Supporting Information

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Experimental Section

Caution: Proper safety precautions should be taken when handling these compounds. Laboratories and personnel should be properly grounded, and safety equipment such as Kevlar gloves, leather coats, faceshields, and ear plugs are recommended

General methods: All chemical reagents and solvents (analytical grade) were used as supplied unless otherwise stated. ^{1}H and ^{13}C NMR spectra were measured with a Bruker Avance III 300 MHz Digital NMR Spectrometer operating at 300 MHz, 75 MHz or 500M, 100Hz). All chemical shifts are quoted in ppm relative to TMS (^{1}H, ^{13}C). The decomposition point was recorded on a DSC823e at a heating rate of $5^{o}C \cdot min^{-1}$ in closed Al containers with a nitrogen flow of 30 mL·min-1. Sensitivity data were determined using a BAM drop- hammer and a BAM friction tester. The electrostatic sensitivity test was carried out using an Electric Spark Tester ESD JGY-50 III.

The DSC curves for compounds **3a**-**5**

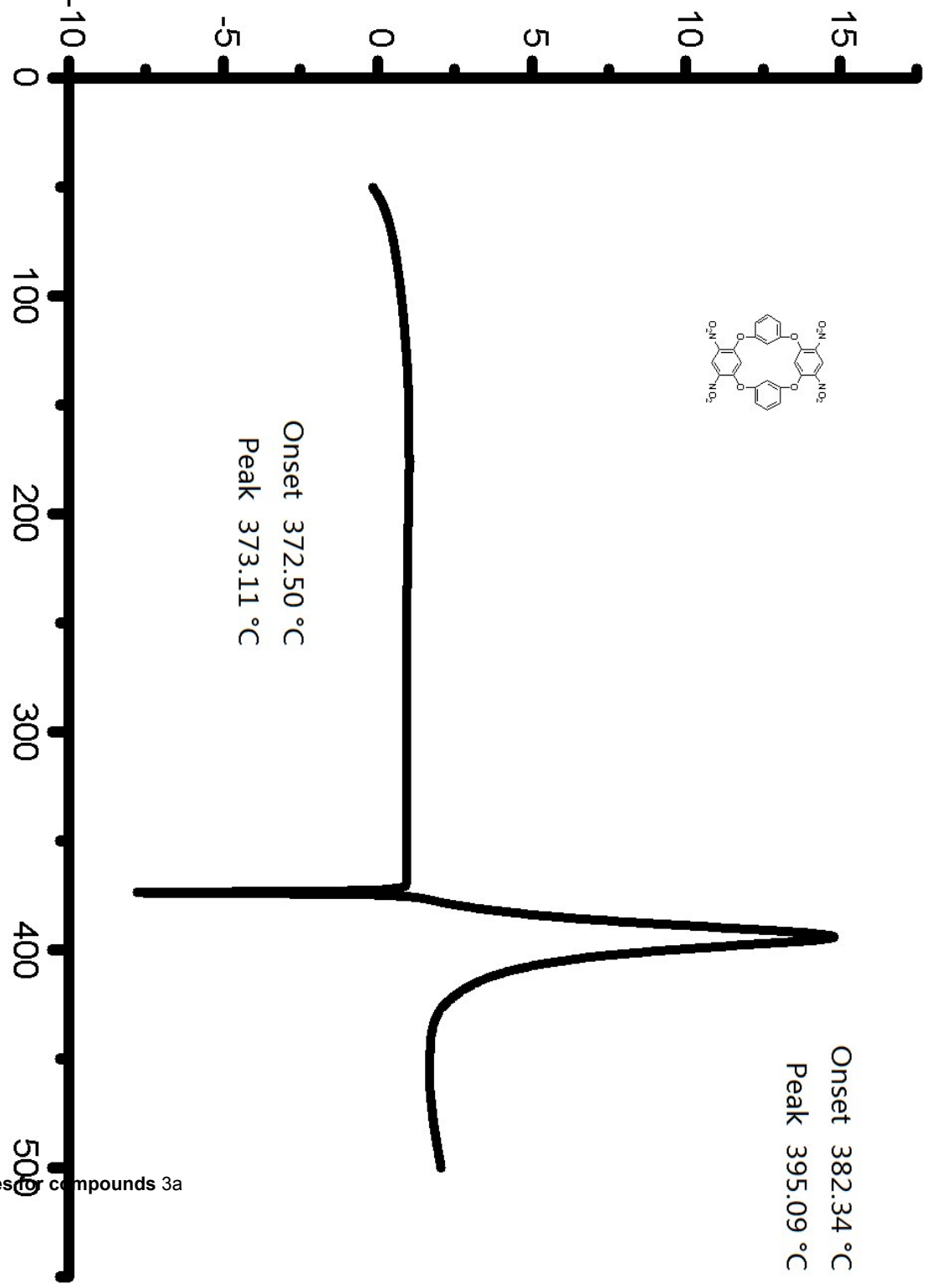


Figure 1 The DSC curves for compounds 3a

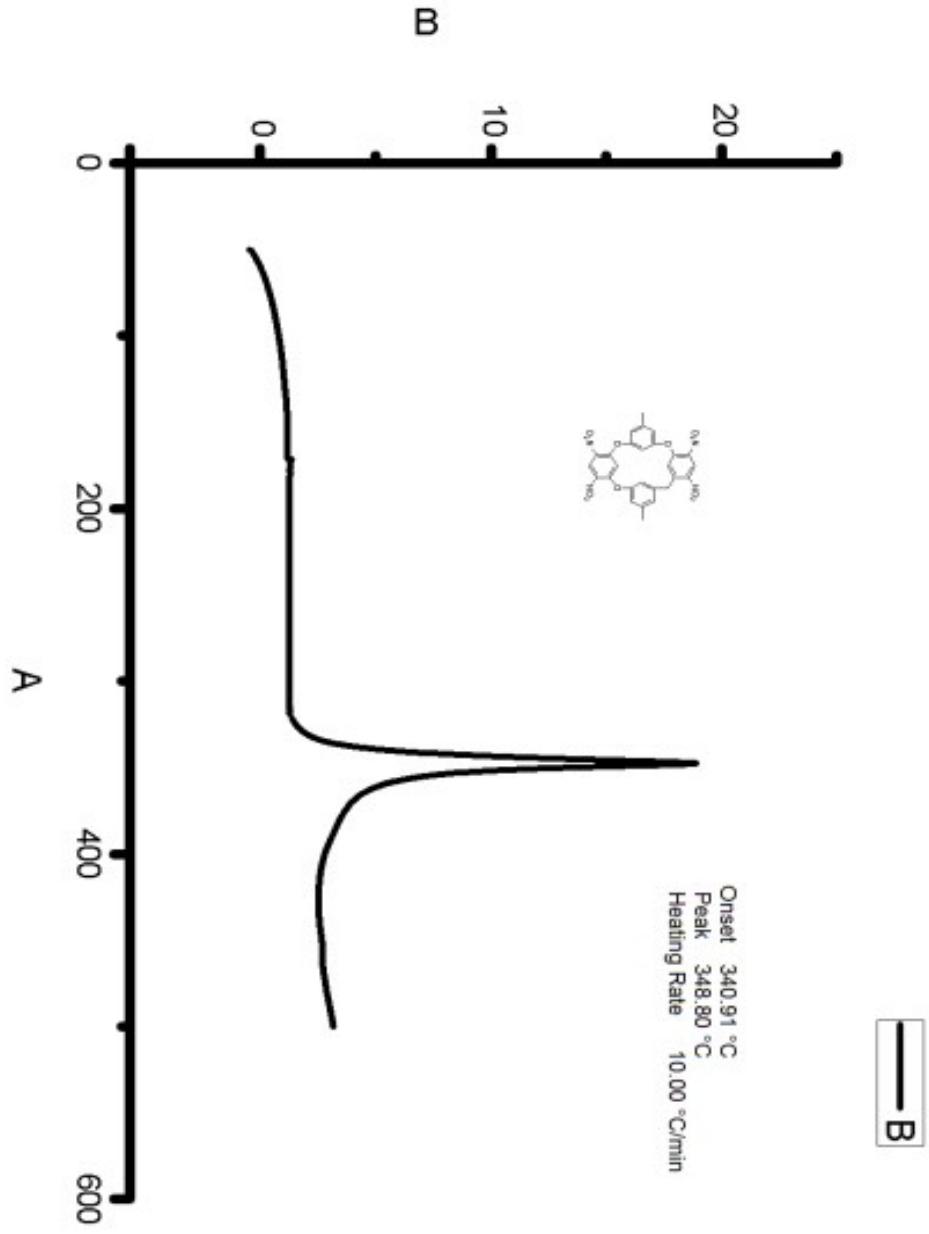


Figure 2 The DSC curves for compound 3b

Figure 3 The DSC curves for compound 3c

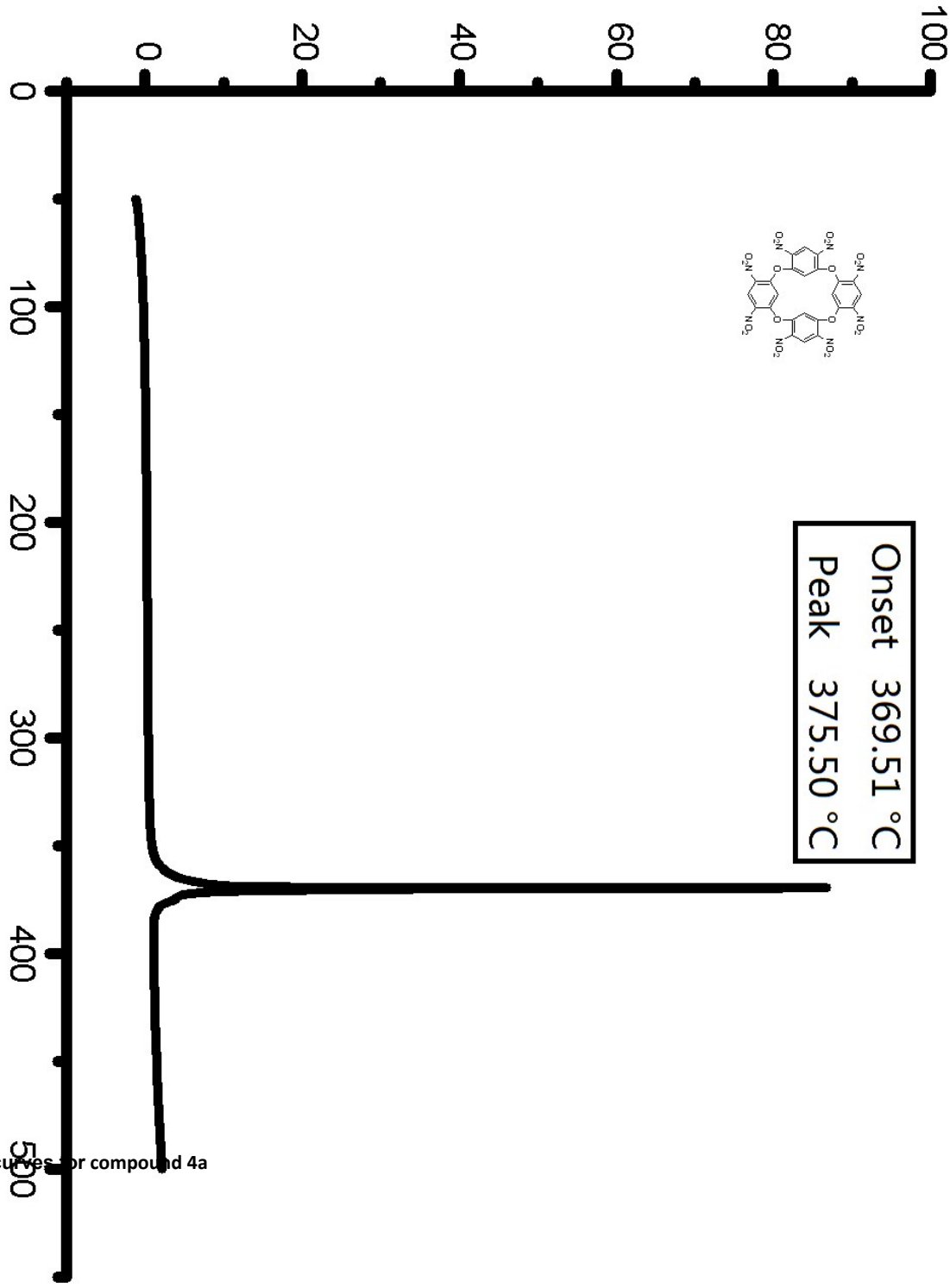


Figure 4 The DSC curves for compound 4a

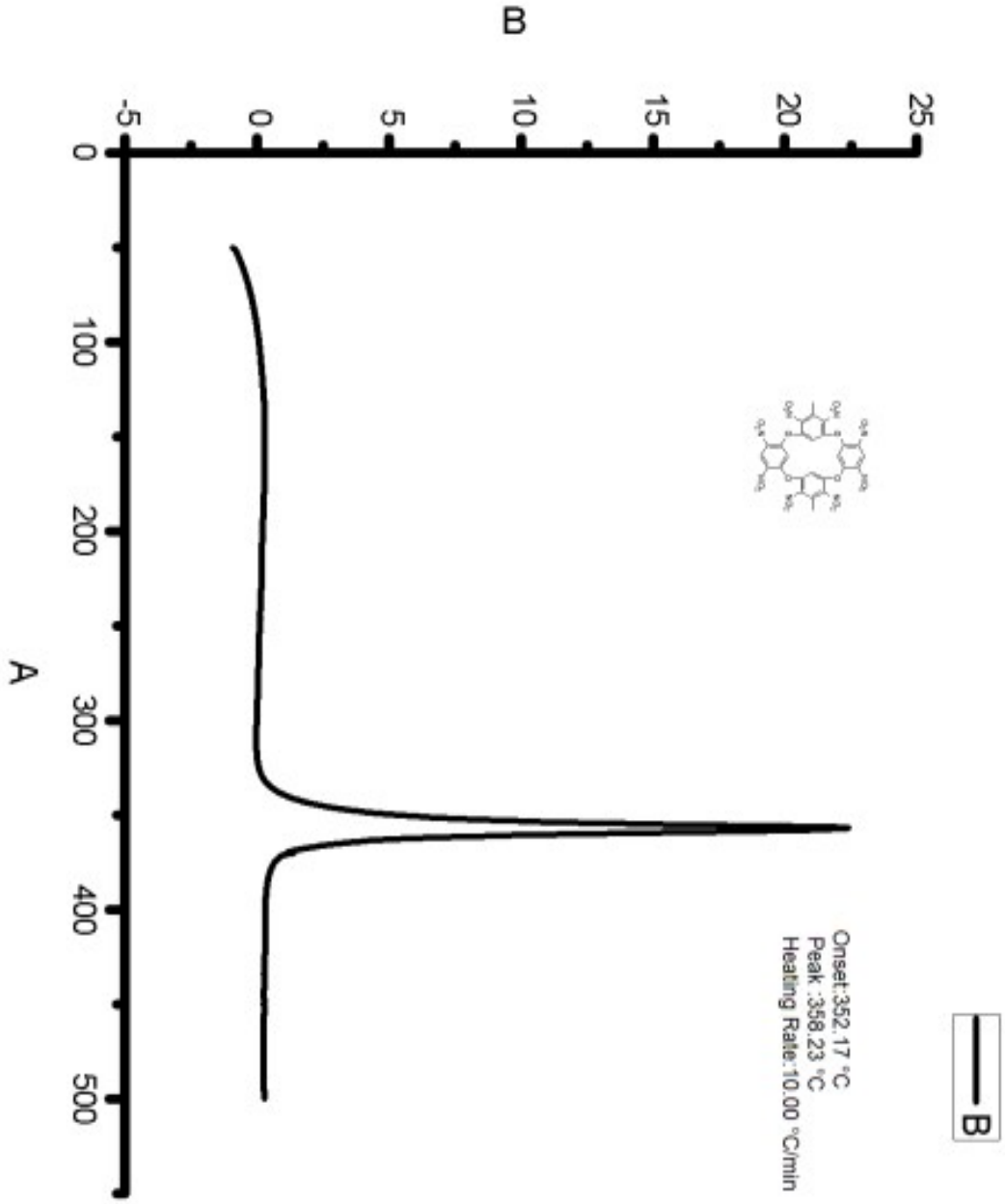


Figure 5 The DSC curves for compound 4b

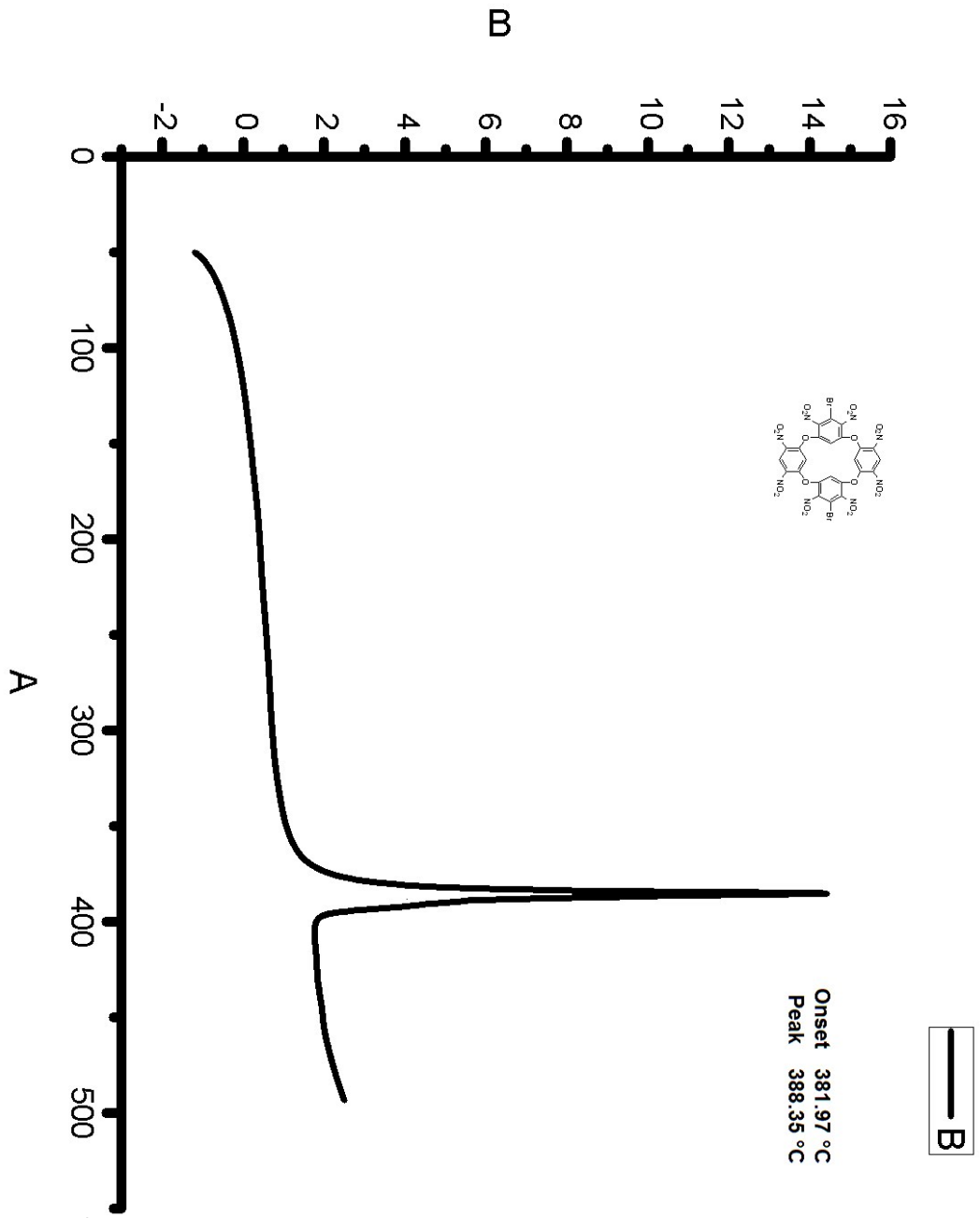


Figure 6 The DSC curves for compound 4c

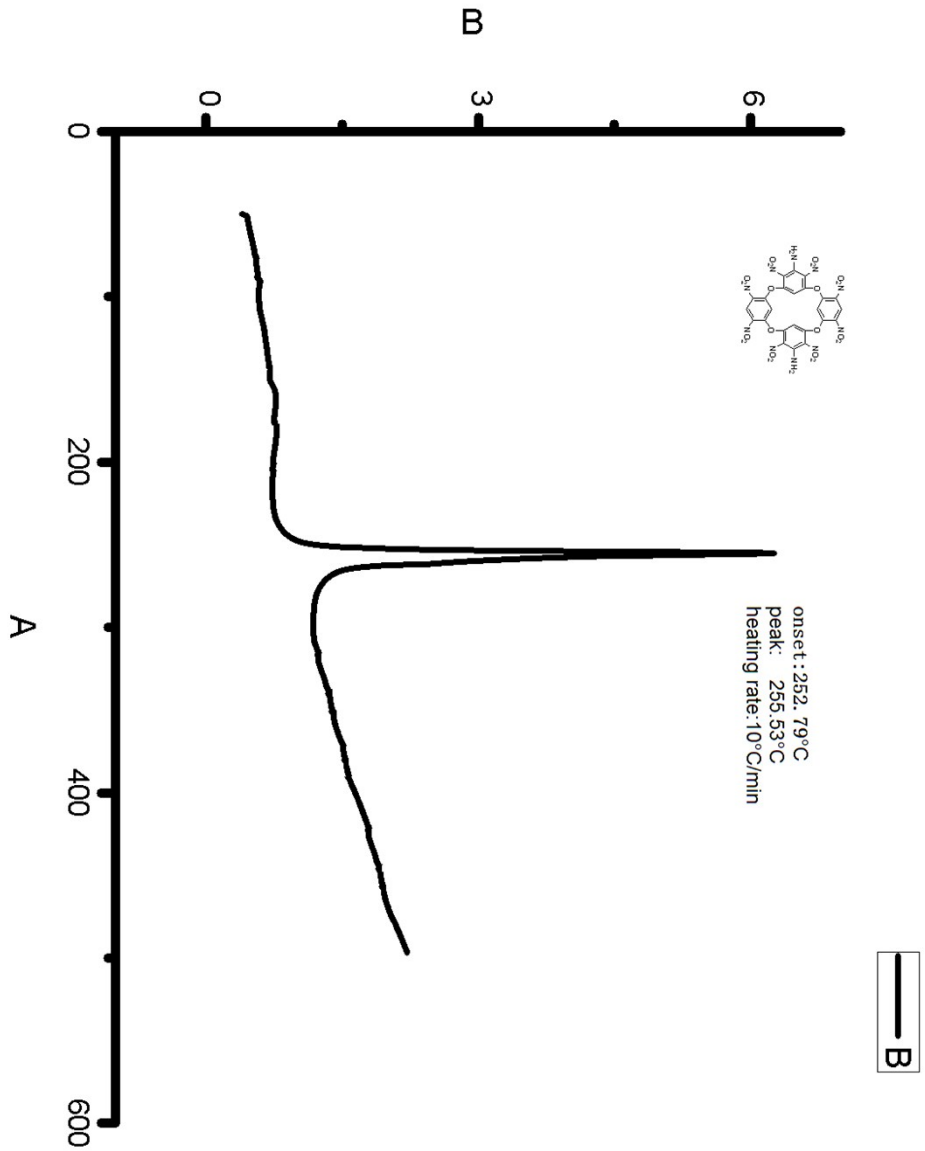


Figure 7：The DSC curves for compound 5

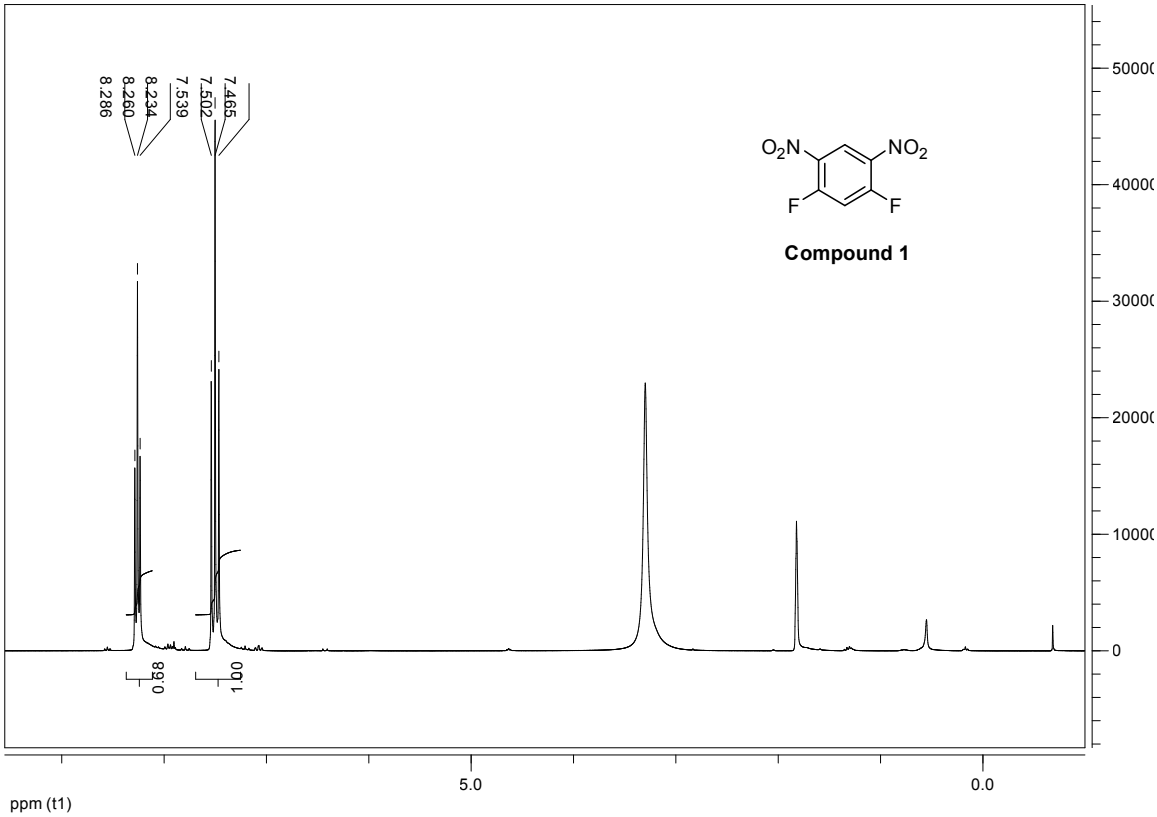


Figure 8 ^{1}H NMR spectrum of 1 (DMSO).

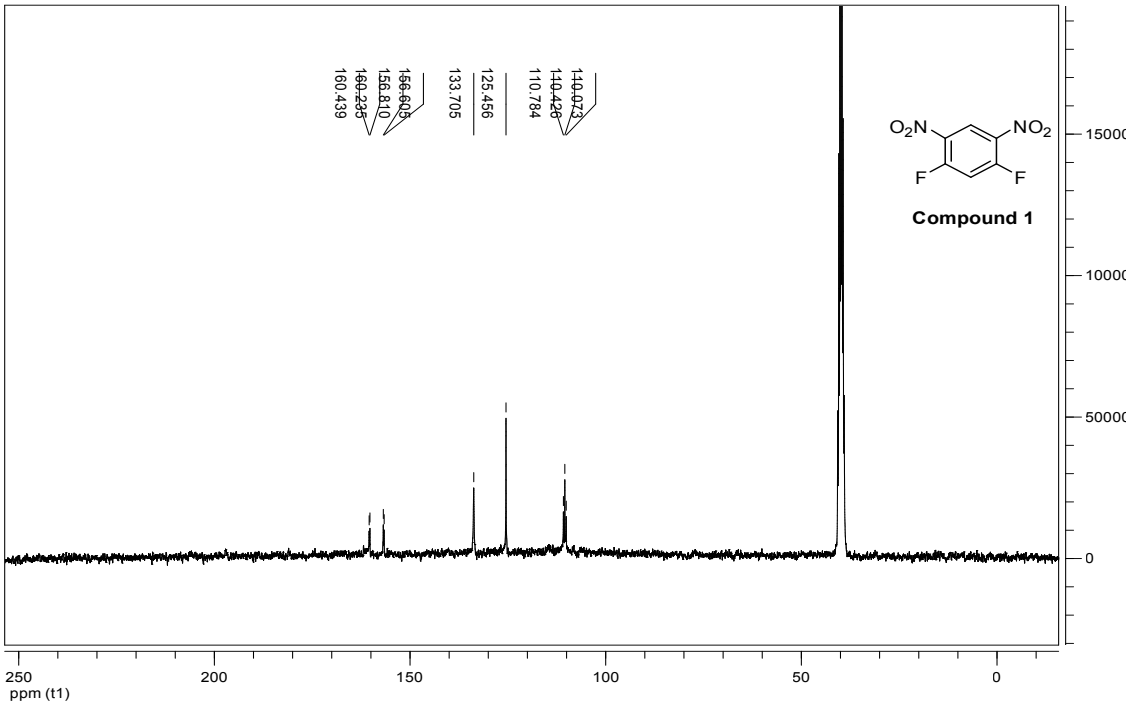


Figure 9 ^{13}C NMR spectrum of 1 (DMSO).

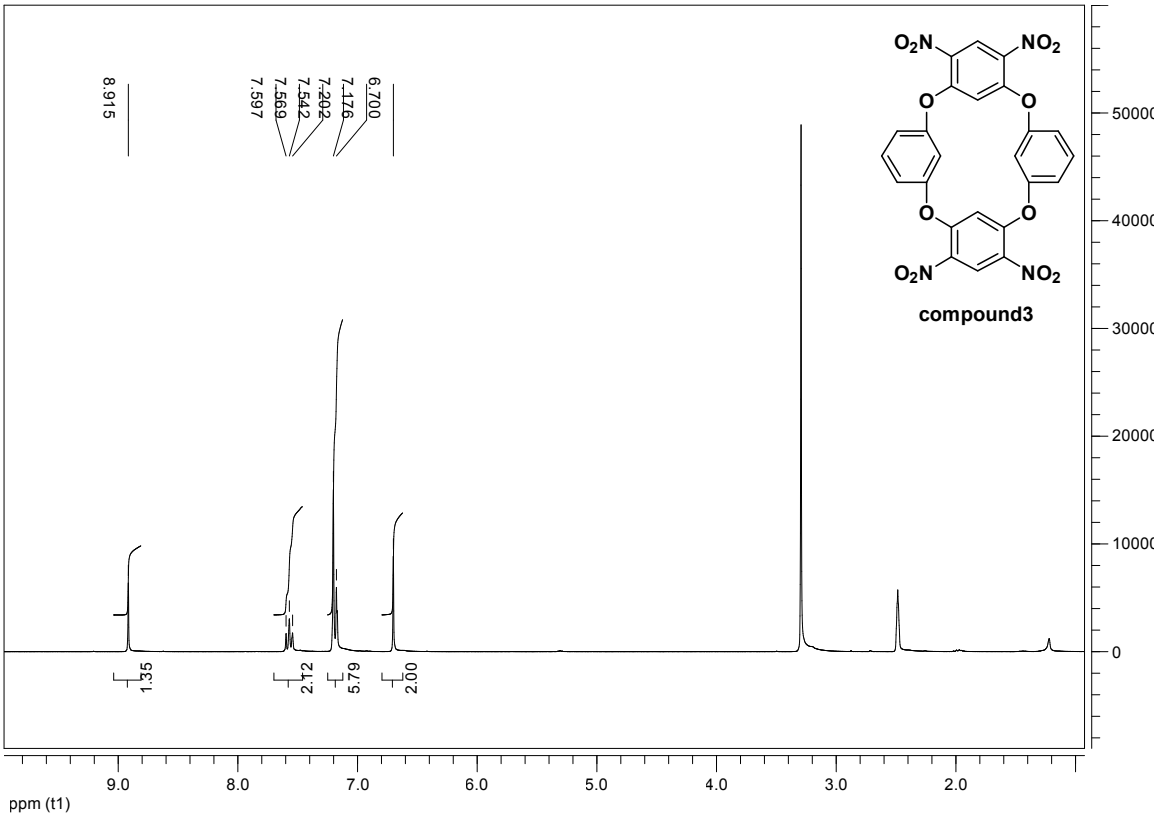


Figure 10 ^{1}H NMR spectrum of 3a (DMSO).

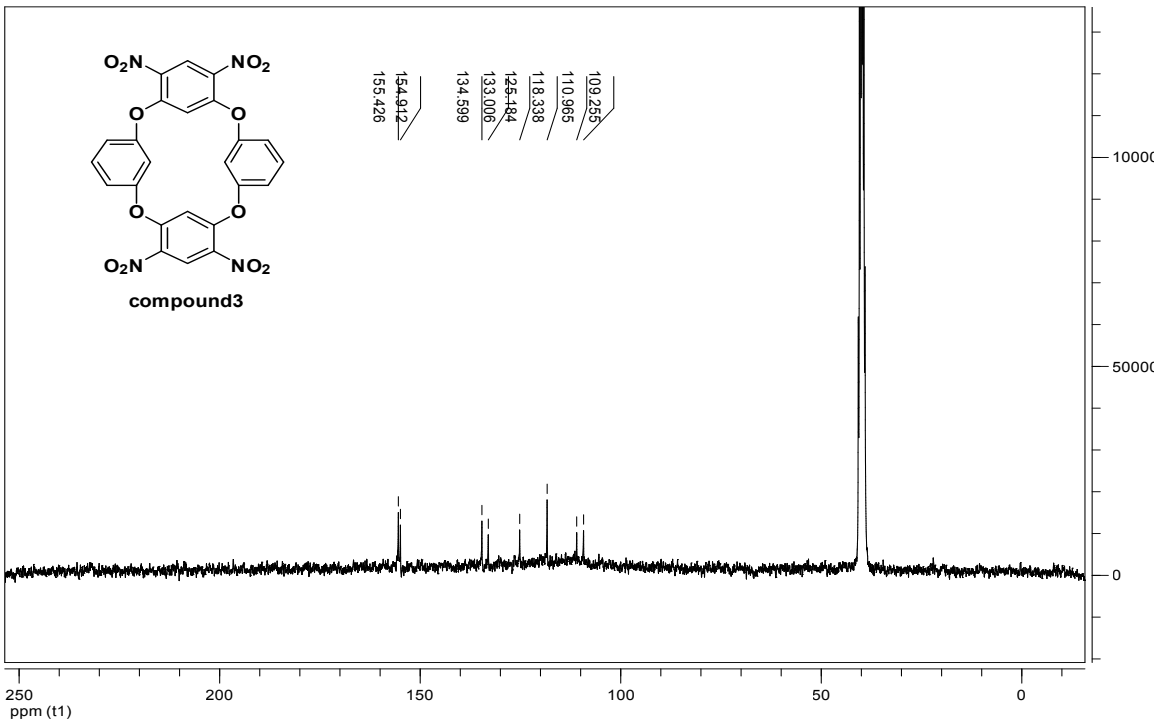


Figure 11 ^{13}C NMR spectrum of 3a (DMSO).

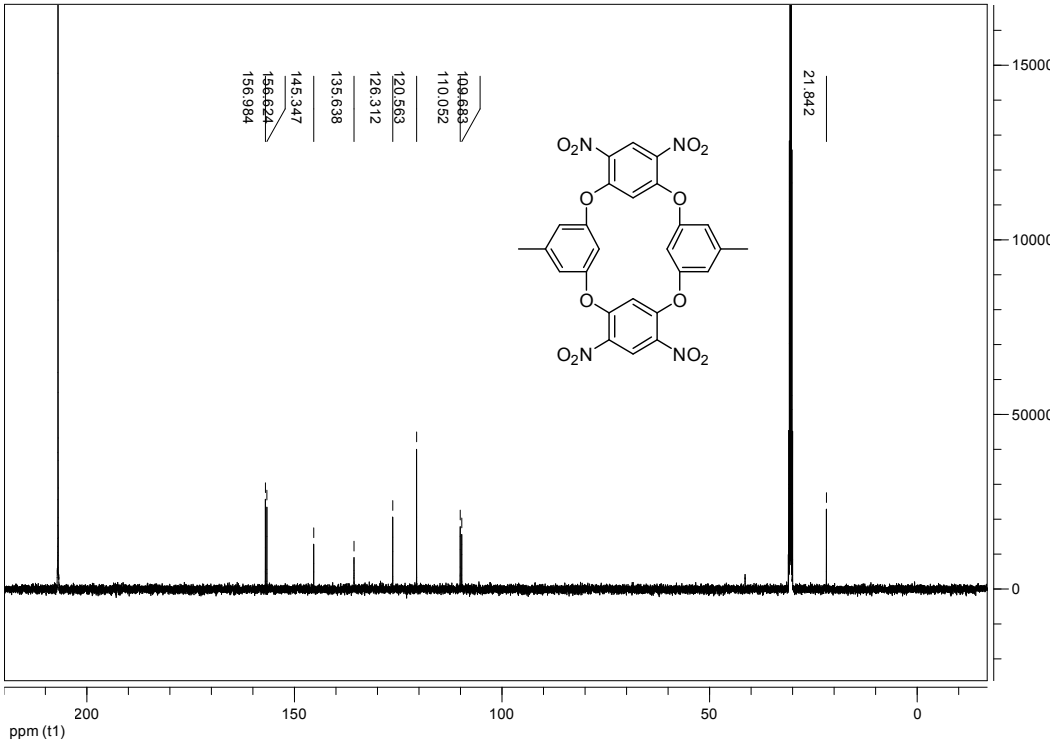


Figure 12 **^{13}C NMR spectrum of 3b (DMSO)**

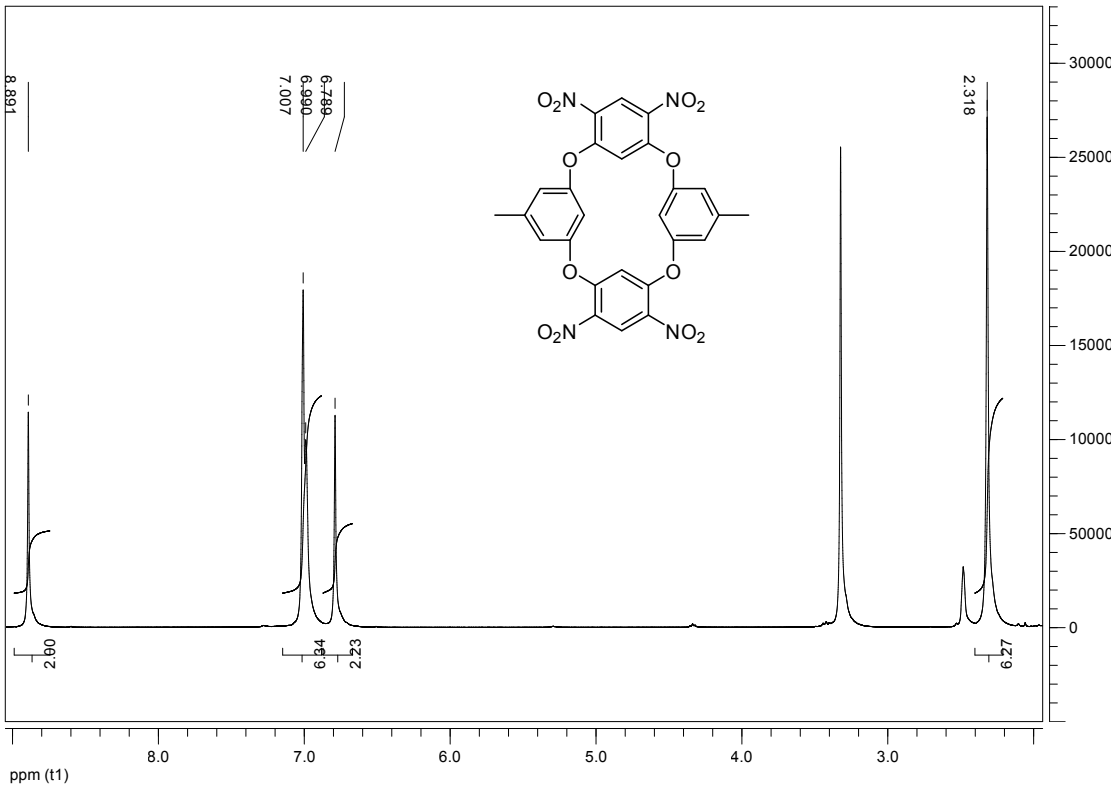


Figure 13 ^{1}HNMR spectrum of 3b (DMSO)

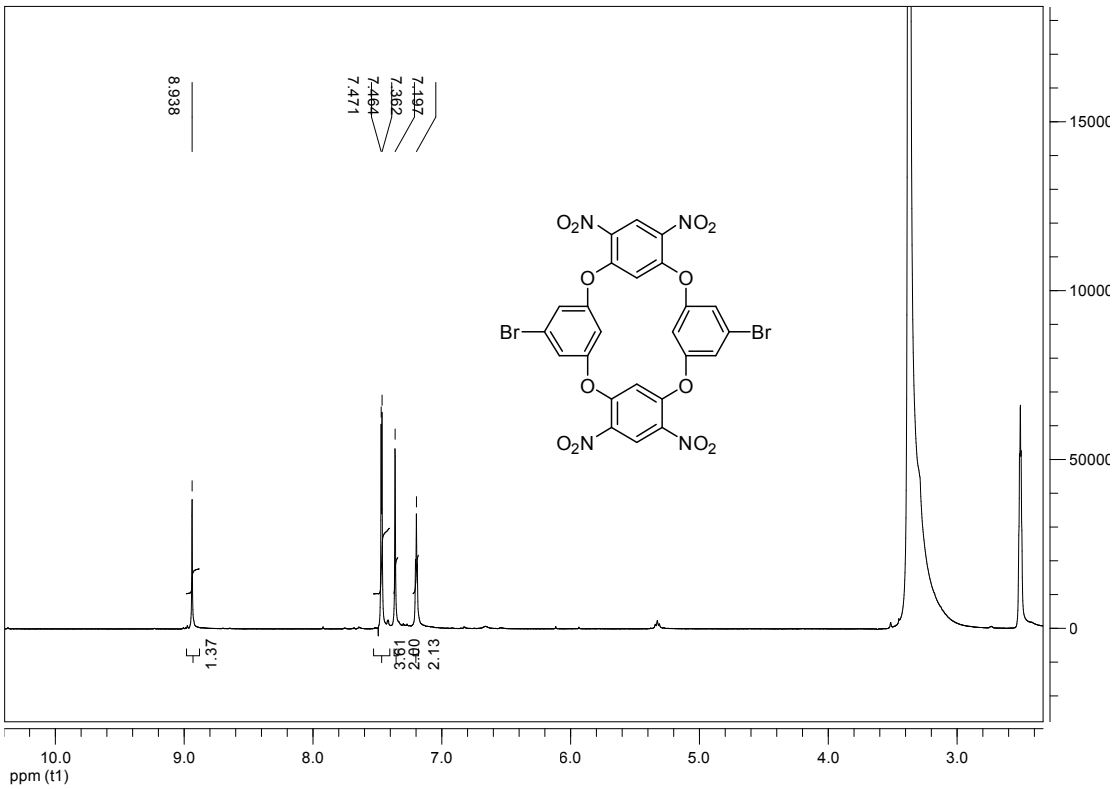


Figure 14 ^{1}H NMR spectrum of 3c (DMSO).

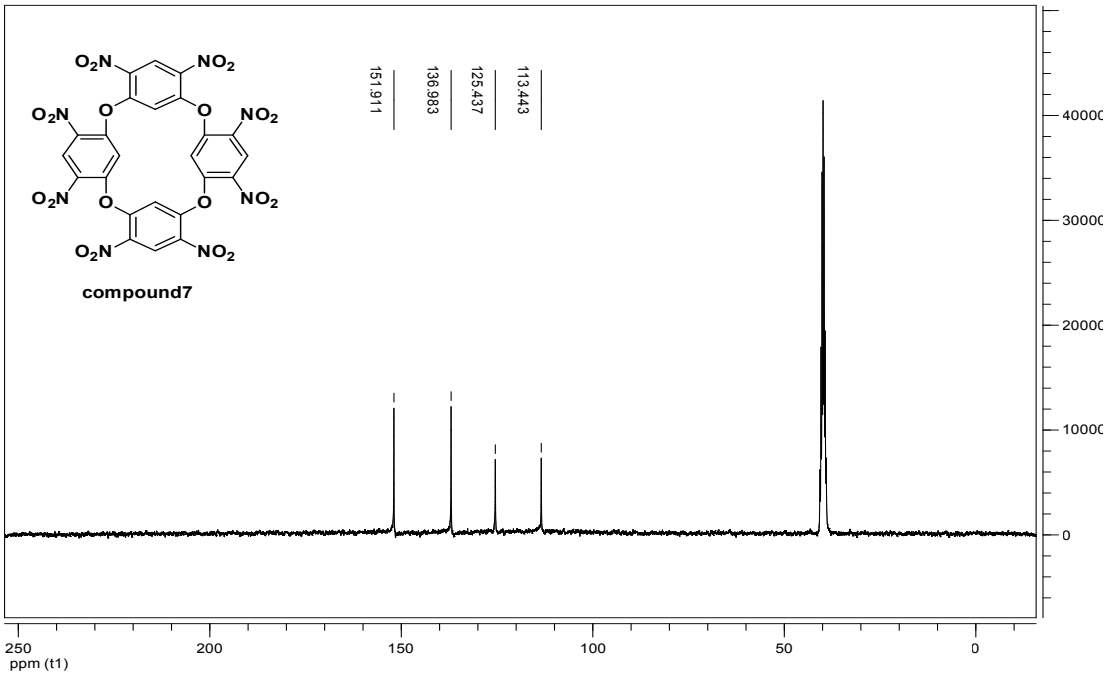


Figure 15 ^{13}CNMR spectrum of 4a (DMSO).

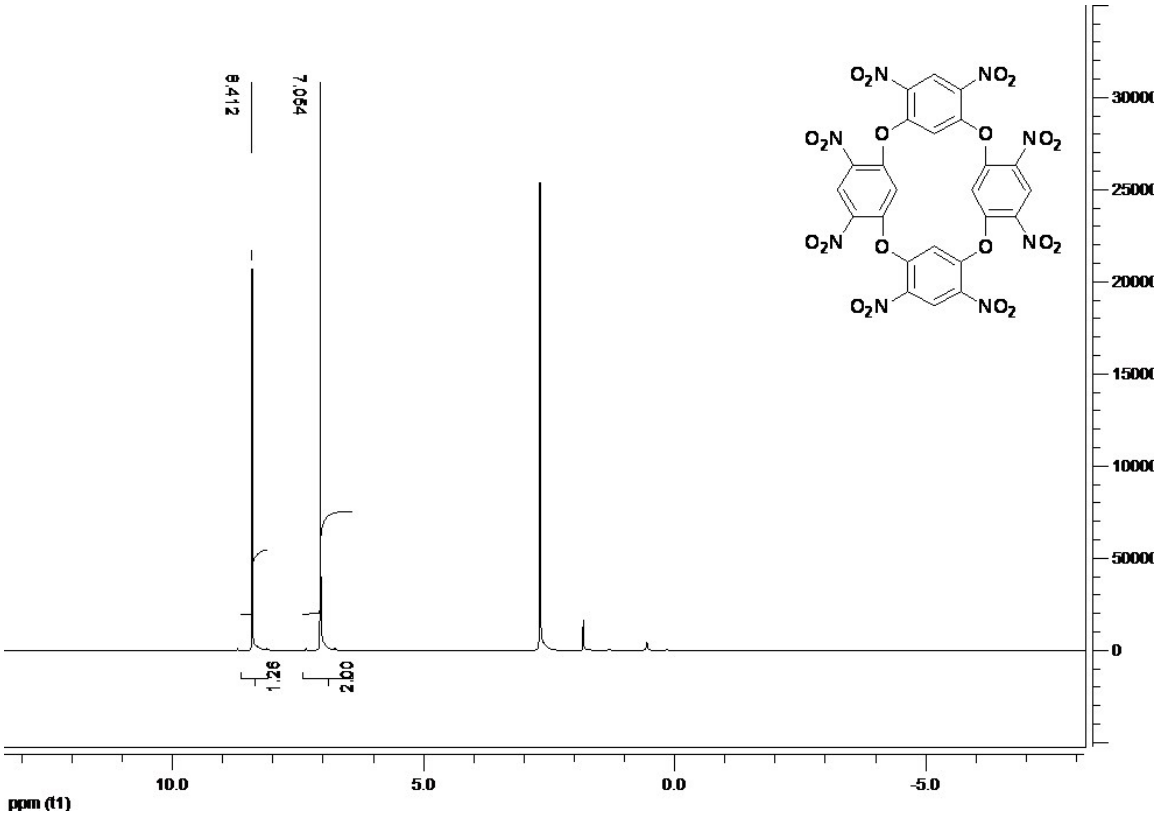


Figure 16 **^{1}H NMR spectrum of 4a (DMSO)**

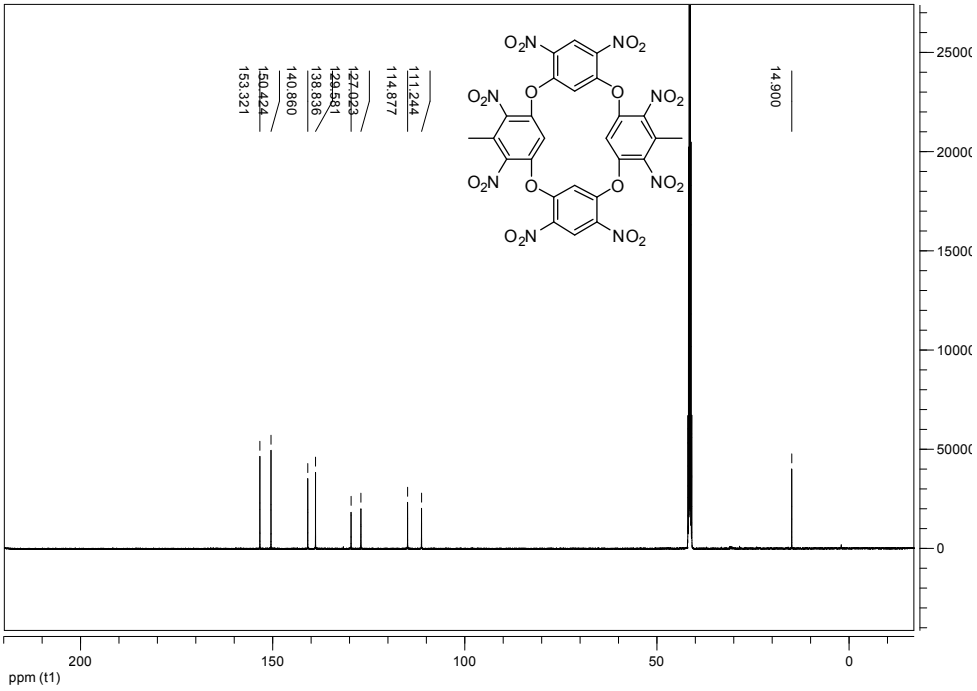


Figure 17 **^{3}C NMR spectrum of 4b (DMSO)**

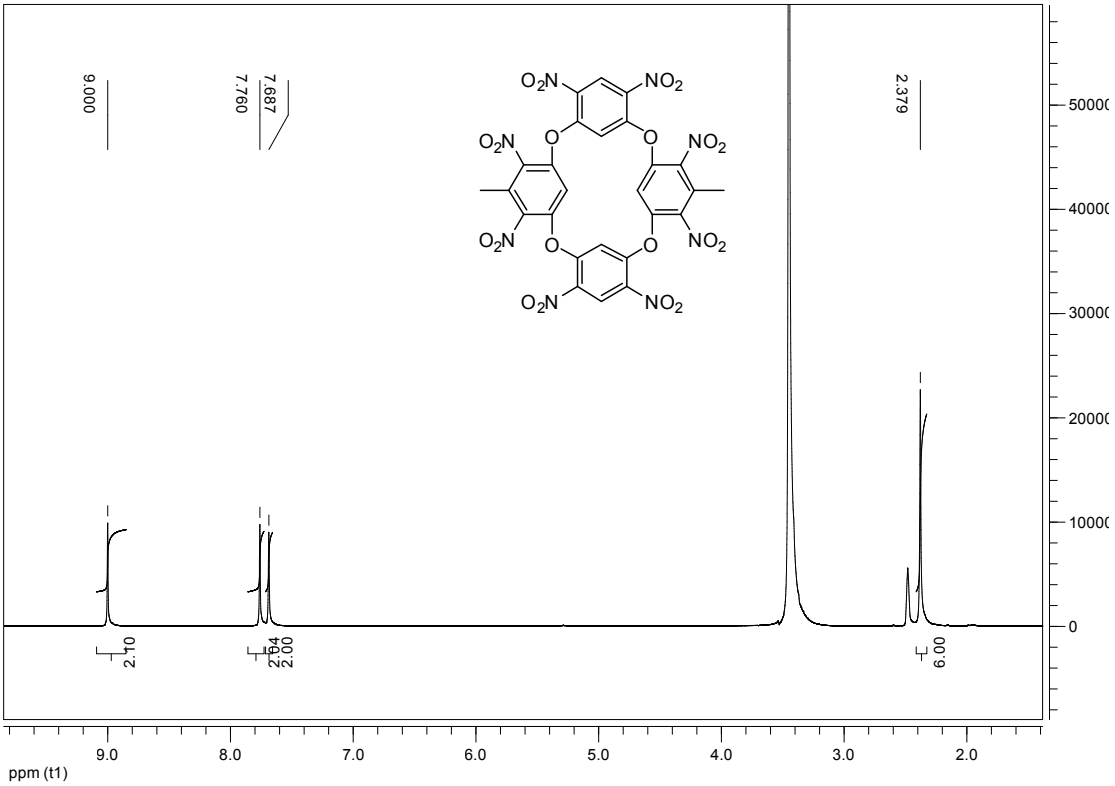


Figure 18 **^{1}H NMR spectrum of 4b (DMSO).**

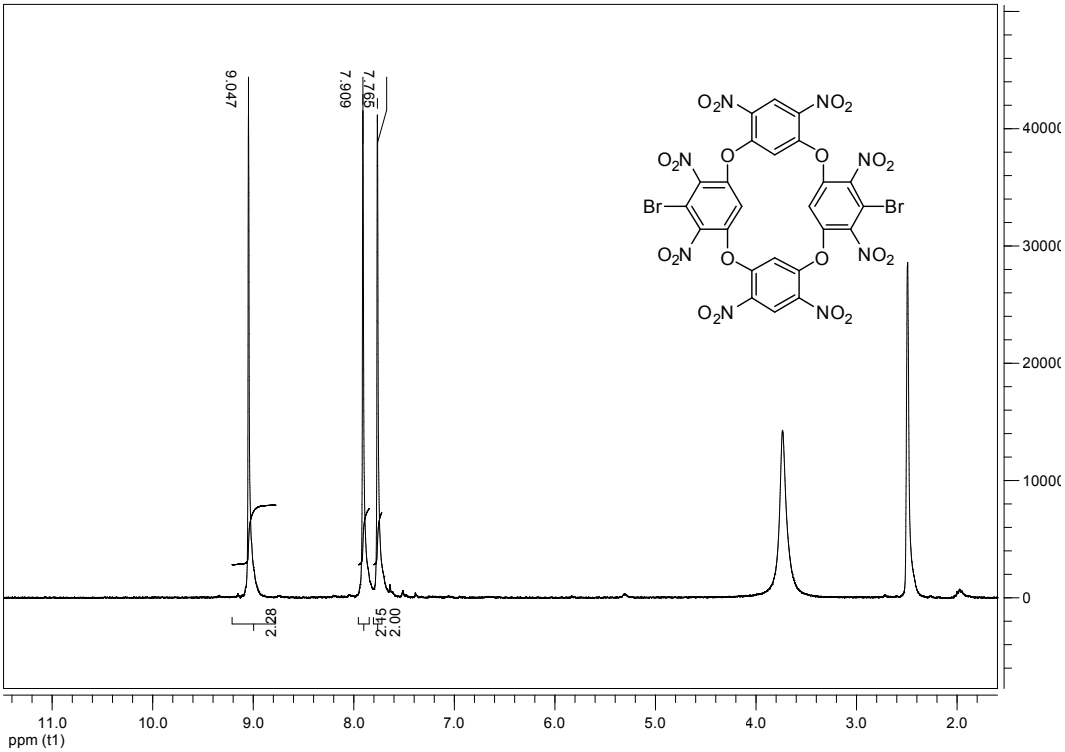


Figure 19 **^{1}H NMR spectrum of 4c (DMSO)**

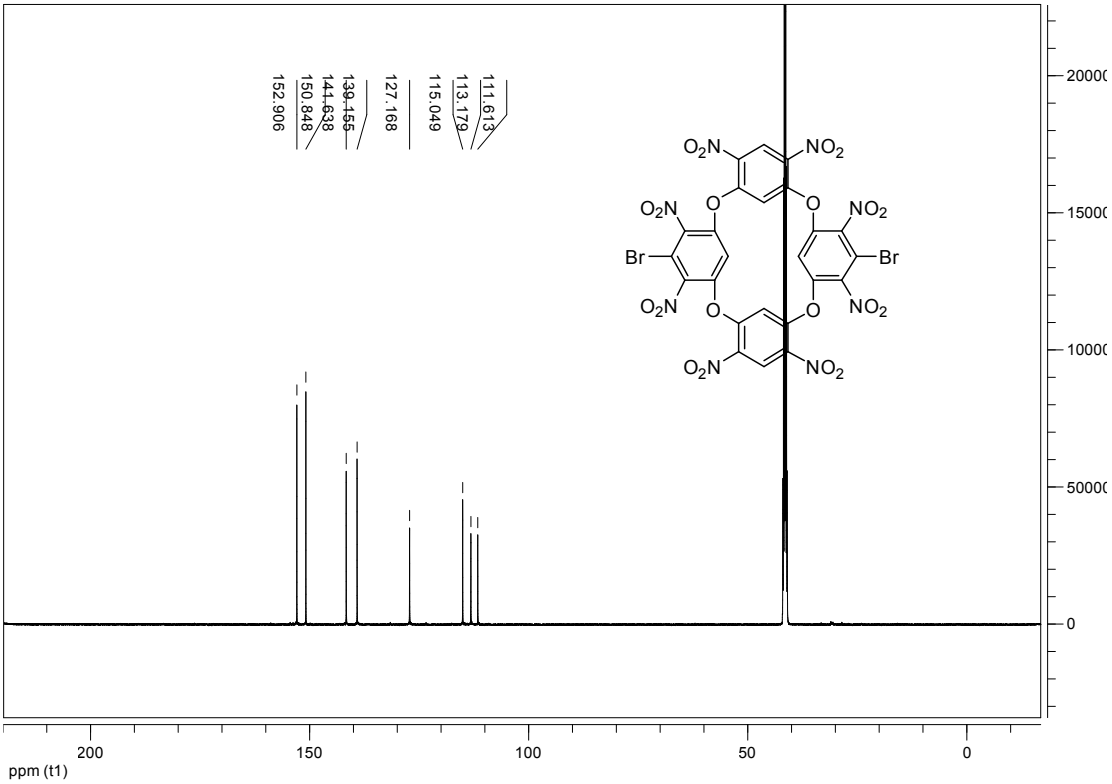


Figure 20 **^{13}C NMR spectrum of 4c (DMSO)**

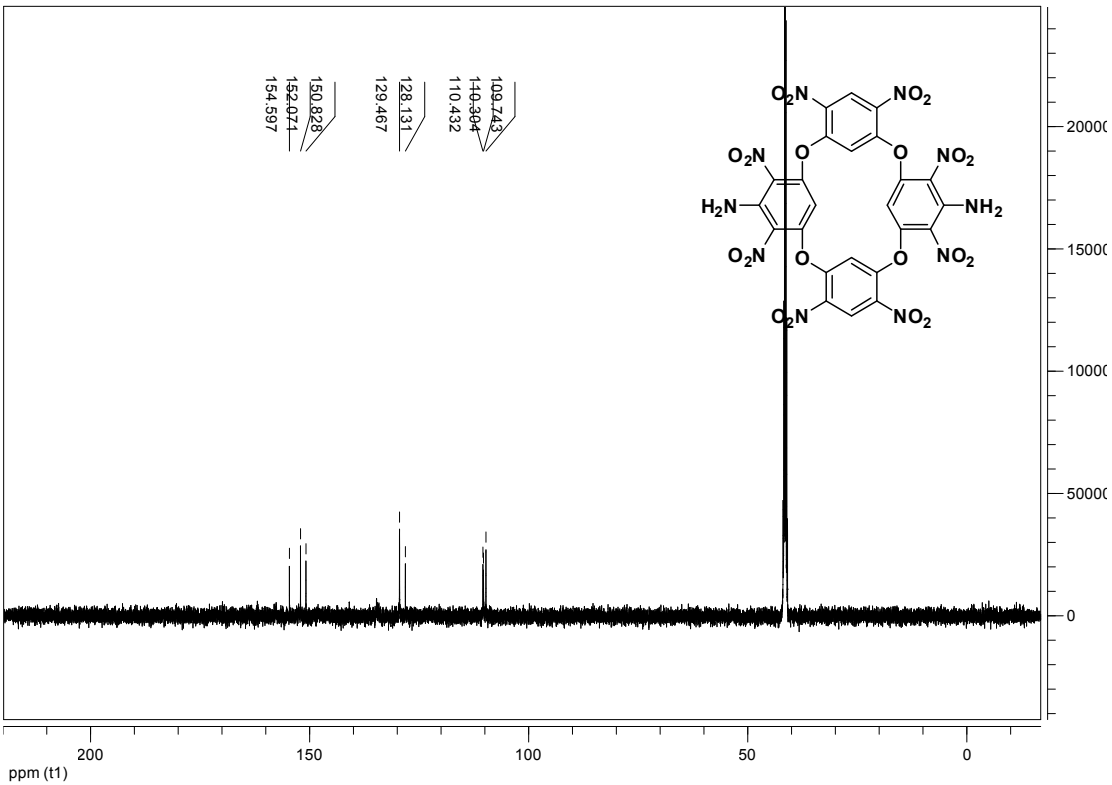


Figure 21 **^{13}C NMR spectrum of 5 (DMSO)**

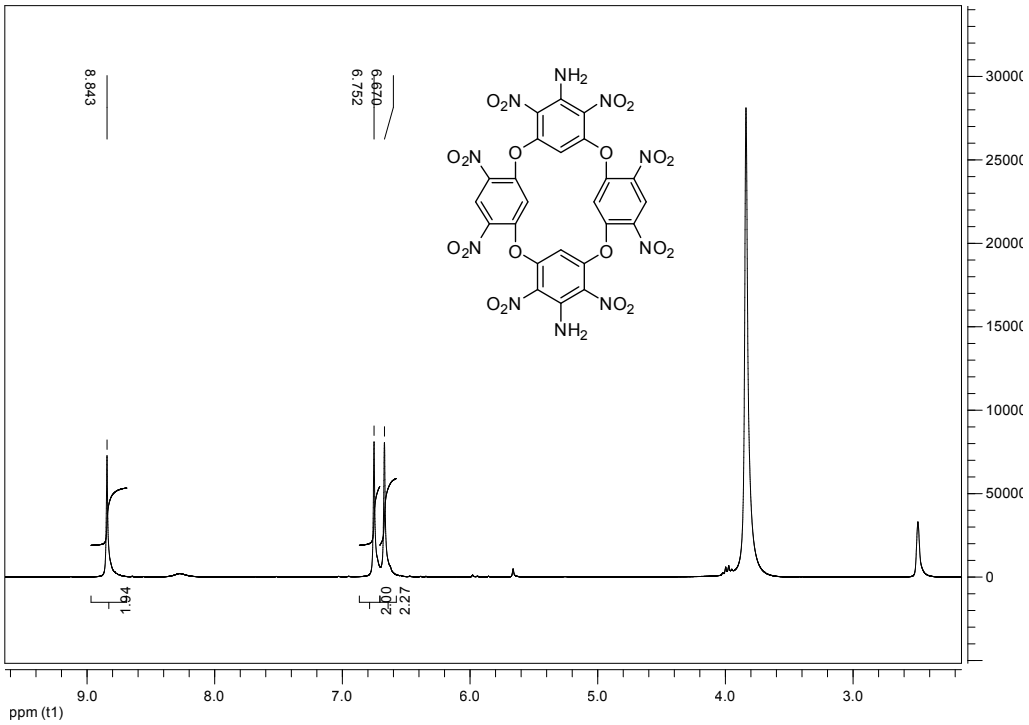


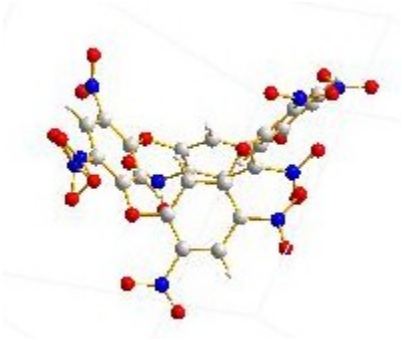
Figure 22 **^{1}HNMR spectrum of 5 (DMSO)**

X-ray Structural Analysis of compound 4a

The selected crystal was mounted with epoxy to the tip of a glass rod drawn out to a fiber. The X-ray intensity data for this colorless needle of C_{24} H_8 N_8 O_{20} with approximate dimensions 0.23 x 0.14 x 0.14 mm were measured with phi and omega scans at 173 K on a Bruker SMART APEX CCD-based X-ray diffract meter system equipped with a Mo-target X-ray tube (λ = 0.71073 Å). The detector was placed at a distance of 5.00 cm from the crystal. A total of 5059 frames were collected (a hemisphere of data) with an exposure time package using a narrow-frame integration algorithm giving a total of 4399 reflections to a maximum (angle of 25.360° of which 3147 reflections were independent. The structure was solved (direct methods) and refined using the Bruker SHELXTL version 6.1 Software Package using literature scattering factors (Wilson, A. J. C., Ed. *International Tables for Crystallography*; Kluwer Academic Publishers: Dordrecht, The Netherlands, 1992; Vol. C.), and the orthorhombic space group *Cc* with Z = 4. No absorption correction was applied. The final anisotropic full-matrix least-squares refinement of F2 converged at R1 =6.21%, wR2 = 14.16% and a goodness-of-fit of 1.060. All non-hydrogen atoms were modeled anisotropically. Hydrogen atoms were placed at calculated distances. All hydrogen atoms use a riding model, which means that the positional and thermal parameters are derived from the atom each hydrogen atom is bound to, while maintaining the calculated or determined distance and

optimal angles. The calculated density is 1.753g/cm^3. Thermal ellipsoid drawings (15%) in this report were generated with the Bruker SHELXTL software.

a



b

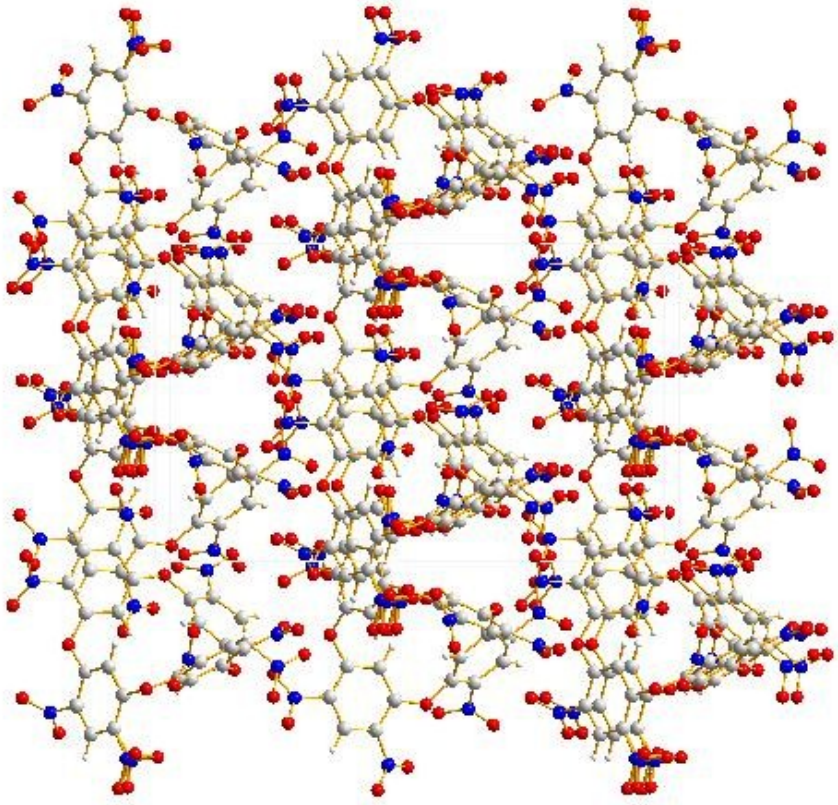


Figure 23. (a) Dimer and (b) packing structures of compound 4a.

Table S4 Selected geometric informations

Atoms 1,2	d 1,2 [Å]	Atoms 1,2	d 1,2 [Å]
C1A—O1A	1.369(7)	C5C—C6C	1.378(8)
C1A—C2A	1.387(8)	C5C—H5C	0.9500
C1A—C6A	1.401(8)	C6C—N2C	1.473(7)
C2A—C3A	1.382(8)	C1D—O1D	1.359(7)
C2A—H2A	0.9500	C1D—C6D	1.382(8)
C3A—O1D	1.368(7)	C1D—C2D	1.392(8)
C3A—C4A	1.399(8)	C2D—C3D	1.388(8)
C4A—C5A	1.381(8)	C2D—H2D	0.9500
C4A—N1A	1.466(8)	C3D—C4D	1.382(8)
C5A—C6A	1.368(8)	C3D—O1C	1.392(7)
C5A—H5A	0.9500	C4D—C5D	1.369(8)
C6A—N2A	1.463(7)	C4D—N1D	1.474(8)
C1B—O1B	1.366(7)	C5D—C6D	1.381(8)
C1B—C2B	1.392(9)	C5D—H5D	0.9500
C1B—C6B	1.402(8)	C6D—N2D	1.464(8)
C2B—C3B	1.374(8)	N1A—O3A	1.213(7)
C2B—H2B	0.9500	N1A—O2A	1.221(7)
C3B—C4B	1.382(8)	N2A—O5A	1.227(7)
C3B—O1A	1.389(7)	N2A—O4A	1.228(7)
C4B—C5B	1.383(9)	N1B—O3B	1.215(7)
C4B—N1B	1.458(8)	N1B—O2B	1.228(7)
C5B—C6B	1.374(8)	N2B—O4B	1.209(7)
C5B—H5B	0.9500	N2B—O5B	1.231(7)
C6B—N2B	1.470(8)	N2C—O5C	1.215(7)
C1C—O1C	1.373(7)	N2C—O4C	1.222(7)
C1C—C2C	1.374(8)	N1D—O3D	1.213(7)
C1C—C6C	1.391(8)	N1D—O2D	1.232(7)
C2C—C3C	1.379(8)	N2D—O4D	1.220(7)
C2C—H2C	0.9500	N2D—O5D	1.229(7)

C3C—C4C	1.371(8)	N1C—O3C	1.219(11)
C3C—O1B	1.387(6)	N1C—O2C	1.236(11)
C4C—C5C	1.391(8)	N1X—O3X	1.226(14)
C4C—N1C	1.477(10)	N1X—O2X	1.232(14)
C4C—N1X	1.483(15)		

Atoms 1,2,3	Angle 1,2,3 [°]	Atoms 1,2,3	Angle 1,2,3 [°]
O1A—C1A—C2A	122.7(5)	C4C—C5C—H5C	120.800
O1A—C1A—C6A	118.0(5)	C5C—C6C—C1C	121.1(5)
C2A—C1A—C6A	119.2(5)	C5C—C6C—N2C	117.3(5)
C3A—C2A—C1A	119.6(6)	C1C—C6C—N2C	121.6(5)
C3A—C2A—H2A	120.200	O1D—C1D—C6D	116.3(5)
C1A—C2A—H2A	120.200	O1D—C1D—C2D	124.2(5)
O1D—C3A—C2A	123.5(6)	C6D—C1D—C2D	119.4(5)
O1D—C3A—C4A	116.3(5)	C3D—C2D—C1D	119.3(6)
C2A—C3A—C4A	119.8(5)	C3D—C2D—H2D	120.300
C5A—C4A—C3A	120.8(5)	C1D—C2D—H2D	120.300
C5A—C4A—N1A	118.1(6)	C4D—C3D—C2D	120.1(6)
C3A—C4A—N1A	121.1(5)	C4D—C3D—O1C	119.1(6)
C6A—C5A—C4A	118.8(6)	C2D—C3D—O1C	120.6(5)
C6A—C5A—H5A	120.600	C5D—C4D—C3D	120.7(6)
C4A—C5A—H5A	120.600	C5D—C4D—N1D	115.3(6)
C5A—C6A—C1A	121.5(6)	C3D—C4D—N1D	124.0(6)
C5A—C6A—N2A	118.9(6)	C4D—C5D—C6D	119.3(6)
C1A—C6A—N2A	119.6(5)	C4D—C5D—H5D	120.400
O1B—C1B—C2B	122.6(5)	C6D—C5D—H5D	120.400
O1B—C1B—C6B	118.3(5)	C5D—C6D—C1D	121.0(6)
C2B—C1B—C6B	119.2(5)	C5D—C6D—N2D	116.6(5)
C3B—C2B—C1B	119.6(5)	C1D—C6D—N2D	122.4(6)

C3B—C2B—H2B	120.200	O3A—N1A—O2A	124.2(6)
C1B—C2B—H2B	120.200	O3A—N1A—C4A	117.6(5)
C2B—C3B—C4B	121.0(6)	O2A—N1A—C4A	118.1(6)
C2B—C3B—O1A	116.9(5)	O5A—N2A—O4A	124.8(5)
C4B—C3B—O1A	122.0(5)	O5A—N2A—C6A	117.6(5)
C3B—C4B—C5B	119.9(6)	O4A—N2A—C6A	117.5(6)
C3B—C4B—N1B	121.9(6)	O3B—N1B—O2B	124.0(6)
C5B—C4B—N1B	118.2(5)	O3B—N1B—C4B	117.8(6)
C6B—C5B—C4B	119.9(5)	O2B—N1B—C4B	118.2(5)
C6B—C5B—H5B	120.000	O4B—N2B—O5B	125.4(6)
C4B—C5B—H5B	120.000	O4B—N2B—C6B	117.5(6)
C5B—C6B—C1B	120.4(6)	O5B—N2B—C6B	117.2(5)
C5B—C6B—N2B	118.6(5)	O5C—N2C—O4C	126.1(6)
C1B—C6B—N2B	121.0(5)	O5C—N2C—C6C	117.0(6)
O1C—C1C—C2C	122.9(5)	O4C—N2C—C6C	117.0(6)
O1C—C1C—C6C	117.5(5)	O3D—N1D—O2D	124.9(6)
C2C—C1C—C6C	119.5(5)	O3D—N1D—C4D	116.7(6)
C1C—C2C—C3C	119.9(5)	O2D—N1D—C4D	118.4(6)
C1C—C2C—H2C	120.000	O4D—N2D—O5D	123.2(6)
C3C—C2C—H2C	120.000	O4D—N2D—C6D	118.3(6)
C4C—C3C—C2C	120.4(5)	O5D—N2D—C6D	118.4(5)
C4C—C3C—O1B	120.7(5)	C1A—O1A—C3B	118.4(4)
C2C—C3C—O1B	118.8(5)	C1B—O1B—C3C	115.4(4)
C3C—C4C—C5C	120.7(5)	C1C—O1C—C3D	120.2(4)
C3C—C4C—N1C	120.4(6)	C1D—O1D—C3A	126.2(5)
C5C—C4C—N1C	118.8(6)	O3C—N1C—O2C	123.9(11)
C3C—C4C—N1X	124.8(8)	O3C—N1C—C4C	118.4(9)
C5C—C4C—N1X	113.8(8)	O2C—N1C—C4C	117.7(8)
N1C—C4C—N1X	13.7(14)	O3X—N1X—O2X	124.4(17)
C6C—C5C—C4C	118.4(5)	O3X—N1X—C4C	117.8(14)

C6C—C5C—H5C	120.800	O2X—N1X—C4C	117.8(12)

[i] x,y,1+z; [ii] 1/2-x,y,-1/2+z; [iii] 1-x,1/2-y,-1/2+z; [iv] 3/2-x,y,1/2+z

X-ray Structural Analysis of compound 4b

The selected crystal was mounted with epoxy to the tip of a glass rod drawn out to a fiber. The X-ray intensity data for this colorless needle of $C_{26}H_{12}N_8O_{20}$ with approximate dimensions 0.13 x 0.23 x 0.24 mm were measured with phi and omega scans at 173 K on a Bruker SMART APEX CCD-based X-ray diffract meter system equipped with a Mo-target X-ray tube (λ = 0.71073 Å). The detector was placed at a distance of 5.00 cm from the crystal. A total of 15169 frames were collected (a hemisphere of data) with an exposure time package using a narrow-frame integration algorithm giving a total of 15887 reflections to a maximum (angle of 25.387° of which 8131 reflections were independent. The structure was solved (direct methods) and refined using the Bruker SHELXTL version 6.1 Software Package using literature scattering factors (Wilson, A. J. C., Ed. *International Tables for Crystallography*; Kluwer Academic Publishers: Dordrecht, The Netherlands, 1992; Vol. C.), and the orthorhombic space group *Cc* with Z = 4. No absorption correction was applied. The final anisotropic full-matrix least-squares refinement of F2 converged at R1 =5.80%, wR2 = 14.29% and a goodness-of-fit of 1.068. All non-hydrogen atoms were modeled anisotropically. Hydrogen atoms were placed at calculated distances. All hydrogen atoms use a riding model, which means that the positional and thermal parameters are derived from the atom each hydrogen atom is bound to, while maintaining the

calculated or determined distance and optimal angles. The calculated density is 1.759g/cm^3. Thermal ellipsoid drawings (15%) in this report were generated with the Bruker SHELXTL software.

c

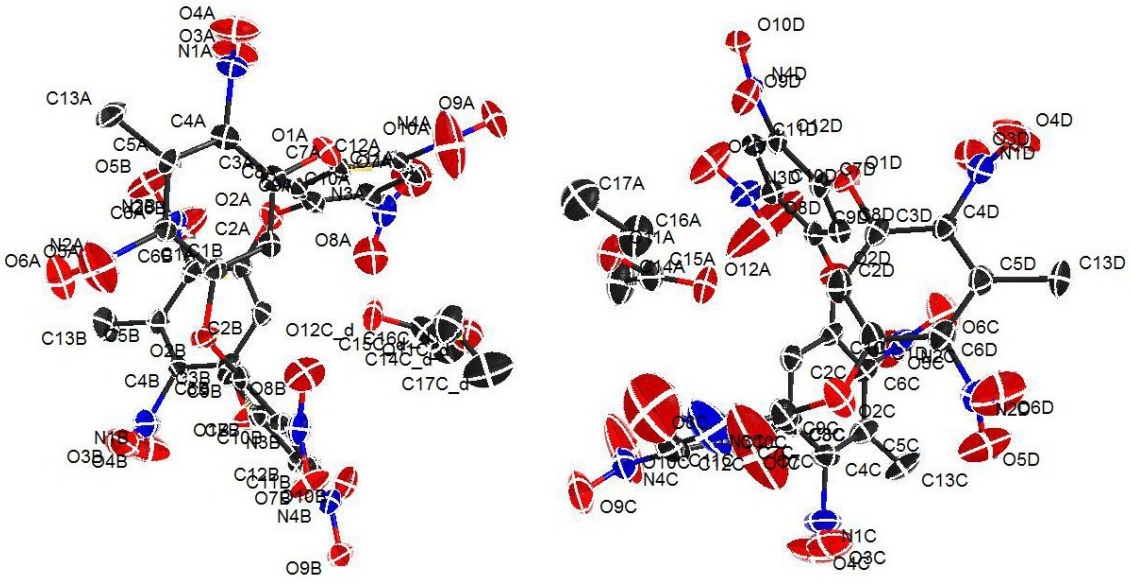


Figure S24. (a) Dimer structures of compound 4b • 2CH_3CO_2Et

Atomic parameters

Atom	Ox.	Wyck.	Site	x/a	y/b	z/c
C1A		2i	1	0.79089	0.08054	0.03172
C2A		2i	1	0.72019	0.12612	0.06083
C3A		2i	1	0.60665	0.12843	0.02638
C4A		2i	1	0.56257	0.08517	-0.03478
C5A		2i	1	0.63145	0.03740	-0.06433
C6A		2i	1	0.74589	0.03737	-0.02894
C7A		2i	1	0.56590	0.24004	0.07020
C8A		2i	1	0.64762	0.27296	0.03844
C9A		2i	1	0.67952	0.34407	0.05583
C10A		2i	1	0.62767	0.38222	0.10401
C11A		2i	1	0.54392	0.35151	0.13547
C12A		2i	1	0.51387	0.27851	0.11841
C13A		2i	1	0.58547	-0.01115	-0.13065
C1B		2i	1	0.87277	0.36526	0.02583
C2B		2i	1	0.93026	0.33666	0.07709
C3B		2i	1	1.04985	0.32770	0.07774
C4B		2i	1	1.11113	0.34849	0.02915
C5B		2i	1	1.05745	0.37761	-0.02311
C6B		2i	1	0.93599	0.38465	-0.02286
C7B		2i	1	1.07425	0.24062	0.14278
C8B		2i	1	1.00352	0.18899	0.09446
C9B		2i	1	0.96812	0.12551	0.11078
C10B		2i	1	1.00489	0.11148	0.17398

C11B	2i	1	1.08071	0.16070	0.22188
C12B	2i	1	1.11176	0.22545	0.20632
C13B	2i	1	1.12187	0.39818	-0.07670
C1C	2i	1	0.49448	0.42184	0.62714
C2C	2i	1	0.56036	0.37296	0.59884
C3C	2i	1	0.67247	0.36777	0.63409
C4C	2i	1	0.71829	0.41033	0.69477
C5C	2i	1	0.65527	0.46137	0.72277
C6C	2i	1	0.54168	0.46476	0.68646
C7C	2i	1	0.71145	0.25549	0.58397
C8C	2i	1	0.62734	0.22012	0.61311
C9C	2i	1	0.60045	0.14865	0.59367
C10C	2i	1	0.66036	0.11230	0.54610
C11C	2i	1	0.74287	0.14837	0.51710
C12C	2i	1	0.76750	0.22008	0.53515
C13C	2i	1	0.69976	0.51006	0.78927
C1D	2i	1	0.40691	0.13488	0.62250
C2D	2i	1	0.35125	0.16437	0.57040
C3D	2i	1	0.23575	0.18124	0.57390
C4D	2i	1	0.17626	0.16816	0.62497
C5D	2i	1	0.23075	0.13737	0.67738
C6D	2i	1	0.34620	0.12172	0.67328
C7D	2i	1	0.21224	0.27119	0.51012
C8D	2i	1	0.28317	0.31980	0.55907
C9D	2i	1	0.31791	0.38575	0.54564
C10D	2i	1	0.28098	0.40238	0.48343
C11D	2i	1	0.20553	0.35406	0.43444
C12D	2i	1	0.17230	0.28887	0.44846
C13D	2i	1	0.16907	0.12714	0.73702
N1A	2i	1	0.44159	0.09267	-0.06929
N2A	2i	1	0.82659	-0.00977	-0.05750
N3A	2i	1	0.66597	0.45697	0.12445
N4A	2i	1	0.42497	0.24802	0.15397
N1B	2i	1	1.24057	0.33964	0.03410
N2B	2i	1	0.86952	0.41510	-0.07576
N3B	2i	1	0.96622	0.04563	0.19389
N4B	2i	1	1.18367	0.27880	0.25991
N1C	2i	1	0.83620	0.39843	0.72981
N2C	2i	1	0.46955	0.51823	0.71217
N3C	2i	1	0.64200	0.03802	0.52713
N4C	2i	1	0.85129	0.25481	0.50040
N1D	2i	1	0.05446	0.18922	0.62549
N2D	2i	1	0.40922	0.09011	0.72599
N3D	2i	1	0.31644	0.46994	0.46590
N4D	2i	1	0.09672	0.23864	0.39372
O1A	2i	1	0.52814	0.16964	0.05412
O2A	2i	1	0.75488	0.37910	0.02079
O3A	2i	1	0.42766	0.14911	-0.08378
O4A	2i	1	0.36564	0.04207	-0.08040
O5A	2i	1	0.81474	-0.06934	-0.04911
O6A	2i	1	0.89805	0.01394	-0.08967
O7A	2i	1	0.58829	0.49550	0.12778
O8A	2i	1	0.77374	0.47593	0.13872
O9A	2i	1	0.36226	0.28701	0.18050
O10A	2i	1	0.42329	0.18818	0.15862
O1B	2i	1	1.11561	0.30340	0.12967
O2B	2i	1	0.90573	0.07253	0.06097
O3B	2i	1	1.26625	0.27988	0.02808
O4B	2i	1	1.31448	0.39064	0.04433
O5B	2i	1	0.80151	0.37638	-0.12062
O6B	2i	1	0.88569	0.47711	-0.07252
O7B	2i	1	1.03712	0.02310	0.23406
O8B	2i	1	0.86284	0.01788	0.17050
O9B	2i	1	1.25597	0.25765	0.30057
O10B	2i	1	1.16566	0.33885	0.26212
O1C	2i	1	0.74894	0.32598	0.60490

O2C	2i	1	0.51999	0.11207	0.62329
O3C	2i	1	0.84748	0.33854	0.73815
O4C	2i	1	0.91348	0.44932	0.74840
O5C	2i	1	0.50684	0.57910	0.71464
O6C	2i	1	0.37409	0.49900	0.72915
O7C	2i	1	0.62563	0.00255	0.56880
O8C	2i	1	0.64744	0.01342	0.46865
O9C	2i	1	0.92164	0.22074	0.47514
O10C	2i	1	0.84657	0.31461	0.49616
O1D	2i	1	0.17331	0.20623	0.52094
O2D	2i	1	0.38508	0.43538	0.59566
O3D	2i	1	0.04058	0.24942	0.62058
O4D	2i	1	-0.02664	0.14492	0.62962
O5D	2i	1	0.49060	0.12618	0.76563
O6D	2i	1	0.37706	0.02971	0.72798
O7D	2i	1	0.29024	0.47925	0.41193
O8D	2i	1	0.36471	0.51511	0.50715
O9D	2i	1	0.11061	0.17741	0.38813
O10D	2i	1	0.02523	0.26278	0.35455
C14A	2i	1	0.55504	0.31844	0.39448
C15A	2i	1	0.50109	0.25309	0.41310
O11A	2i	1	0.48298	0.20066	0.36225
C16A	2i	1	0.41827	0.13528	0.37199
C17A	2i	1	0.39145	0.08902	0.30361
O12A	2i	1	0.47292	0.24797	0.46605
C14D	2i	1	0.19075	0.37439	0.74026
C15D	2i	1	0.29223	0.33143	0.75471
O11D	2i	1	0.30405	0.31946	0.81666
C16D	2i	1	0.40466	0.28467	0.84139
C17D	2i	1	0.51310	0.33845	0.86741
O12D	2i	1	0.35721	0.30874	0.71657
C14W	2i	1	0.18151	0.35604	0.74099
C15W	2i	1	0.30541	0.33416	0.75129
O11W	2i	1	0.34835	0.33777	0.81579
C16W	2i	1	0.47094	0.32015	0.83236
C17W	2i	1	0.49687	0.32682	0.90719
O12W	2i	1	0.36643	0.31589	0.70916
C14B	2i	1	1.10138	0.15910	0.91917
C15B	2i	1	0.97171	0.17076	0.90193
O11B	2i	1	0.93459	0.15834	0.83766
C16B	2i	1	0.80805	0.17163	0.81547
C17B	2i	1	0.78128	0.13453	0.74353
O12B	2i	1	0.90462	0.19112	0.94147
C14Y	2i	1	1.10289	0.13693	0.91709
C15Y	2i	1	1.00351	0.17963	0.90069
O11Y	2i	1	0.99071	0.18795	0.83743
C16Y	2i	1	0.87191	0.20421	0.80860
C17Y	2i	1	0.78538	0.13821	0.81023
O12Y	2i	1	0.93920	0.20579	0.93812
C14C	2i	1	0.82808	0.36131	0.27582
C15C	2i	1	0.79576	0.28434	0.24298
O11C	2i	1	0.75612	0.24706	0.28534
C16C	2i	1	0.72474	0.17240	0.26178
C17C	2i	1	0.75633	0.13670	0.32081
O12C	2i	1	0.80614	0.26071	0.18738
C14X	2i	1	0.83871	0.36112	0.27227
C15X	2i	1	0.78788	0.28725	0.23893
O11X	2i	1	0.70978	0.25969	0.27246
C16X	2i	1	0.65932	0.18706	0.24941
C17X	2i	1	0.75314	0.14437	0.27929
O12X	2i	1	0.81301	0.25622	0.18836

Anisotropic displacement parameters, in Å²

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C1A	0.03113	0.03017	0.02475	0.00655	0.00302	0.00637
C2A	0.03330	0.02946	0.02979	0.00317	0.00987	0.00264

C3A	0.03225	0.02383	0.03715	0.00103	0.00813	0.00350
C4A	0.03090	0.02480	0.04074	0.00328	0.00307	0.00755
C5A	0.03454	0.02566	0.02703	0.00306	0.00488	0.00286
C6A	0.03424	0.03093	0.02371	0.00934	0.00526	0.00260
C7A	0.02744	0.02796	0.03533	0.00763	0.00736	0.00135
C8A	0.03088	0.03702	0.03767	0.01287	0.00901	0.00787
C9A	0.02733	0.03411	0.03882	0.00692	0.00977	0.01305
C10A	0.03476	0.02902	0.04421	0.00729	0.00846	0.00708
C11A	0.03438	0.03397	0.04155	0.00571	0.00813	0.00483
C12A	0.02207	0.03912	0.03879	0.01024	0.00788	0.00860
C13A	0.04592	0.04407	0.02883	0.00518	-0.01067	-0.00824
C1B	0.03448	0.03211	0.02895	0.00131	0.00982	0.00849
C2B	0.03438	0.03849	0.03170	0.00537	0.01144	0.01302
C3B	0.03594	0.02810	0.02918	0.00139	0.00414	0.00827
C4B	0.02891	0.04266	0.03698	0.00657	0.01238	0.01047
C5B	0.03950	0.04797	0.02898	0.00278	0.00902	0.01468
C6B	0.03897	0.04113	0.02266	0.00528	0.00530	0.01054
C7B	0.02518	0.03547	0.02822	0.00507	0.01003	0.00951
C8B	0.03597	0.04011	0.02378	0.01032	0.00542	0.00680
C9B	0.02768	0.02786	0.02629	0.00965	0.00516	-0.00506
C10B	0.02836	0.02594	0.02652	0.00646	0.00624	0.00632
C11B	0.03076	0.03184	0.02635	0.00297	0.00673	0.00783
C12B	0.03044	0.03570	0.01973	0.00326	0.00414	0.00182
C13B	0.06032	0.10589	0.05589	0.01907	0.03292	0.04711
C1C	0.03577	0.02422	0.02653	-0.00130	0.00017	0.00780
C2C	0.03619	0.03237	0.03414	-0.00008	0.00909	0.00864
C3C	0.03601	0.03751	0.04453	0.00415	0.01522	0.01033
C4C	0.03283	0.04104	0.04539	0.00486	0.00093	0.01597
C5C	0.04829	0.03346	0.03587	-0.00172	-0.00310	0.01027
C6C	0.04059	0.02474	0.03043	0.00300	0.00091	0.00583
C7C	0.03058	0.03889	0.04445	0.01300	0.00899	0.01138
C8C	0.04134	0.04032	0.04015	0.01482	0.01671	0.01331
C9C	0.04513	0.04013	0.05581	0.01287	0.01964	0.02427
C10C	0.04509	0.04484	0.06977	0.02046	0.02430	0.01091
C11C	0.04323	0.05739	0.05178	0.01671	0.01345	0.00420
C12C	0.02831	0.05695	0.04165	0.01476	0.01537	0.01422
C13C	0.08004	0.05518	0.03256	0.00027	-0.02076	0.00140
C1D	0.04668	0.02703	0.04605	0.00419	0.01926	0.01431
C2D	0.04954	0.02637	0.03928	0.00685	0.01783	0.01140
C3D	0.04098	0.02752	0.02571	-0.00239	0.00385	0.00548
C4D	0.03674	0.03266	0.02912	-0.00311	0.00500	0.00772
C5D	0.03669	0.04084	0.03162	-0.00324	0.00818	0.01163
C6D	0.04480	0.02843	0.03612	0.00235	0.00753	0.01302
C7D	0.03318	0.02545	0.02659	0.00237	0.00730	0.00522
C8D	0.03123	0.03077	0.02967	0.00391	0.00881	0.00620
C9D	0.03038	0.02556	0.02968	0.00738	0.00580	-0.00275
C10D	0.03261	0.02463	0.03230	-0.00005	0.00434	0.00922
C11D	0.03194	0.02822	0.03342	0.00170	0.00600	0.00446
C12D	0.03216	0.02990	0.02376	0.00271	0.00894	0.00189
C13D	0.05550	0.09311	0.04215	0.00736	0.02149	0.03701
N1A	0.03142	0.04209	0.04632	0.01005	0.00206	0.01019
N2A	0.03899	0.03100	0.03088	0.01479	0.00073	-0.00170
N3A	0.06729	0.03089	0.05297	0.00781	0.01510	0.00105
N4A	0.03639	0.03752	0.05030	0.00403	0.02096	0.00313
N1B	0.04387	0.05441	0.04592	0.00374	0.01007	0.01489
N2B	0.04554	0.05191	0.03548	0.00580	0.00769	0.02129
N3B	0.05100	0.03041	0.03727	0.00268	0.01225	-0.00014
N4B	0.03819	0.03381	0.02425	-0.00207	0.00905	0.00383
N1C	0.04715	0.08103	0.06580	0.02109	-0.01056	0.01594
N2C	0.05253	0.03369	0.03205	0.00709	0.00195	0.00126
N3C	0.09119	0.04784	0.14758	0.03027	0.06042	0.00907
N4C	0.05031	0.07294	0.05535	0.01332	0.02620	0.01921
N1D	0.04182	0.05409	0.03757	0.00378	0.00663	0.01447
N2D	0.04407	0.05501	0.05162	0.00525	0.00830	0.02820
N3D	0.05799	0.03099	0.04066	-0.01181	-0.00550	0.01014
N4D	0.03416	0.03798	0.02340	-0.00668	0.00956	0.00389

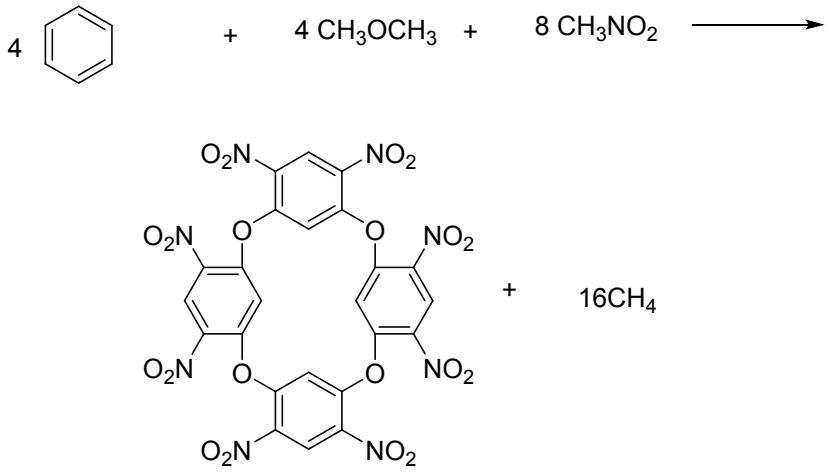
O1A	0.03313	0.02848	0.05803	0.00398	0.01851	0.00156
O2A	0.03736	0.04295	0.04134	0.00723	0.01476	0.01900
O3A	0.05183	0.05572	0.09757	0.02181	-0.00333	0.03267
O4A	0.04026	0.05051	0.09468	-0.01006	-0.01581	0.01091
O5A	0.09173	0.03684	0.10632	0.03319	0.04204	0.01875
O6A	0.07730	0.06334	0.07440	0.03049	0.04613	0.01622
O7A	0.10281	0.03620	0.11503	0.02218	0.00644	-0.00174
O8A	0.07719	0.04571	0.08631	-0.01922	0.02502	0.00203
O9A	0.05148	0.07121	0.07696	0.01094	0.04247	0.00728
O10A	0.16861	0.04318	0.13798	0.01046	0.11428	0.02214
O1B	0.03959	0.03677	0.03574	-0.00161	-0.00059	0.01811
O2B	0.03539	0.03359	0.03039	0.01102	-0.00651	-0.00564
O3B	0.05047	0.08146	0.08514	0.02496	-0.00137	-0.01100
O4B	0.03874	0.08581	0.12594	-0.01202	0.00379	0.04773
O5B	0.10806	0.07565	0.05672	0.00110	-0.03861	0.01548
O6B	0.13376	0.05558	0.06961	0.01910	-0.02796	0.02881
O7B	0.07339	0.04732	0.04622	0.00416	-0.00830	0.02399
O8B	0.05640	0.04625	0.06050	-0.01636	0.00065	0.01193
O9B	0.03301	0.05307	0.02987	-0.00128	0.00083	0.01005
O10B	0.06396	0.03544	0.03269	-0.00153	0.01191	0.00195
O1C	0.03177	0.04210	0.07233	0.00667	0.02109	0.00882
O2C	0.05003	0.04782	0.08229	0.01959	0.03379	0.03770
O3C	0.07813	0.08128	0.09037	0.03875	-0.00839	0.02962
O4C	0.05076	0.09486	0.12942	-0.00320	-0.02974	0.00353
O5C	0.09723	0.03246	0.06543	0.01089	0.01041	0.00266
O6C	0.08457	0.06408	0.09812	0.02040	0.04268	0.00261
O7C	0.18866	0.05811	0.30658	0.06070	0.16928	0.08004
O8C	0.17212	0.06910	0.16743	0.02521	0.04959	-0.03565
O9C	0.06003	0.10671	0.06514	-0.00252	0.03944	-0.00256
O10C	0.17229	0.10686	0.23281	0.06902	0.16355	0.10526
O1D	0.04567	0.03144	0.02827	-0.00751	-0.00193	0.01307
O2D	0.04130	0.02376	0.03931	0.00285	-0.00449	-0.00176
O3D	0.05691	0.04699	0.06267	0.01714	0.00772	0.00158
O4D	0.03361	0.08615	0.13093	-0.00912	0.01068	0.05670
O5D	0.08988	0.08398	0.07496	-0.00036	-0.03234	0.02664
O6D	0.10556	0.05466	0.10043	-0.00247	-0.00896	0.05080
O7D	0.14642	0.06026	0.05290	-0.04385	-0.01887	0.03303
O8D	0.43695	0.10266	0.10652	-0.16577	-0.12667	0.06598
O9D	0.06657	0.02968	0.03253	-0.00084	0.00872	0.00606
O10D	0.03351	0.05059	0.03237	-0.00376	0.00213	0.00575
C14A	0.09969	0.04651	0.05823	-0.00665	0.03380	0.01402
C15A	0.04506	0.03700	0.03997	0.00603	0.01195	0.00538
O11A	0.06414	0.03710	0.03765	0.00260	0.01573	0.00252
C16A	0.08262	0.03678	0.05832	-0.01494	0.01886	-0.00556
C17A	0.07888	0.05886	0.06804	-0.00314	0.00905	-0.01736
O12A	0.07433	0.04922	0.03150	-0.00319	0.02066	0.00593
C14D	0.05424	0.05703	0.05877	0.00070	-0.00774	0.00865
C15D	0.07908	0.04561	0.03186	0.00472	-0.00048	0.00428
O11D	0.09800	0.05990	0.04010	0.02093	0.00936	0.01406
C16D	0.11055	0.07182	0.05400	0.03126	-0.01272	0.02141
C17D	0.11431	0.11330	0.08444	0.03444	-0.03528	0.00273
O12D	0.08220	0.06980	0.04499	0.02602	0.00467	0.00677
C14W	0.08080	0.05620	0.05545	0.01214	-0.00986	-0.00458
C15W	0.08179	0.05053	0.03292	0.00394	-0.00081	0.00343
O11W	0.10786	0.07628	0.04941	0.01738	-0.01325	0.01264
C16W	0.10929	0.08978	0.04717	0.03171	-0.01017	-0.00010
C17W	0.12205	0.10917	0.04925	0.01630	-0.02324	0.01608
O12W	0.08659	0.07960	0.03805	0.01517	0.00165	0.01616
C14B	0.07940	0.06932	0.05302	0.01776	-0.00408	0.00150
C15B	0.06722	0.05061	0.03331	0.00307	0.00549	0.00391
O11B	0.06669	0.09803	0.03960	0.01136	-0.00461	0.01472
C16B	0.08329	0.12607	0.07344	-0.00021	0.01533	0.01064
C17B	0.08571	0.19653	0.07358	0.00135	-0.00307	0.00797
O12B	0.08678	0.06565	0.04438	0.00349	0.00669	0.01834
C14C	0.09730	0.05695	0.07801	0.02115	-0.00144	-0.00344
C15C	0.03507	0.07409	0.05736	0.01528	0.01393	0.01209

O11C	0.07039	0.07258	0.05074	0.01223	0.01721	0.01112
C16C	0.07197	0.05718	0.05280	-0.00386	0.01541	0.01153
C17C	0.08490	0.05595	0.08476	0.00041	-0.01357	0.01952
O12C	0.07030	0.07257	0.02927	0.00840	0.02666	0.00181

Computation details

Computations were carried out by using the Gaussian03 suite of programs. The elementary geometric optimization and the frequency analysis were performed at the level of Becke three Lee-Yan-Parr (B3LYP) Functionals [1]. All of the optimized structures were characterized to be local energy minima on the potential surface without any imaginary frequencies.

The gas phase heat of formation (HOF) (Table S6) was determined by using the method of isodesmic reactions [3]. For the compounds reported here, the isodesmic reactions were carried out as Hakima Abou-Rachid did [4] The accuracy of the method was also proved by the HOF prediction, as shown in Table S6. According to the optimized structures, the total energy (E_0) and thermodynamic parameters, including zero point energy (ZPE) and thermal correction to enthalpy (HT), were obtained at the B3LYP/6-311+G** level [5] .298 K



Scheme1. Isodesmic reactions for compound **4a**

$A_aB_bC_c(g) \rightarrow aA(g)+bB(g)+cC(g)$

$$\Delta H_{298} = \sum \Delta_f H_P - \sum \Delta_f H_R$$

$$\Delta H_{298} = \Delta E_{298} + \Delta(PV) = \Delta E_0 + \Delta E_{ZPE} + \Delta H_T + \Delta nRT$$

Table 10 Table Theoretical total energies, zero-point vibrational energies, thermal corrections for enthalpies and heat of formation (HOF) for 8 and the reference compounds

compound	E_0 (a.u.)	**zero-point(KJ/**mol**)**	**HT(KJ/mol)**	**HOF(KJ/mol)**
4a	**-2861.52**	**885.36**	**114.22**	**613.58**
CH4	**-40.53**	**112.26**	**10.04**	**-74.6**
CH3NO2	**-245.09**	**124.93**	**11.6**	**-80.8**

benzene	**-232.31**	**252.53**	**14.44**	**82.93**
CH_3OCH_3	**-155.07**	**199.82**	**14.05**	**-184.1**

In addition, Detonation velocity (D) and detonation pressure (P) were evaluated by the empirical Kamlet formula as

$P = 1.558\ \rho^2\ \Phi$ (1)

$D = 1.01\ \Phi^{1/2}\ (1+1.30\ \rho_0)$ (2)

$\Phi = 0.4889\ N\ (MQ)^{1/2}$ (3)

Where D is the predicted detonation velocity (km/s) and P is the detonation pressure (GPa), ρ is the density of a compound (cm^3 /mol). Φ, N, M and Q are characteristic parameters of an explosive, Q is chemical energy of detonation (kJ/g). The crystal densities and the calculated heats of formation were used in computing the D and P values

Table 11 heoretical total energies, zero-point vibrational energies, thermal corrections for enthalpies and heat of formation 6-8

Compound	E_0 (a.u.)	ZPE (kJ·mol^{-1})	ΔH_T (kJ·mol^{-1})	HOF (kJ·mol^{-1})
4a	**-2861.52**	**885.36**	**114.22**	**613.58**
4b	**-2940.32**	**1028.68**	**126.15**	**404.46**
5	**-2972.44**	**976.67**	**122.82**	**287.85**

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