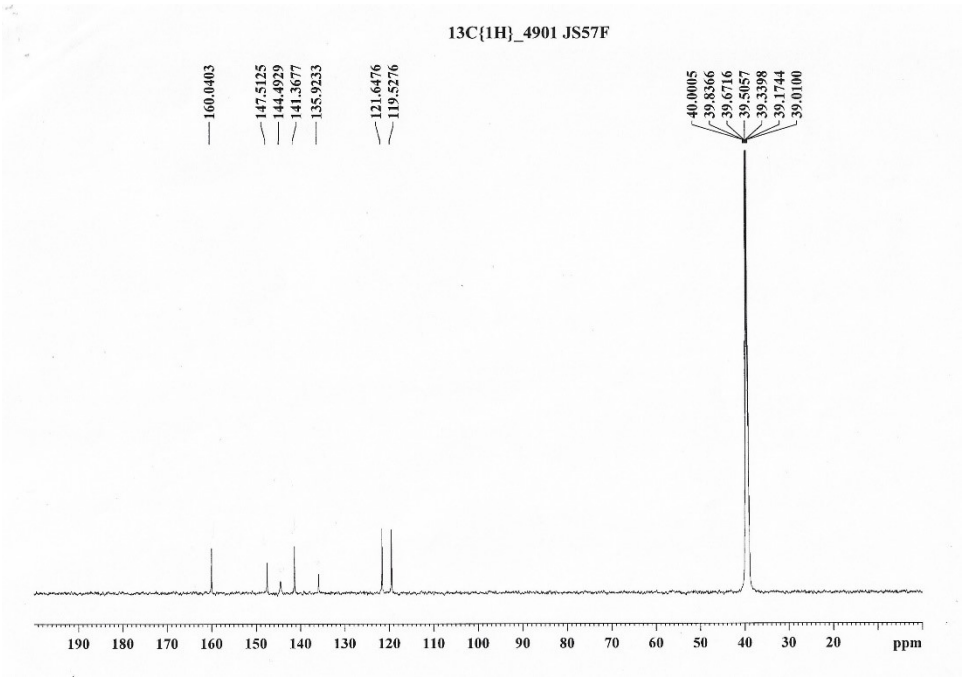

Figure S14: ^{13}C NMR of compound **7**

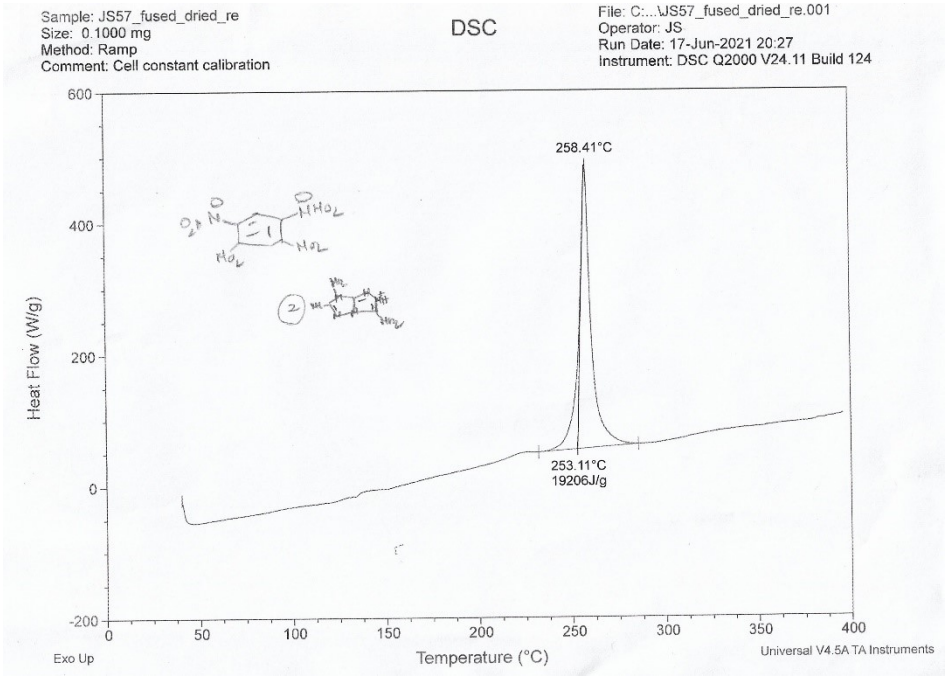

Figure S15: DSC of compound **7**

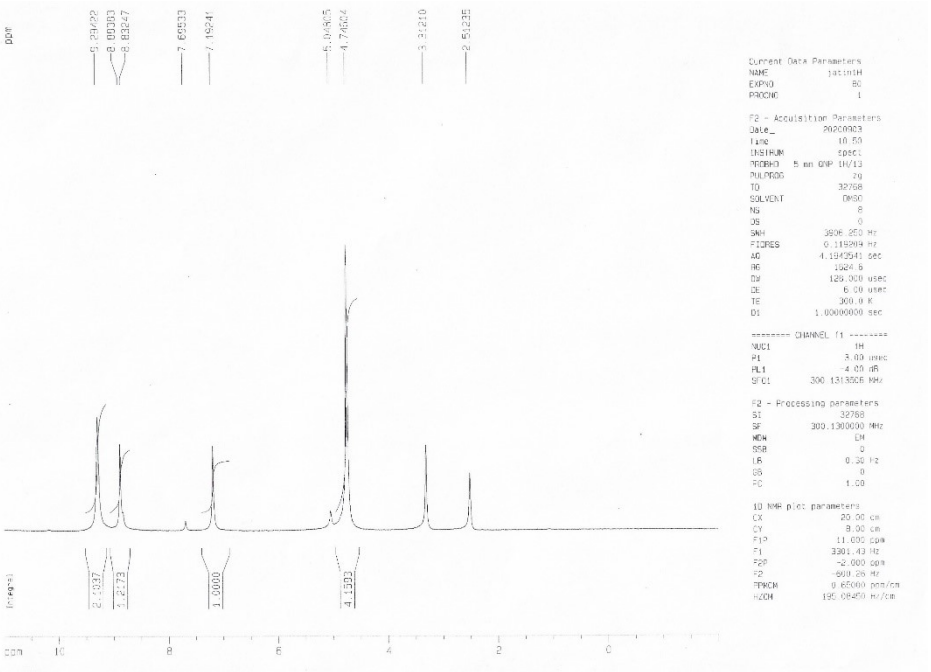

Figure S16: ^{1}H NMR of compound **8**

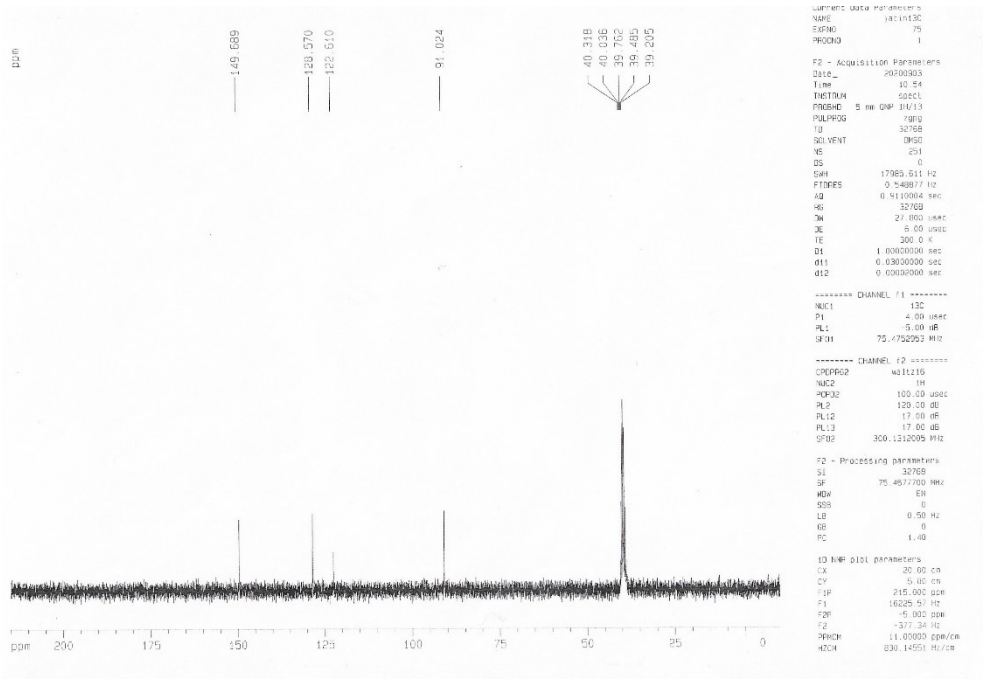

Figure S17: ^{13}C NMR of compound **8**

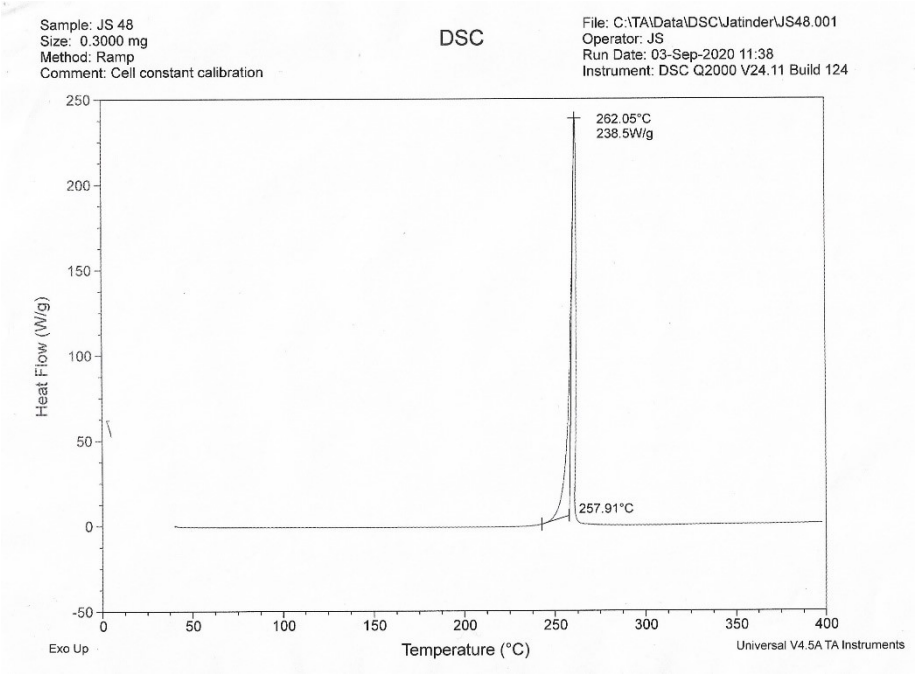

Figure S18: DSC of compound **8**

Crystal Structure Data

Table S1: Crystal data and structure refinement for compounds **3, 5**·0.5CH_3CN and **7**.

Compound	**3**	**5**·0.5CH_3CN	**7**
CCDC #	2100986	2100987	2100988
Formula	$C_6H_4N_6O_8$	$C_7H_{13.5}N_{10.5}O_8$	$C_{12}H_{16}N_{22}O_8$
$d_{calc.}$/ g cm^{-3}	1.907	1.736	1.800
μ/mm^{-1}	1.599	1.371	1.331
Formula Weight	288.15	372.78	596.47
Colour	orange	yellow	yellow
Shape	block	block	needle-shaped
Size/mm^3	0.11×0.09×0.06	0.07×0.05×0.02	0.20×0.04×0.03
T/K	100.00(10)	100.00(10)	100.0(2)
Crystal System	orthorhombic	triclinic	triclinic
Flack Parameter	0.1(3)	-	-
Hooft Parameter	0.15(12)	-	-
Space Group	$Pca2_1$	P-1	P-1
a/Å	15.9214(2)	6.7679(2)	6.74834(15)
b/Å	6.89576(10)	10.3865(4)	8.47996(19)
c/Å	9.14257(12)	11.1358(5)	20.5330(3)
α/°	90	114.135(4)	92.5744(15)
β/°	90	92.458(3)	94.2528(16)
γ/°	90	91.245(3)	109.608(2)
V/Å^3	1003.76(2)	713.04(5)	1100.78(4)
Z	4	2	2
Z'	1	1	1
Wavelength/Å	1.54184	1.54184	1.54184
Radiation type	Cu K□	Cu K□	Cu K_a
Θ_{min}/°	5.557	4.670	4.330
Θ_{max}/°	77.084	77.362	80.222
Measured Refl's.	10587	7238	14565
Indep't Refl's	2013	2825	4679
Refl's I≥2 σ(I)	1942	2424	4085
R_{int}	0.0463	0.0327	0.0411
Parameters	190	268	435
Restraints	1	1	0
Largest Peak	0.212	0.401	0.279
Deepest Hole	-0.157	-0.710	-0.283
GooF	1.031	1.091	1.058
wR_2 (all data)	0.0779	0.1442	0.1013
wR_2	0.0767	0.1386	0.0975
R_1 (all data)	0.0307	0.0606	0.0431
R_1	0.0294	0.0519	0.0377

Table S2: Bond Lengths in Å for **3**.

Atom	Atom	Length/Å
O1	N2	1.227(3)
O2	N2	1.216(3)
O3	N4	1.216(3)
O4	N4	1.233(3)
O5	N5	1.235(3)
O6	N5	1.223(3)
O7	N6	1.215(3)
O8	N6	1.232(3)
N1	N2	1.371(3)
N1	C1	1.392(3)
N3	N4	1.368(3)
N3	C3	1.394(3)
N5	C4	1.460(3)
N6	C6	1.462(3)
C1	C2	1.393(4)
C1	C6	1.407(3)
C2	C3	1.392(4)
C3	C4	1.406(3)
C4	C5	1.376(4)
C5	C6	1.381(4)

Table S3: Bond Angles in ° for **3**.

Atom	Atom	Atom	Angle/°
N2	N1	C1	125.6(2)
O1	N2	N1	113.2(2)
O2	N2	O1	126.4(2)
O2	N2	N1	120.4(2)
N4	N3	C3	127.6(2)
O3	N4	O4	125.4(2)
O3	N4	N3	121.0(2)
O4	N4	N3	113.6(2)
O5	N5	C4	119.1(2)
O6	N5	O5	122.9(2)
O6	N5	C4	118.0(2)
O7	N6	O8	123.1(2)
O7	N6	C6	117.5(2)
O8	N6	C6	119.4(2)
N1	C1	C2	122.4(2)
N1	C1	C6	118.8(2)
C2	C1	C6	118.7(2)
C3	C2	C1	121.5(2)
N3	C3	C4	119.0(2)
C2	C3	N3	122.7(2)
C2	C3	C4	118.2(2)
C3	C4	N5	123.8(2)
C5	C4	N5	115.4(2)
C5	C4	C3	120.9(2)
C4	C5	C6	120.4(2)
C1	C6	N6	123.7(2)
C5	C6	N6	116.0(2)
C5	C6	C1	120.2(2)

Table S4: Torsion Angles in ° for **3**.

Atom	Atom	Atom	Atom	Angle/°
O5	N5	C4	C3	-15.3(4)
O5	N5	C4	C5	163.9(2)
O6	N5	C4	C3	165.9(2)
O6	N5	C4	C5	-14.9(3)
O7	N6	C6	C1	165.1(3)
O7	N6	C6	C5	-13.9(4)
O8	N6	C6	C1	-14.8(4)
O8	N6	C6	C5	166.2(2)
N1	C1	C2	C3	177.2(2)
N1	C1	C6	N6	6.4(4)
N1	C1	C6	C5	-174.7(2)
N2	N1	C1	C2	28.7(4)
N2	N1	C1	C6	-153.6(3)
N3	C3	C4	N5	1.3(4)
N3	C3	C4	C5	-177.9(2)
N4	N3	C3	C2	8.7(4)
N4	N3	C3	C4	-170.7(2)
N5	C4	C5	C6	-179.4(2)
C1	N1	N2	O1	165.9(3)
C1	N1	N2	O2	-15.3(4)
C1	C2	C3	N3	178.3(2)
C1	C2	C3	C4	-2.3(4)
C2	C1	C6	N6	-175.7(2)
C2	C1	C6	C5	3.2(4)
C2	C3	C4	N5	-178.1(2)
C2	C3	C4	C5	2.7(4)
C3	N3	N4	O3	3.5(4)
C3	N3	N4	O4	-176.7(2)
C3	C4	C5	C6	-0.2(4)
C4	C5	C6	N6	176.2(2)
C4	C5	C6	C1	-2.9(4)
C6	C1	C2	C3	-0.6(4)

Table S5: Bond Lengths in Å for **5**·0.5CH_3CN.

Atom	Atom	Length/Å
O1	N2	1.265(3)
O2	N2	1.274(3)
O3	N4	1.273(3)
O4	N4	1.261(3)
O5	N5	1.232(3)
O6	N5	1.226(3)
O7	N6	1.224(3)
O8	N6	1.232(3)
N1	N2	1.301(3)
N1	C1	1.404(3)
N3	N4	1.301(3)
N3	C3	1.404(3)
N5	C4	1.460(3)
N6	C6	1.463(3)
C1	C2	1.399(3)
C1	C6	1.413(3)
C2	C3	1.402(3)
C3	C4	1.410(3)
C4	C5	1.375(3)
C5	C6	1.380(3)
N7	N8	1.449(3)
N9	N10	1.439(3)

Table S6: Bond Angles in ° for **5**·0.5CH_3CN.

Atom	Atom	Atom	Angle/°
N2	N1	C1	118.03(2)
O1	N2	O2	118.57(2)
O1	N2	N1	125.27(2)
O2	N2	N1	116.09(2)
N4	N3	C3	118.45(2)
O3	N4	N3	115.93(2)
O4	N4	O3	119.06(2)
O4	N4	N3	124.9(2)
O5	N5	C4	116.81(2)
O6	N5	O5	123.5(2)
O6	N5	C4	119.6(2)
O7	N6	O8	123.6(2)
O7	N6	C6	119.4(2)
O8	N6	C6	117.00(2)
N1	C1	C6	116.9(2)
C2	C1	N1	125.3(2)
C2	C1	C6	117.1(2)
C1	C2	C3	122.6(2)
N3	C3	C4	117.1(2)
C2	C3	N3	125.2(2)
C2	C3	C4	117.0(2)
C3	C4	N5	122.2(2)
C5	C4	N5	115.6(2)
C5	C4	C3	122.2(2)
C4	C5	C6	119.2(2)
C1	C6	N6	122.9(2)
C5	C6	N6	115.3(2)
C5	C6	C1	121.8(2)
N1S	C2S	C1S	170.6(1)

Table S7: Torsion Angles in ° for **5**·0.5CH_3CN.

Atom	Atom	Atom	Atom	Angle/°
O5	N5	C4	C3	149.6(2)
O5	N5	C4	C5	-30.0(3)
O6	N5	C4	C3	-31.6(3)
O6	N5	C4	C5	148.8(2)
O7	N6	C6	C1	32.7(3)
O7	N6	C6	C5	-147.9(2)
O8	N6	C6	C1	-148.9(2)
O8	N6	C6	C5	30.4(3)
N1	C1	C2	C3	170.8(2)
N1	C1	C6	N6	8.0(3)
N1	C1	C6	C5	-171.3(2)
N2	N1	C1	C2	35.1(3)
N2	N1	C1	C6	-154.6(2)
N3	C3	C4	N5	-8.8(3)
N3	C3	C4	C5	170.7(2)
N4	N3	C3	C2	-36.7(3)
N4	N3	C3	C4	153.4(2)
N5	C4	C5	C6	179.91(2)
C1	N1	N2	O1	2.9(3)
C1	N1	N2	O2	179.86(2)
C1	C2	C3	N3	-170.4(2)
C1	C2	C3	C4	-0.6(3)
C2	C1	C6	N6	179.08(2)
C2	C1	C6	C5	-0.2(3)
C2	C3	C4	C5	0.0(3)
C3	N3	N4	O3	178.63(2)
C3	N3	N4	O4	-4.4(3)
C3	C4	C5	C6	0.4(3)
C4	C5	C6	C1	-0.3(3)
C6	C1	C2	C3	0.6(3)

Table S8: Bond Lengths in Å for **7**.

Atom	Atom	Length/Å
O1	N2	1.2736(2)
O2	N2	1.2830(2)
O3	N4	1.2569(2)
O4	N4	1.2716(2)
O5	N5	1.2271(2)
O6	N5	1.2312(2)
O7	N6	1.2324(2)
O8	N6	1.2254(2)
N1	N2	1.2867(2)
N1	C1	1.4039(2)
N3	N4	1.3080(2)
N3	C3	1.3939(2)
N5	C4	1.4601(2)
N6	C6	1.4583(2)
C1	C2	1.393(2)
C1	C6	1.405(2)
C2	C3	1.398(2)
C3	C4	1.409(2)
C4	C5	1.383(2)
C5	C6	1.381(2)
N7	N8	1.3966(2)
N7	C7	1.3947(2)
N7	C8	1.3575(2)
N9	N10	1.4081(2)
N9	C8	1.304(2)
N10	C9	1.3414(2)
N11	N12	1.4016(2)
N11	C8	1.3547(2)
N11	C9	1.3500(2)
N12	C7	1.3270(2)
N13	C7	1.3369(2)
N14	C9	1.325(2)
N15	N16	1.3956(2)
N15	C10	1.3904(2)
N15	C11	1.3639(2)
N17	N18	1.4048(2)
N17	C11	1.3043(2)
N18	C12	1.338(2)
N19	N20	1.4010(2)
N19	C11	1.3533(2)
N19	C12	1.3499(2)
N20	C10	1.3278(2)
N21	C12	1.323(2)
N22	C10	1.3332(2)

Table S9: Bond Angles in ° for **7**.

Atom	Atom	Atom	Angle/°
N2	N1	C1	115.76(12)
O1	N2	O2	117.90(11)
O1	N2	N1	117.68(12)
O2	N2	N1	124.38(12)
N4	N3	C3	117.86(12)
O3	N4	O4	120.75(12)
O3	N4	N3	124.59(12)
O4	N4	N3	114.64(12)
O5	N5	O6	123.67(13)
O5	N5	C4	117.91(12)
O6	N5	C4	118.29(12)
O7	N6	C6	117.25(12)
O8	N6	O7	124.21(12)
O8	N6	C6	118.49(12)
N1	C1	C6	126.84(13)
C2	C1	N1	116.08(13)
C2	C1	C6	116.91(13)
C1	C2	C3	123.11(13)
N3	C3	C2	114.40(13)
N3	C3	C4	128.49(13)
C2	C3	C4	116.91(13)
C3	C4	N5	122.18(13)
C5	C4	N5	115.84(13)
C5	C4	C3	121.53(13)
C6	C5	C4	119.22(13)
C1	C6	N6	122.15(13)
C5	C6	N6	115.96(12)
C5	C6	C1	121.89(13)
C7	N7	N8	129.71(13)
C8	N7	N8	123.72(12)
C8	N7	C7	106.46(12)
C8	N9	N10	100.64(11)
C9	N10	N9	113.17(12)
C8	N11	N12	113.93(12)
C9	N11	N12	138.65(12)
C9	N11	C8	107.22(12)
C7	N12	N11	100.97(11)
N12	C7	N7	113.54(13)
N12	C7	N13	125.35(13)
N13	C7	N7	121.09(13)
N9	C8	N7	140.52(14)
N9	C8	N11	114.39(13)
N11	C8	N7	105.08(12)
N10	C9	N11	104.56(12)
N14	C9	N10	129.90(14)
N14	C9	N11	125.53(14)
C10	N15	N16	123.05(12)
C11	N15	N16	130.87(12)
C11	N15	C10	105.99(12)
C11	N17	N18	100.81(11)

Atom	Atom	Atom	Angle/°
C12	N18	N17	113.26(12)
C11	N19	N20	114.01(12)
C12	N19	N20	138.55(12)
C12	N19	C11	107.38(12)
C10	N20	N19	100.72(11)
N20	C10	N15	114.06(12)
N20	C10	N22	125.58(13)
N22	C10	N15	120.30(13)
N17	C11	N15	140.75(14)
N17	C11	N19	114.08(13)
N19	C11	N15	105.16(12)
N18	C12	N19	104.47(13)
N21	C12	N18	128.45(14)
N21	C12	N19	127.07(14)

Table S10: Torsion Angles in ° 7.

Atom	Atom	Atom	Atom	Angle/°
O5	N5	C4	C3	30.06(19)
O5	N5	C4	C5	-142.37(13)
O6	N5	C4	C3	-153.82(13)
O6	N5	C4	C5	33.74(18)
O7	N6	C6	C1	-143.91(13)
O7	N6	C6	C5	36.26(18)
O8	N6	C6	C1	38.47(19)
O8	N6	C6	C5	-141.36(13)
N1	C1	C2	C3	-179.45(13)
N1	C1	C6	N6	1.4(2)
N1	C1	C6	C5	-178.77(13)
N2	N1	C1	C2	-137.06(13)
N2	N1	C1	C6	47.9(2)
N3	C3	C4	N5	8.5(2)
N3	C3	C4	C5	-179.50(13)
N4	N3	C3	C2	-143.07(14)
N4	N3	C3	C4	42.3(2)
N5	C4	C5	C6	168.63(12)
C1	N1	N2	O1	-174.99(12)
C1	N1	N2	O2	7.4(2)
C1	C2	C3	N3	-177.27(13)
C1	C2	C3	C4	-2.0(2)
C2	C1	C6	N6	-173.61(12)
C2	C1	C6	C5	6.2(2)
C2	C3	C4	N5	-166.02(13)
C2	C3	C4	C5	6.0(2)
C3	N3	N4	O3	4.2(2)
C3	N3	N4	O4	-177.54(12)
C3	C4	C5	C6	-3.9(2)
C4	C5	C6	N6	177.35(12)
C4	C5	C6	C1	-2.5(2)
C6	C1	C2	C3	-3.9(2)
N8	N7	C7	N12	174.85(14)
N8	N7	C7	N13	-7.1(2)
N8	N7	C8	N9	6.6(3)
N8	N7	C8	N11	-174.87(13)
N9	N10	C9	N11	0.71(16)
N9	N10	C9	N14	179.36(15)
N10	N9	C8	N7	177.32(19)
N10	N9	C8	N11	-1.13(16)
N11	N12	C7	N7	0.45(15)
N11	N12	C7	N13	-177.50(14)
N12	N11	C8	N7	-1.48(16)
N12	N11	C8	N9	177.49(12)
N12	N11	C9	N10	-175.58(16)
N12	N11	C9	N14	5.7(3)
C7	N7	C8	N9	-176.91(19)
C7	N7	C8	N11	1.63(15)
C8	N7	C7	N12	-1.37(17)

Atom	Atom	Atom	Atom	Angle/°
C8	N7	C7	N13	176.68(13)
C8	N9	N10	C9	0.23(16)
C8	N11	N12	C7	0.65(15)
C8	N11	C9	N10	-1.33(16)
C8	N11	C9	N14	179.93(15)
C9	N11	N12	C7	174.64(17)
C9	N11	C8	N7	-177.33(12)
C9	N11	C8	N9	1.65(17)
N16	N15	C10	N20	-179.05(13)
N16	N15	C10	N22	-1.8(2)
N16	N15	C11	N17	-0.2(3)
N16	N15	C11	N19	178.80(14)
N17	N18	C12	N19	0.17(16)
N17	N18	C12	N21	179.26(15)
N18	N17	C11	N15	179.23(19)
N18	N17	C11	N19	0.25(16)
N19	N20	C10	N15	1.02(15)
N19	N20	C10	N22	-176.08(14)
N20	N19	C11	N15	-1.80(16)
N20	N19	C11	N17	177.53(12)
N20	N19	C12	N18	-176.83(16)
N20	N19	C12	N21	4.1(3)
C10	N15	C11	N17	-176.79(19)
C10	N15	C11	N19	2.24(15)
C11	N15	C10	N20	-2.15(17)
C11	N15	C10	N22	175.11(13)
C11	N17	N18	C12	-0.25(16)
C11	N19	N20	C10	0.51(15)
C11	N19	C12	N18	-0.01(16)
C11	N19	C12	N21	-179.12(15)
C12	N19	N20	C10	177.19(17)
C12	N19	C11	N15	-179.50(12)
C12	N19	C11	N17	-0.16(18)