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Supporting Information

$C_8N_{12}O_{10}$: A Promising Energetic Compound with Excellent Detonation Performance and Desirable Sensitivity

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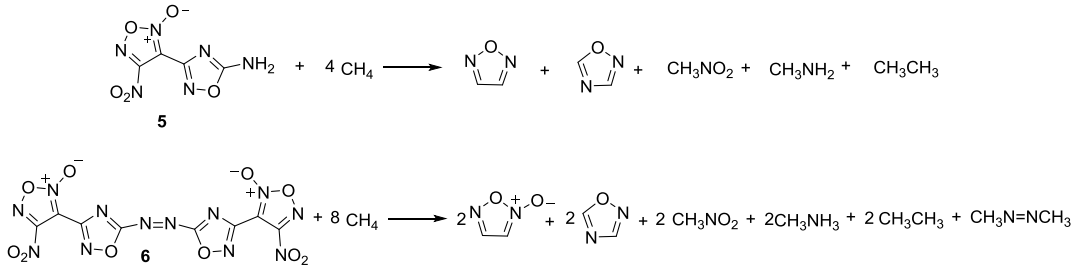
1. Computational Details

The geometric optimization, frequency analysis and single-point energies were accomplished by using Gaussian 09 package at the B3LYP 6-311+G** level. [1-4] All of the optimized structures were characterized to be local energy minima on the potential surface without any imaginary frequencies. Atomization energies were calculated by the CBS-4M.[5] All the optimized structures were characterized to be true local energy minima on the potential-energy surface without imaginary frequencies.

The predictions of heats of formation (HOF) of compounds through designed isodesmic reactions. The isodesmic reaction processes, that is, the number of each kind of formal bond is conserved, were used with the application of the bond separation reaction (BSR) rules. The molecule was broken down into a set of two heavy-atom molecules containing the same component bonds. The isodesmic reactions used to derive the HOF of neutral compounds **5** and **6** are shown in Scheme S1.



Scheme S1. The isodesmic reactions for calculating heat of formation for **5** and **6**

Table S1. Calculated zero-point energy (ZPE), thermal correction to enthalpy (H_T), total energy (E_0) and heats of formation (HOF)

Compound	E_0 / a. u	*ZPE* / kJ mol^{-1}	ΔH_T / kJ mol^{-1}	HOF/kJ mol^{-1}
5	-858.1683916	239.37	35.47	411.66
6	-1713.817052	366.40	66.50	1188.78
CH_4	-40.5339263	112.26	10.04	-74.60
furazan	-262.1183629	114.62	11.84	215.72
furoxan	-337.3042877	124.09	14.34	224.73
1,2,4-oxadiazole	-262.1529348	116.90	11.67	99.80
$CH_3N{=}NCH_3$	-189.3337358	211.85	16.32	147.85
CH_3NO_2	-245.0915559	124.93	11.60	-80.80
CH_3CH_3	-79.8565413	187.31	11.79	-84.01

2. Crystallographic data for 5 and 6

Table S2 Crystallographic data for **5 and 6**

empirical formula	$C_4H_2N_6O_5$	$C_8N_{12}O_{10}$
formula weight	214.12	424.20
temperature/K	173(2)	173(2)
crystal system	monoclinic	monoclinic
space group	$P2_1/c$	$P2_1/c$
a/Å	6.0977(4)	11.2116(12)
b/Å	8.2774(6)	5.9944(8)
c/Å	15.1568(10)	10.8652(11)
α/°	90	90
β/°	97.006(3)	95.429(4)

γ/°	90	90
Volume/Å^3	759.30(9)	726.94(14)
Z	4	2
ρ_{calc} mg/mm^3	1.873	1.938
m/mm^{-1}	0.172	0.179
F(000)	432.0	424.0
Crystal size/mm^3	0.25×0.21×0.18	0.32×0.23×0.04
2Θ range for data collection	5.618 to 50.81°	7.302 to 50.926°
Index ranges	-7≤h≤7,-9≤k≤9, -18≤l≤17	-13 ≤ h ≤ 13, -7 ≤k ≤ 6, -13 ≤l≤ 12
Reflections collected	6683	5466
Independent reflections	1397[R(int) = 0.0495]	1330[R(int) = 0.0555]
Data/restraints/parameters	1397/0/142	1330/0/136
Goodness-of-fit on F^2	1.043	1.051
Final R indexes [I>=2σ (I)]	0.0363, 0.0749	0.0525， 0.1299
Final R indexes [all data]	0.0590, 0.0831	0.0764， 0.1349
CCDC	1572565	1850981

Table S3 Selected bond lengths [Å] and angles [°] for compound **5**

C(1)-C(2)	1.411(3)	N(1)-O(2)	1.215(2)
C(1)-C(3)	1.455(3)	N(2)-O(1)	1.367(2)
C(1)-N(1)	1.331(2)	N(3)-O(3)	1.431(2)
C(2)-N(2)	1.293(2)	N(5)-H(5A)	0.84(2)
C(2)-N(6)	1.458(2)	N(5)-H(5B)	0.86(2)
C(3)-N(3)	1.302(3)	N(6)-O(4)	1.214(2)
C(3)-N(4)	1.361(2)	N(6)-O(5)	1.213(2)
C(4)-N(4)	1.316(2)	C(2)-C(1)-C(3)	132.24(18)
C(4)-N(5)	1.310(2)	N(1)-C(1)-C(2)	104.77(16)
C(4)-O(3)	1.348(2)	N(1)-C(1)-C(3)	122.96(17)
N(1)-O(1)	1.466(2)	C(1)-C(2)-N(6)	127.84(17)
N(2)-C(2)-C(1)	114.56(18)	C(2)-N(2)-O(1)	105.78(15)
N(2)-C(2)-N(6)	117.31(16)	C(3)-N(3)-O(3)	101.53(14)
N(3)-C(3)-C(1)	118.99(17)	C(4)-N(4)-C(3)	101.43(16)
N(3)-C(3)-N(4)	117.44(17)	C(4)-N(5)-H(5A)	118.7(15)
N(4)-C(3)-C(1)	123.57(18)	C(4)-N(5)-H(5B)	119.2(15)
N(4)-C(4)-O(3)	113.19(16)	H(5A)-N(5)-H(5B)	122(2)
N(5)-C(4)-N(4)	128.85(19)	O(4)-N(6)-C(2)	117.94(16)
N(5)-C(4)-O(3)	117.96(17)	O(5)-N(6)-C(2)	115.80(16)
C(1)-N(1)-O(1)	107.05(14)	O(5)-N(6)-O(4)	126.21(18)
O(2)-N(1)-C(1)	136.26(16)	N(2)-O(1)-N(1)	107.84(12)
O(2)-N(1)-O(1)	116.68(15)	C(4)-O(3)-N(3)	106.41(14)

Table S4. Selected bond lengths [Å] and angles [°] for compound **6**

O1-N2	1.407(3)	N2-C1	1.304(4)
O1-C2	1.341(4)	N3-C1	1.378(4)
O2-N4	1.468(3)	N3-C2	1.292(4)
O2-N5	1.357(4)	N4-C3	1.333(4)
O3-N4	1.209(4)	N5-C4	1.290(4)
O4-N6	1.221(4)	N6-C4	1.455(5)
O5-N6	1.218(5)	C1-C3	1.464(5)
N1-C2	1.406(4)	C3-C4	1.411(5)
N1-N1_a	1.257(3)	N2-C1-N3	115.5(3)
N2 -O1-C2	105.5(2)	N2-C1-C3	120.4(3)
N4 -O2-N5	108.4(2)	N3-C1-C3	124.0(3)
N1_a-N1-C2	112.2(2)	O1-C2-N1	121.1(3)
O1 -N2-C1	103.1(2)	O1-C2-N3	115.0(3)
C1 -N3-C2	101.0(3)	N1-C2-N3	123.9(3)
O2 -N4-O3	118.0(2)	N4-C3-C1	120.7(3)
O2 -N4-C3	106.2(3)	N4-C3-C4	105.3(3)
O3 -N4-C3	135.8(3)	C1-C3-C4	134.0(3)
O2 -N5-C4	106.0(3)	N5-C4-N6	118.6(3)
O4 -N6-O5	126.3(3)	N5-C4-C3	114.2(3)
O4 -N6-C4	115.9(3)	N6-C4-C3	127.0(3)
O5 -N6-C4	117.7(3)	O2 -N4-C3 -C1	176.8(3)
N2 -O1-C2 -N3	-0.1(4)	O3 -N4-C3 -C4	-179.4(3)
C2 -O1-N2 -C1	0.2(3)	O3 -N4-C3 -C1	-1.2(6)
N2 -O1-C2 -N1	-179.5(3)	O2 -N4-C3 -C4	-1.4(3)
N5 -O2-N4 -O3	179.9(3)	O2 -N5-C4 -N6	174.9(3)
N4 -O2-N5 -C4	-0.9(3)	O2 -N5-C4 -C3	0.0(4)
N5 -O2-N4 -C3	1.5(3)	O4 -N6-C4 -C3	21.8(5)
N1_a-N1-C2 -O1	-0.7(4)	O5 -N6-C4 -C3	-160.6(4)
C2 -N1-N1_a-C2_a	-180.0(3)	O4 -N6-C4 -N5	-152.4(3)
N1_a-N1-C2 -N3	179.9(3)	O5 -N6-C4 -N5	25.3(5)
O1 -N2-C1 -N3	-0.3(4)	N2 -C1-C3 -C4	-152.6(4)
O1 -N2-C1 -C3	-177.7(3)	N2 -C1-C3 -N4	29.7(5)
C1 -N3-C2 -N1	179.3(3)	N3 -C1-C3 -C4	30.2(6)
C2 -N3-C1 -C3	177.6(3)	N3-C1-C3-N4	-147.5(3)
C1 -N3-C2 -O1	-0.1(4)	C1-C3-C4-N6	8.7(6)
C2 -N3-C1 -N2	0.3(4)	N4-C3-C4-N5	1.0(4)
N4-C3-C4-N6	-173.4(3)	C1-C3-C4-N5	-177.0(4)

3. Spectrums of compounds 3-6

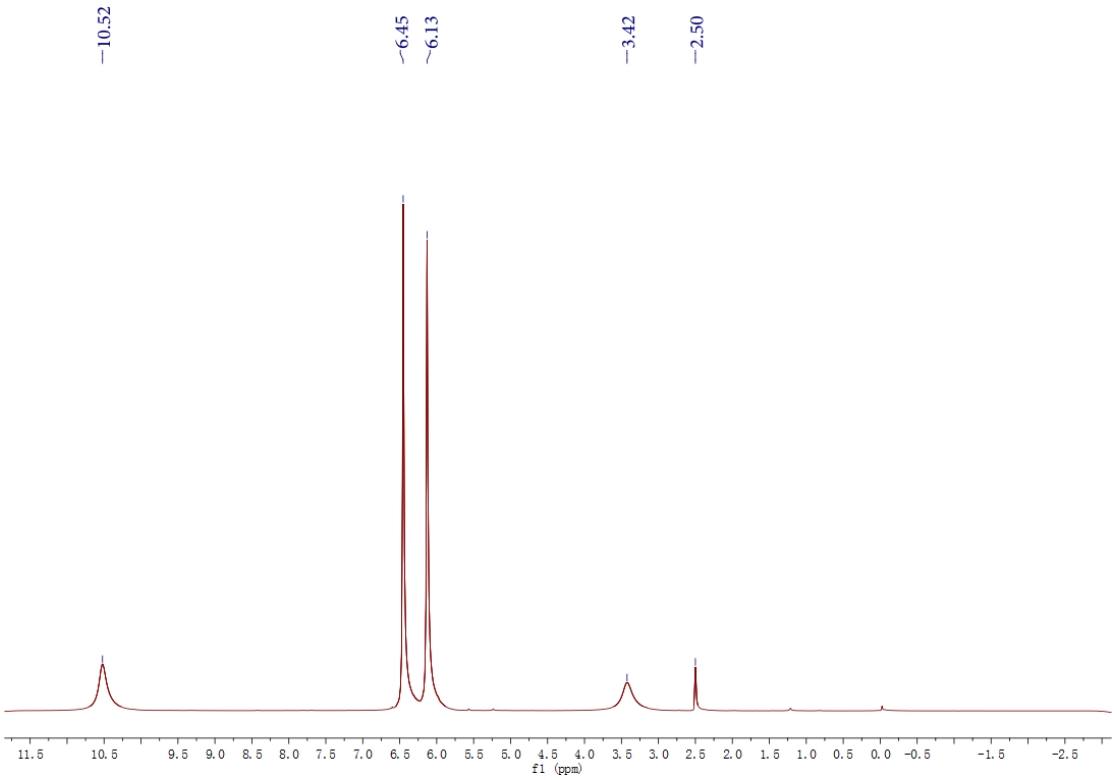


Figure S1. 1H NMR spectra in DMSO-d6 for **3**.

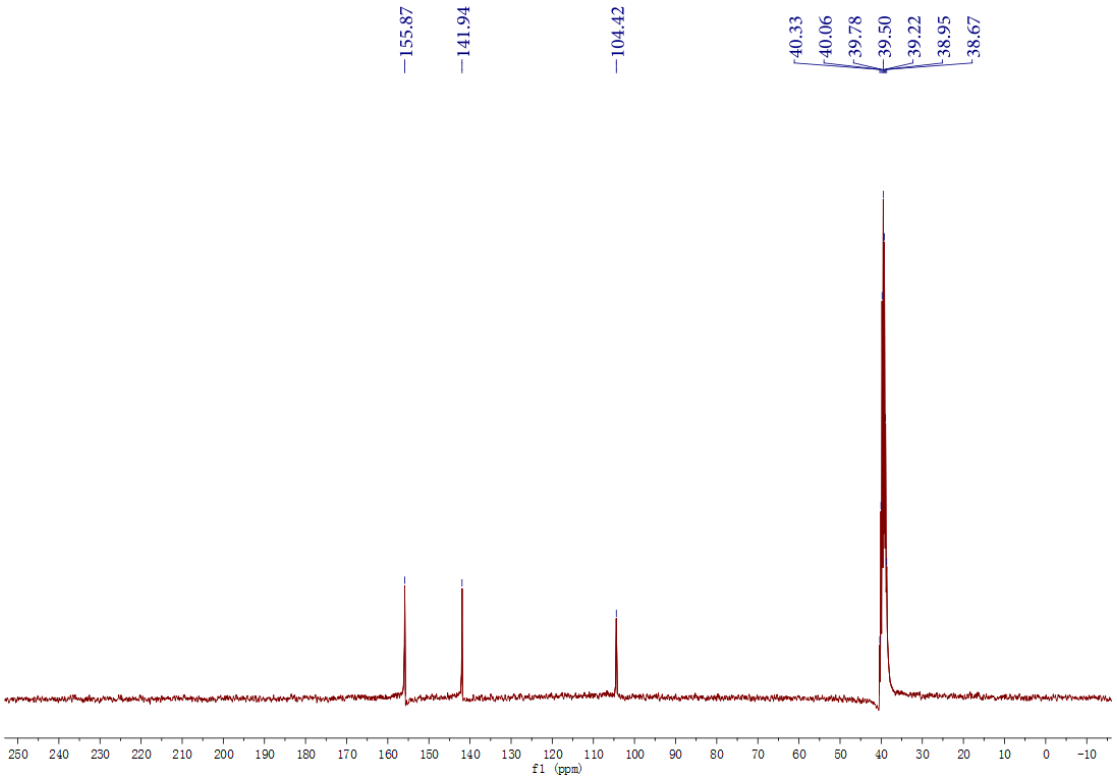


Figure S2. ^{13}C NMR spectra in DMSO-d_6 for **3.**

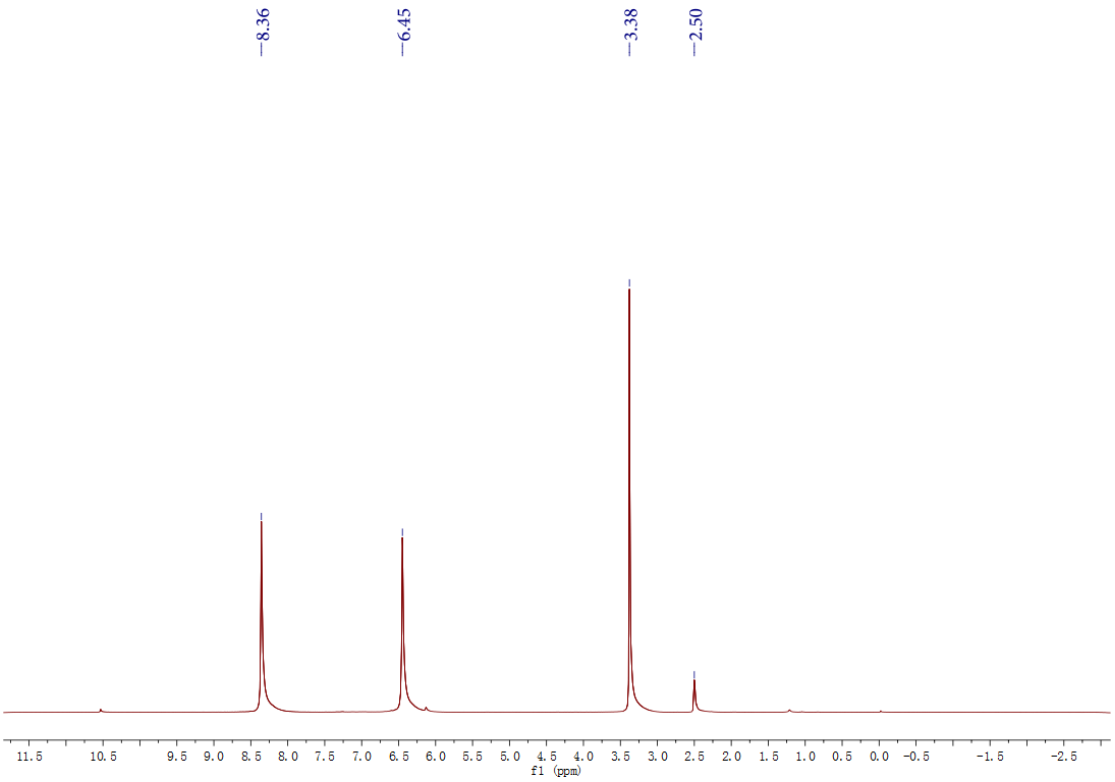


Figure S3. ^{1}H NMR spectra in DMSO-d_6 for **4.**

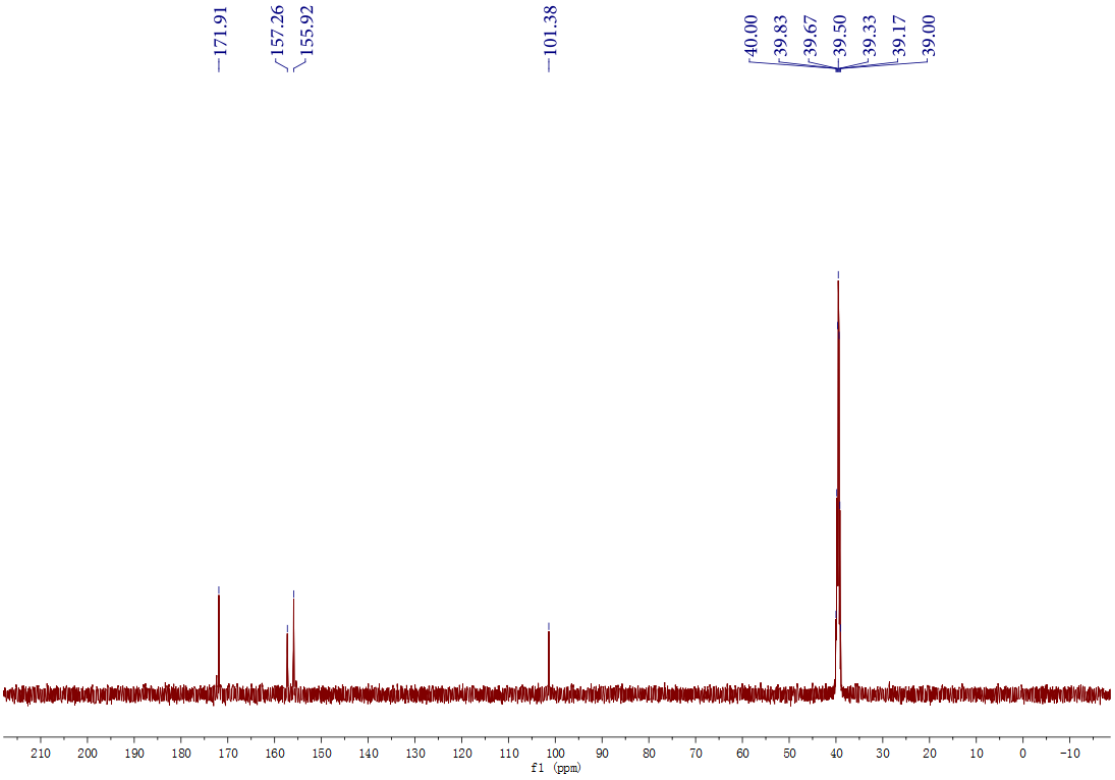


Figure S4. ^{13}C NMR spectra in DMSO-d_6 for **4.**

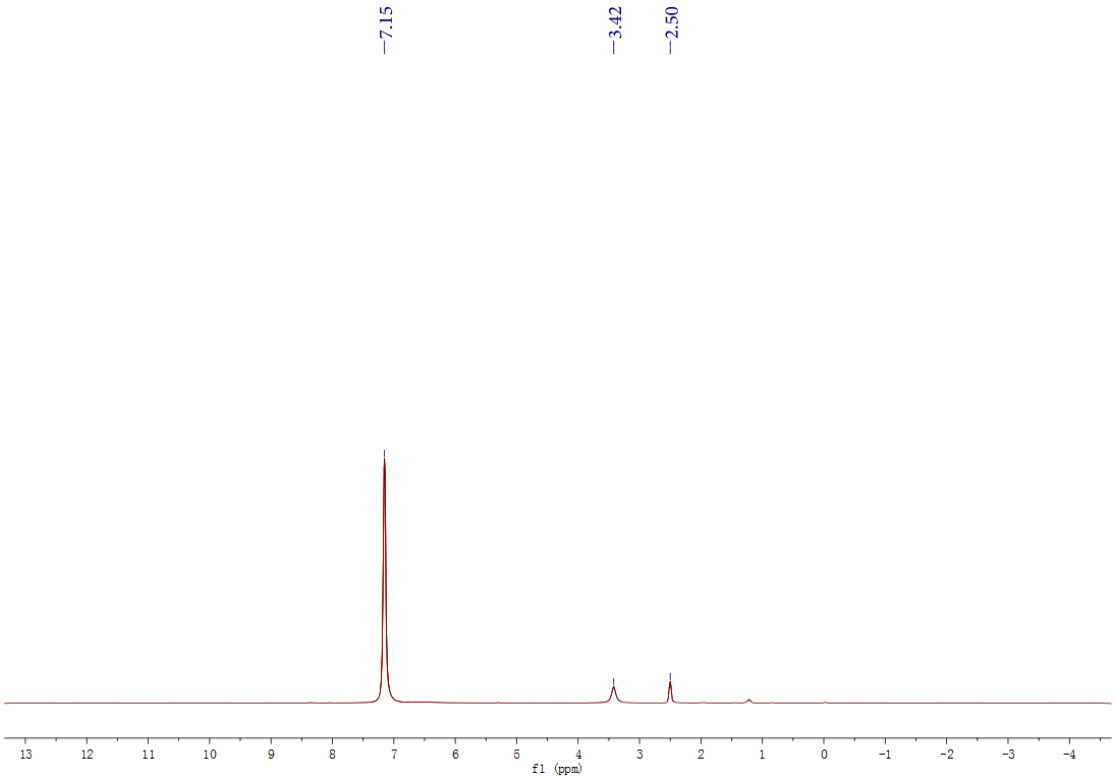


Figure S5. ^{1}H NMR spectra in DMSO-d_6 for **5.**

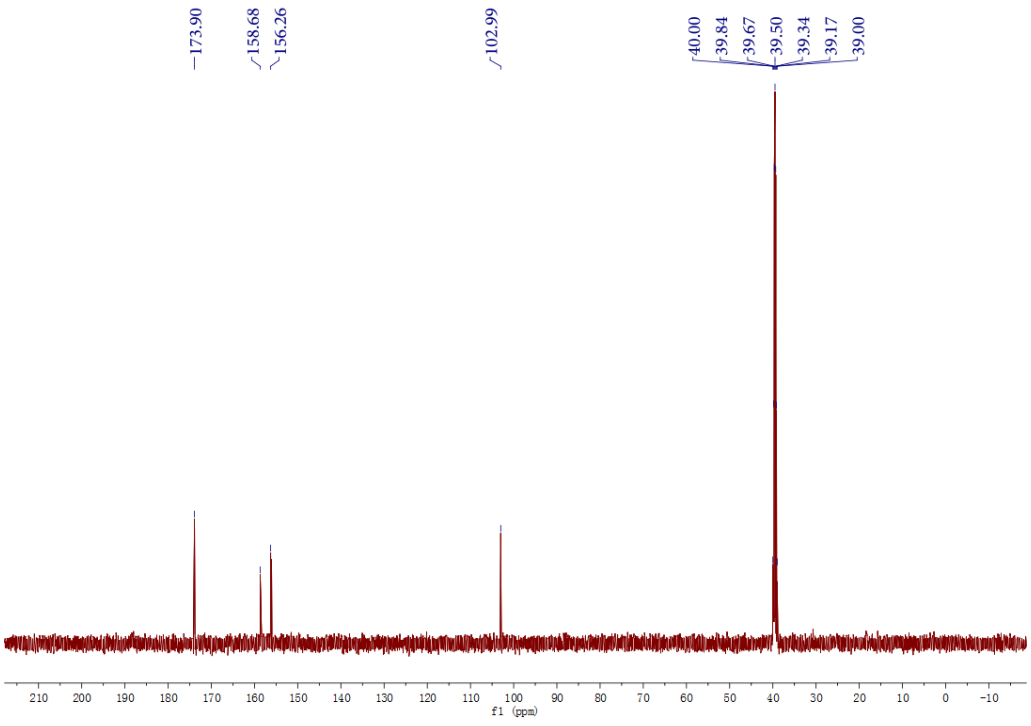


Figure S6. ^{13}C NMR spectra in DMSO-d_6 for **5**.

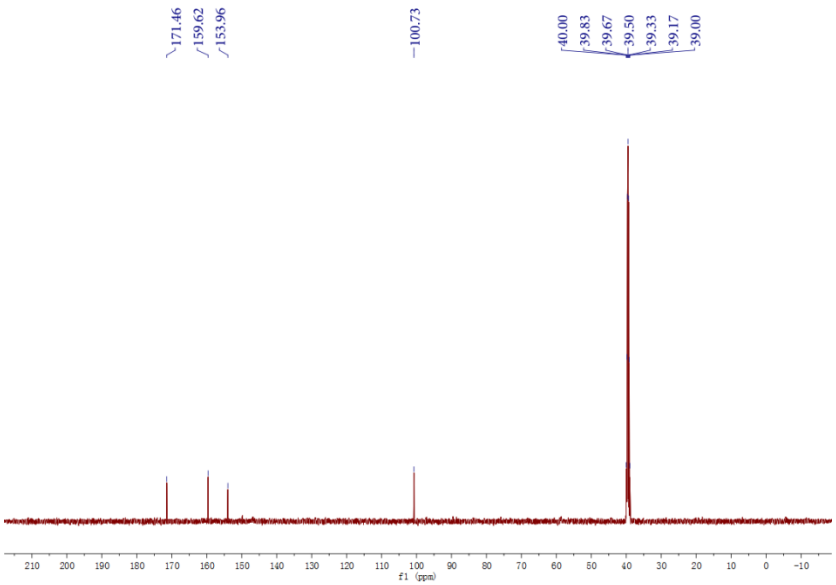


Figure S7. ^{13}C NMR spectra in DMSO-d_6 for **6**.

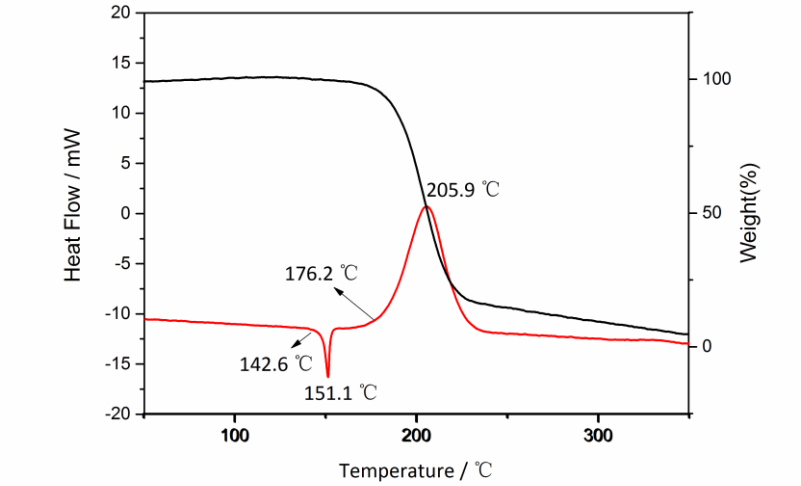


Figure S8: TG and DSC curves of **5** measured at a heating rate of 5 ℃ min^{-1} (exo up).

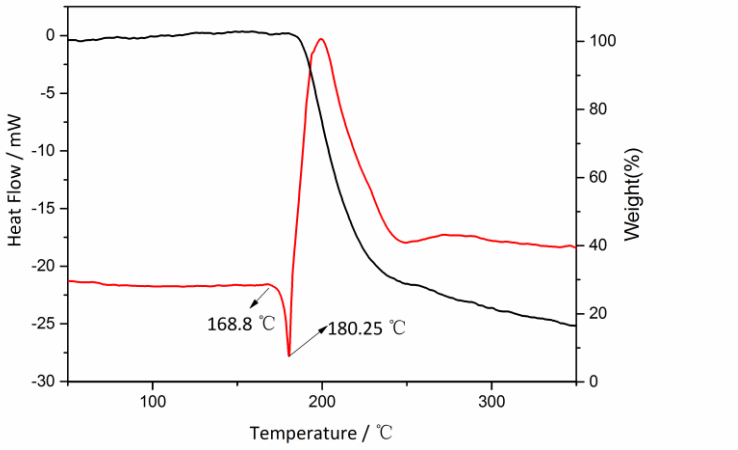


Figure S9: TG and DSC curves of **6** measured at a heating rate of 5 ℃ min^{-1} (exo up).

4. References

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