Electronic Supplementary Material (ESI) for Dalton Transactions.

Electronic Supporting Information

N,N'-Methylenebis(N-(1,2,5-oxadiazol-3-yl)nitramide) Derivatives as Metal-free Green Primary Explosives

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Crystallographic data

Table S1. Selected crystal parameters of **6**.

Empirical formula	$C_7H_{10}N_{14}O_{16}$ (**6**)
CCDC Number	1846164
Formula weight	546.29
Temperature/K	150(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	11.8644(10)
b/Å	12.1879(10)
c/Å	19.9991(16)
α/º	90
β/º	98.3080(10)
γ/º	90
Volume/Å^3	1892.8(3)
Z	4
ρ_{calc} g/cm^3 (-123 ºC)	1.917
ρ_{calc} g/cm^3 (20 ºC)	1.886
μ/mm^{-1}	0.186
F(000)	1112
Crystal size/mm^3	0.330 x 0.145 x 0.117
θ range/º	3.153 - 30.027
Reflections collected	20793
Independent reflections	5335 [R_{int} = 0.0367]
Data/restraints/parameters	5335/0/342
Goodness-of-fit on F^2	1.018
Final R indexes [I>=2σ (I)]	R_1 = 0.0373, wR_2 = 0.0847
Final R indexes [all data]	R_1 = 0.0575, wR_2 = 0.0932
Largest diff. peak/hole / e Å^{-3}	0.377/-0.306

Figures S1 to S6

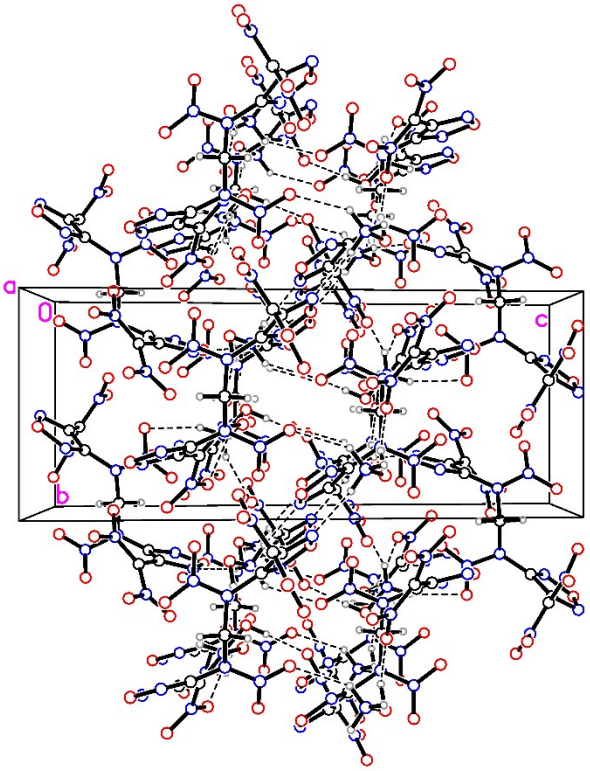


Fig. S1. Unit cell view for **6** along *a* axis, hydrogen bonds are marked as dotted lines.

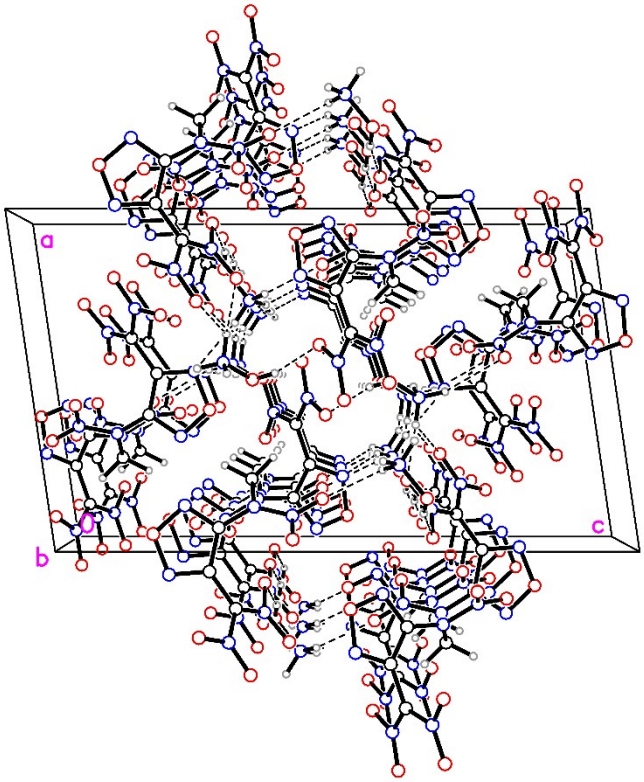


Fig. S2. Unit cell view for **6** along *b* axis, hydrogen bonds are marked as dotted lines.

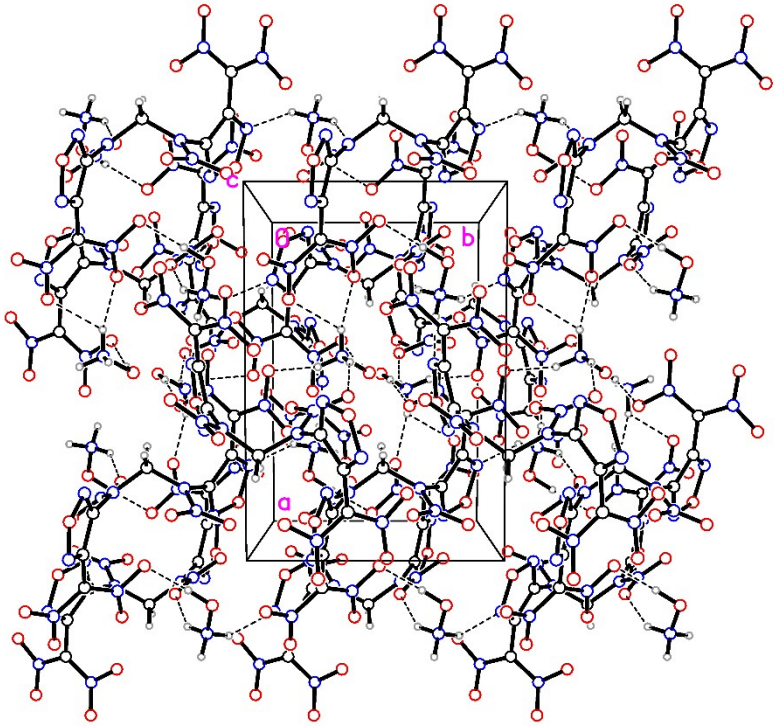


Fig. S3. Unit cell view for **6** along *c* axis, hydrogen bonds are marked as dotted lines.

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **6**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z
O(1)	11818(1)	449(1)	7504(1)
O(2)	12887(1)	1397(1)	6803(1)
N(3)	12019(1)	1475(2)	7074(1)
C(4)	11203(1)	2751(2)	6909(1)
N(5)	11379(1)	4011(1)	6481(1)
O(6)	12197(1)	4101(1)	6151(1)
O(7)	10637(1)	5161(1)	6422(1)
C(8)	10195(1)	2807(2)	7245(1)
N(9)	10255(1)	2421(2)	7884(1)
O(10)	9161(1)	2536(1)	8043(1)
N(11)	8406(1)	2995(1)	7488(1)
C(12)	9016(1)	3188(2)	7002(1)
N(13)	8471(1)	3874(1)	6398(1)
N(14)	8689(1)	3196(2)	5796(1)
O(15)	9283(1)	1959(1)	5836(1)
O(16)	8255(1)	3906(1)	5281(1)
C(17)	7745(1)	5324(2)	6386(1)
N(18)	8351(1)	6893(1)	6358(1)
N(19)	8956(1)	7491(2)	6952(1)

O(20)	9033(1)	6568(1)	7440(1)
O(21)	9356(1)	8889(1)	6943(1)
C(22)	8350(1)	7847(2)	5770(1)
N(23)	9238(1)	7960(2)	5459(1)
O(24)	8901(1)	8971(1)	4918(1)
N(25)	7777(1)	9451(2)	4896(1)
C(26)	7426(1)	8771(2)	5421(1)
C(27)	6257(1)	8917(2)	5555(1)
N(28)	5939(1)	10264(1)	5918(1)
O(29)	6709(1)	11256(1)	6135(1)
O(30)	4937(1)	10454(1)	6024(1)
N(31)	5506(1)	7713(1)	5295(1)
O(32)	5971(1)	6486(1)	5033(1)
O(33)	4465(1)	7758(1)	5299(1)
N(34)	2721(1)	7729(2)	6024(1)
O(35)	1816(1)	8025(2)	6377(1)
N(36)	5484(1)	6396(1)	3448(1)
O(37)	5016(1)	5259(1)	3865(1)

Table S3. Bond lengths [Å] and angles [º] for **6**.

O(1)-N(3)	1.2410(16)	O(2)-N(3)	1.2325(16)
N(3)-C(4)	1.4182(18)	C(4)-N(5)	1.3648(17)
C(4)-C(8)	1.4537(19)	N(5)-O(6)	1.2519(15)
N(5)-O(7)	1.2724(15)	C(8)-N(9)	1.3080(17)
C(8)-C(12)	1.4460(19)	N(9)-O(10)	1.3829(16)
O(10)-N(11)	1.3733(15)	N(11)-C(12)	1.3014(18)
C(12)-N(13)	1.3982(17)	N(13)-N(14)	1.3797(16)
N(13)-C(17)	1.4507(17)	N(14)-O(15)	1.2177(15)
N(14)-O(16)	1.2250(15)	C(17)-N(18)	1.4600(17)
C(17)-H(17A)	0.9900	C(17)-H(17B)	0.9900
N(18)-N(19)	1.3828(16)	N(18)-C(22)	1.4056(17)
N(19)-O(20)	1.2208(15)	N(19)-O(21)	1.2241(15)
C(22)-N(23)	1.3008(19)	C(22)-C(26)	1.4221(19)
N(23)-O(24)	1.3687(16)	O(24)-N(25)	1.3830(16)
N(25)-C(26)	1.3049(17)	C(26)-C(27)	1.4555(19)
C(27)-N(31)	1.3687(17)	C(27)-N(28)	1.3880(17)
N(28)-O(29)	1.2437(16)	N(28)-O(30)	1.2477(15)
N(31)-O(33)	1.2357(15)	N(31)-O(32)	1.2807(15
N(34)-O(35)	1.3882(17)	N(34)-H(34A)	0.9100
N(34)-H(34B)	0.9100	N(34)-H(34C)	0.9100
O(35)-H(35)	0.98(2)	N(36)-O(37)	1.4068(15)
N(36)-H(36A)	0.9100	N(36)-H(36B)	0.9100

N(36)-H(36C)	0.9100	O(37)-H(37)	0.82(2)
O(2)-N(3)-O(1)	121.73(12)	O(2)-N(3)-C(4)	121.42(12)
O(1)-N(3)-C(4)	116.84(12)	N(5)-C(4)-N(3)	121.60(12)
N(5)-C(4)-C(8)	118.53(12)	N(3)-C(4)-C(8)	119.68(12)
O(6)-N(5)-O(7)	119.21(11)	O(6)-N(5)-C(4)	125.12(12)
O(7)-N(5)-C(4)	115.68(12)	N(9)-C(8)-C(12)	106.97(12)
N(9)-C(8)-C(4)	120.76(12)	C(12)-C(8)-C(4)	132.25(12)
C(8)-N(9)-O(10)	106.78(11)	N(11)-O(10)-N(9)	110.87(10)
C(12)-N(11)-O(10)	105.53(11)	N(11)-C(12)-N(13)	117.01(12)
N(11)-C(12)-C(8)	109.84(12)	N(13)-C(12)-C(8)	132.67(12)
N(14)-N(13)-C(12)	118.39(11)	N(14)-N(13)-C(17)	119.37(11)
C(12)-N(13)-C(17)	122.14(11)	O(15)-N(14)-O(16)	127.34(12)
O(15)-N(14)-N(13)	116.56(11)	O(16)-N(14)-N(13)	116.10(12)
N(13)-C(17)-N(18)	113.85(11)	N(13)-C(17)-H(17A)	108.8
N(18)-C(17)-H(17A)	108.8	N(13)-C(17)-H(17B)	108.8
N(18)-C(17)-H(17B)	108.8	H(17A)-C(17)-H(17B)	107.7
N(19)-N(18)-C(22)	117.78(11)	N(19)-N(18)-C(17)	117.77(11)
C(22)-N(18)-C(17)	124.44(11)	O(20)-N(19)-O(21)	126.03(12)
O(20)-N(19)-N(18)	116.39(11)	O(21)-N(19)-N(18)	117.58(11)
N(23)-C(22)-N(18)	122.35(13)	N(23)-C(22)-C(26)	110.44(12)
N(18)-C(22)-C(26)	127.19(13)	C(22)-N(23)-O(24)	104.78(11)
N(23)-O(24)-N(25)	111.23(10)	C(26)-N(25)-O(24)	105.96(11)
N(25)-C(26)-C(22)	107.59(12)	N(25)-C(26)-C(27)	122.53(12)
C(22)-C(26)-C(27)	129.76(12)	N(31)-C(27)-N(28)	122.86(12)
N(31)-C(27)-C(26)	117.28(12)	N(28)-C(27)-C(26)	119.83(12)
O(29)-N(28)-O(30)	122.05(12)	O(29)-N(28)-C(27)	116.45(12)
O(30)-N(28)-C(27)	121.50(12)	O(33)-N(31)-O(32)	120.99(11)
O(33)-N(31)-C(27)	124.96(12)	O(32)-N(31)-C(27)	114.05(12)
O(35)-N(34)-H(34A)	109.5	O(35)-N(34)-H(34B)	109.5
H(34A)-N(34)-H(34B)	109.5	O(35)-N(34)-H(34C)	109.5
H(34A)-N(34)-H(34C)	109.5	H(34B)-N(34)-H(34C)	109.5
N(34)-O(35)-H(35)	102.4(13)	O(37)-N(36)-H(36A)	109.5
O(37)-N(36)-H(36B)	109.5	H(36A)-N(36)-H(36B)	109.5
O(37)-N(36)-H(36C)	109.5	H(36A)-N(36)-H(36C)	109.5
H(36B)-N(36)-H(36C)	109.5	N(36)-O(37)-H(37)	103.3(15)

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}
O(1)	26(1)	27(1)	31(1)	16(1)	11(1)
O(2)	17(1)	22(1)	47(1)	9(1)	17(1)
N(3)	13(1)	16(1)	20(1)	3(1)	4(1)

C(4)	11(1)	15(1)	14(1)	3(1)	2(1)
N(5)	11(1)	16(1)	16(1)	2(1)	2(1)
O(6)	13(1)	26(1)	19(1)	6(1)	7(1)
O(7)	14(1)	17(1)	32(1)	9(1)	7(1)
C(8)	12(1)	11(1)	14(1)	1(1)	1(1)
N(9)	13(1)	21(1)	16(1)	3(1)	4(1)
O(10)	15(1)	25(1)	15(1)	7(1)	5(1)
N(11)	14(1)	17(1)	16(1)	4(1)	2(1)
C(12)	12(1)	10(1)	14(1)	1(1)	1(1)
N(13)	13(1)	13(1)	11(1)	0(1)	1(1)
N(14)	15(1)	18(1)	14(1)	-2(1)	1(1)
O(15)	21(1)	19(1)	23(1)	-6(1)	4(1)
O(16)	30(1)	31(1)	12(1)	2(1)	-2(1)
C(17)	10(1)	13(1)	17(1)	1(1)	0(1)
N(18)	17(1)	13(1)	13(1)	1(1)	-4(1)
N(19)	15(1)	16(1)	16(1)	-2(1)	-1(1)
O(20)	23(1)	20(1)	14(1)	3(1)	-2(1)
O(21)	37(1)	17(1)	25(1)	-1(1)	-3(1)
C(22)	12(1)	13(1)	14(1)	-1(1)	1(1)
N(23)	16(1)	19(1)	21(1)	2(1)	3(1)
O(24)	15(1)	25(1)	20(1)	4(1)	7(1)
N(25)	14(1)	18(1)	16(1)	2(1)	4(1)
C(26)	13(1)	12(1)	12(1)	-1(1)	2(1)
C(27)	12(1)	12(1)	12(1)	0(1)	2(1)
N(28)	16(1)	15(1)	13(1)	1(1)	3(1)
O(29)	24(1)	22(1)	26(1)	-9(1)	3(1)
O(30)	16(1)	23(1)	24(1)	-1(1)	8(1)
N(31)	13(1)	14(1)	12(1)	3(1)	1(1)
O(32)	18(1)	14(1)	19(1)	-4(1)	2(1)
O(33)	10(1)	22(1)	26(1)	3(1)	3(1)
N(34)	18(1)	19(1)	15(1)	1(1)	1(1)
O(35)	30(1)	26(1)	51(1)	-6(1)	23(1)
N(36)	16(1)	16(1)	15(1)	1(1)	3(1)
O(37)	39(1)	21(1)	15(1)	-3(1)	7(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **6 6.**.

	x	y	z
H(17A)	7365	5318	6796
H(17B)	7144	5251	5989
H(34A)	2833	8634	5769
H(34B)	2561	6834	5750
H(34C)	3362	7527	6321

H(35)	1380(20)	6990(30)	6307(11)
H(36A)	5184	7421	3497
H(36B)	5318	6069	3009
H(36C)	6253	6436	3568
H(37)	5191(18)	5650(30)	4243(11)

Table S6. Torsion angles [º] for **6**.

O(2)-N(3)-C(4)-N(5)	-4.6(2)	O(1)-N(3)-C(4)-N(5)	175.09(13)
O(2)-N(3)-C(4)-C(8)	-179.44(13)	O(1)-N(3)-C(4)-C(8)	0.27(19)
N(3)-C(4)-N(5)-O(6)	6.5(2)	C(8)-C(4)-N(5)-O(6)	-178.61(12)
N(3)-C(4)-N(5)-O(7)	-173.62(12)	C(8)-C(4)-N(5)-O(7)	1.25(18)
N(5)-C(4)-C(8)-N(9)	-137.34(14)	N(3)-C(4)-C(8)-N(9)	37.64(19)
N(5)-C(4)-C(8)-C(12)	44.8(2)	N(3)-C(4)-C(8)-C(12)	-140.20(14)
C(12)-C(8)-N(9)-O(10)	0.49(14)	C(4)-C(8)-N(9)-O(10)	-177.84(11)
C(8)-N(9)-O(10)-N(11)	0.33(14)	N(9)-O(10)-N(11)-C(12)	-1.08(14)
O(10)-N(11)-C(12)-N(13)	-171.72(11)	O(10)-N(11)-C(12)-C(8)	1.36(14)
N(9)-C(8)-C(12)-N(11)	-1.21(15)	C(4)-C(8)-C(12)-N(11)	176.85(14)
N(9)-C(8)-C(12)-N(13)	170.39(14)	C(4)-C(8)-C(12)-N(13)	-11.5(2)
N(11)-C(12)-N(13)-N(14)	-137.96(13)	C(8)-C(12)-N(13)-N(14)	50.9(2)
N(11)-C(12)-N(13)-C(17)	45.81(18)	C(8)-C(12)-N(13)-C(17)	-125.32(16)
C(12)-N(13)-N(14)-O(15)	5.21(18)	C(17)-N(13)-N(14)-O(15)	-178.45(12)
C(12)-N(13)-N(14)-O(16)	-175.18(12)	C(17)-N(13)-N(14)-O(16)	1.15(18)
N(14)-N(13)-C(17)-N(18)	-86.79(14)	C(12)-N(13)-C(17)-N(18)	89.40(15)
N(13)-C(17)-N(18)-N(19)	-78.96(15)	N(13)-C(17)-N(18)-C(22)	101.82(15)
C(22)-N(18)-N(19)-O(20)	-173.26(12)	C(17)-N(18)-N(19)-O(20)	7.47(18)
C(22)-N(18)-N(19)-O(21)	7.28(19)	C(17)-N(18)-N(19)-O(21)	-172.00(12)
N(19)-N(18)-C(22)-N(23)	72.86(17)	C(17)-N(18)-C(22)-N(23)	-107.91(16)
N(19)-N(18)-C(22)-C(26)	-108.60(16)	C(17)-N(18)-C(22)-C(26)	70.62(19)
N(18)-C(22)-N(23)-O(24)	179.59(12)	C(26)-C(22)-N(23)-O(24)	0.84(15)
C(22)-N(23)-O(24)-N(25)	-1.09(14)	N(23)-O(24)-N(25)-C(26)	0.91(14)
O(24)-N(25)-C(26)-C(22)	-0.36(14)	O(24)-N(25)-C(26)-C(27)	-176.71(11)
N(23)-C(22)-C(26)-N(25)	-0.32(16)	N(18)-C(22)-C(26)-N(25)	-178.99(13)
N(23)-C(22)-C(26)-C(27)	175.68(13)	N(18)-C(22)-C(26)-C(27)	-3.0(2)
N(25)-C(26)-C(27)-N(31)	90.92(16)	C(22)-C(26)-C(27)-N(31)	-84.54(18)
N(25)-C(26)-C(27)-N(28)	-87.34(17)	C(22)-C(26)-C(27)-N(28)	97.19(17)
N(31)-C(27)-N(28)-O(29)	178.91(12)	C(26)-C(27)-N(28)-O(29)	-2.93(18)
N(31)-C(27)-N(28)-O(30)	-0.4(2)	C(26)-C(27)-N(28)-O(30)	177.80(11)
N(28)-C(27)-N(31)-O(33)	6.8(2)	C(26)-C(27)-N(31)-O(33)	-171.42(12)
N(28)-C(27)-N(31)-O(32)	-173.56(12)	C(26)-C(27)-N(31)-O(32)	8.24(17)

Table S7. Hydrogen bonds for **6** [Å and º].

D-H...A	d(D-H)	d(H...A)	d(D...A)

N(34)-H(34A)...N(25)#3	0.91	2.10	2.9295(17)
N(34)-H(34B)...O(16)#2	0.91	2.23	3.0028(16)
N(34)-H(34C)...N(9)#1	0.91	2.12	3.0146(18)
O(35)-H(35)...O(7)#4	0.98(2)	1.75(2)	2.7076(16)
N(36)-H(36A)...O(30)#3	0.91	1.98	2.8219(16)
N(36)-H(36B)...O(21)#5	0.91	2.27	3.1201(16)
N(36)-H(36C)...O(2)#7	0.91	2.21	2.7266(16)
N(36)-H(36C)...O(6)#7	0.91	1.89	2.7816(16)
O(37)-H(37)...O(32)	0.82(2)	1.84(2)	2.6371(15)

Symmetry transformations used to generate equivalent atoms:

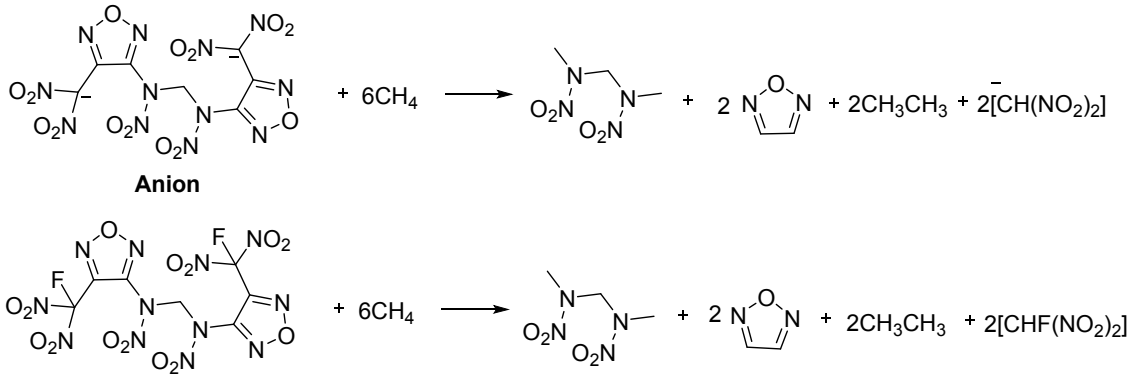
#1 -x+3/2, y+1/2,-z+3/2 #2 -x+1, -y+1, -z+1 #3 -x+1, -y+2, -z+1

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

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

Theoretical calculations

As mentioned in the manuscript, the heats of formation were determined using isodesmic reactions (**Scheme S1**). The calculations were carried out using Gaussian 03 (Revision D.01) suite of programs.[1] The geometric optimization and frequency analyses of the structures were calculated using B3LYP/6-31+G** level,[2] and single energy points were calculated at the MP2/6-311++G** level.[3] The heats of formation for the cations were obtained by an atomization approach using G2 ab initio method.[4] The heats of formation of other compounds in Scheme S1 were obtained from the NIST WebBook.[5]



Scheme S1. Isodesmic reactions.

Table S8 The heats of formation (HOF) for bis(2,5-dinitromethyl)-1,3,4-oxadiazole anion and **11**.[a]

Compounds	**ZPE** [Hartree/Particle]	**Hcorr** [Hartree/Particle]	**Mp-6-311++g**** [Hartree/Particle]	**HoF(gas)** [kJ mol^{-1}]
Anion	0.17775	0.206862	-1973.2013768	-784.8165576
11	0.18574	0.217373	-2172.4104146	298.1216829

[a] The enthalpy of sublimation was calculated by using Trouton's rule. Solid-state heats of formation of the resulting compounds were calculated with Equation (1) in which Tm is the melting temperature. $\Delta H_f = \Delta H_f(g) - \Delta H_{sub} = \Delta Hf(g) - 188[J\ mol^{-1}\ K^{-1}] \times T_m$ (1).

^{1}H and ^{13}C NMR spectra

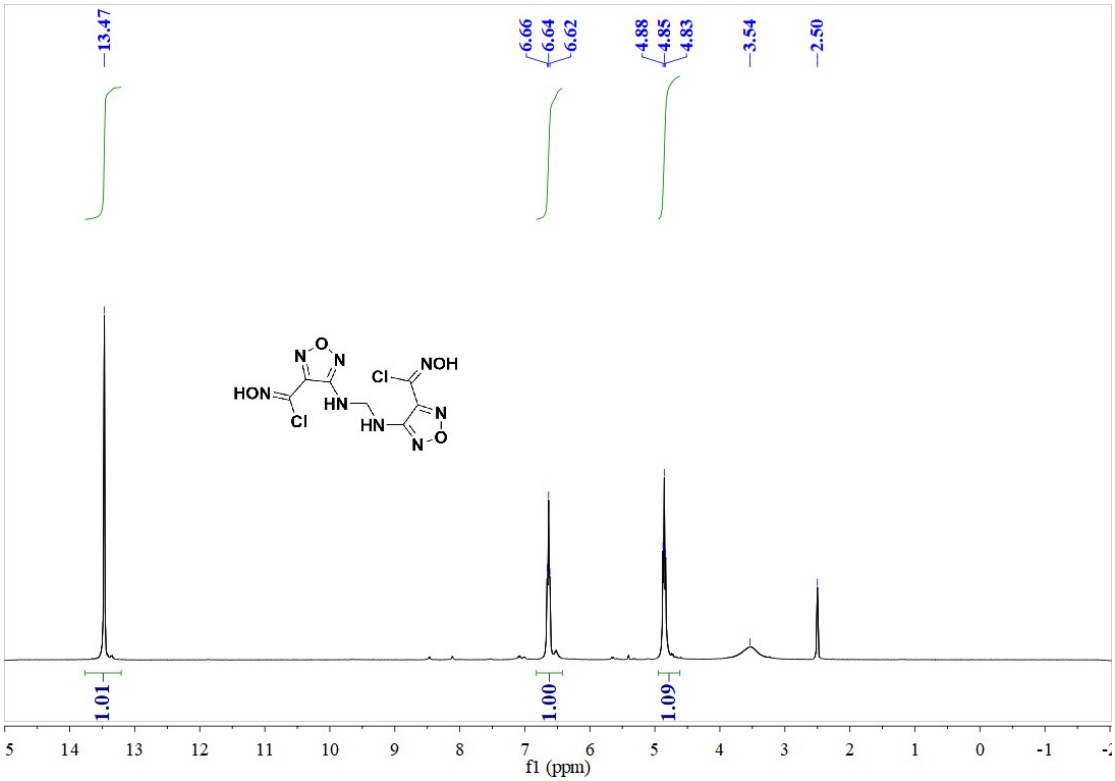


Fig S4 ^{1}H-NMR spectrum of **1** in d_6-DMSO.

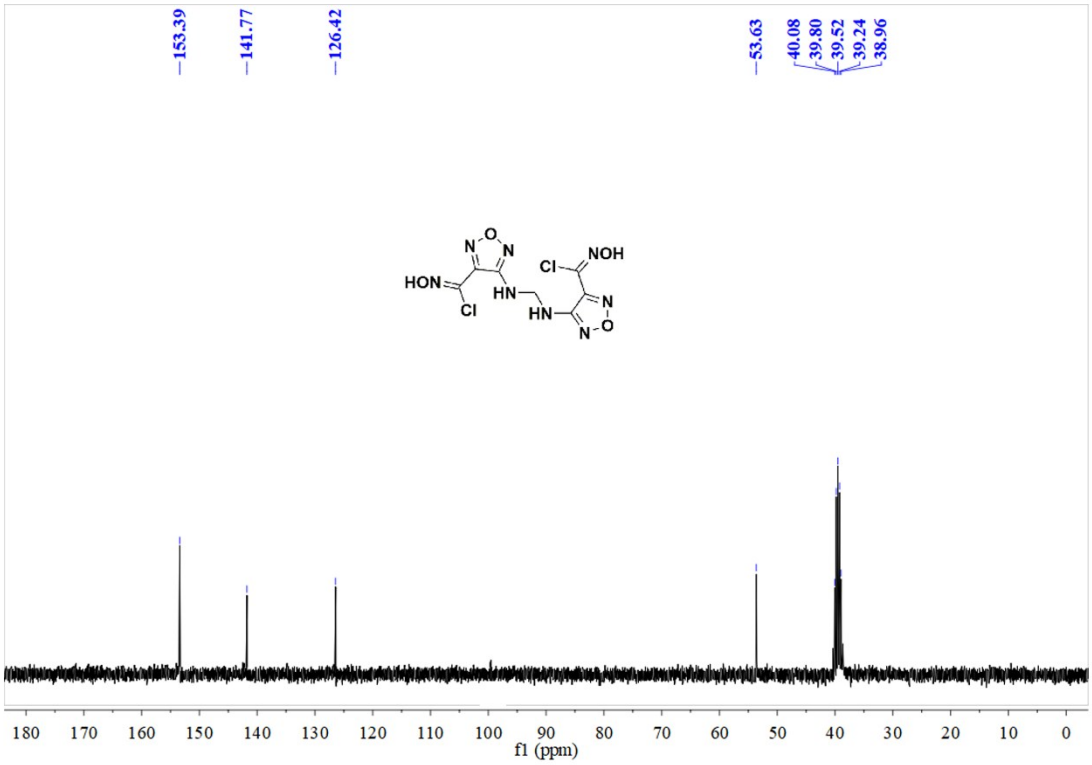


Fig S5 ^{13}C-NMR spectrum of **1** in d_6-DMSO.

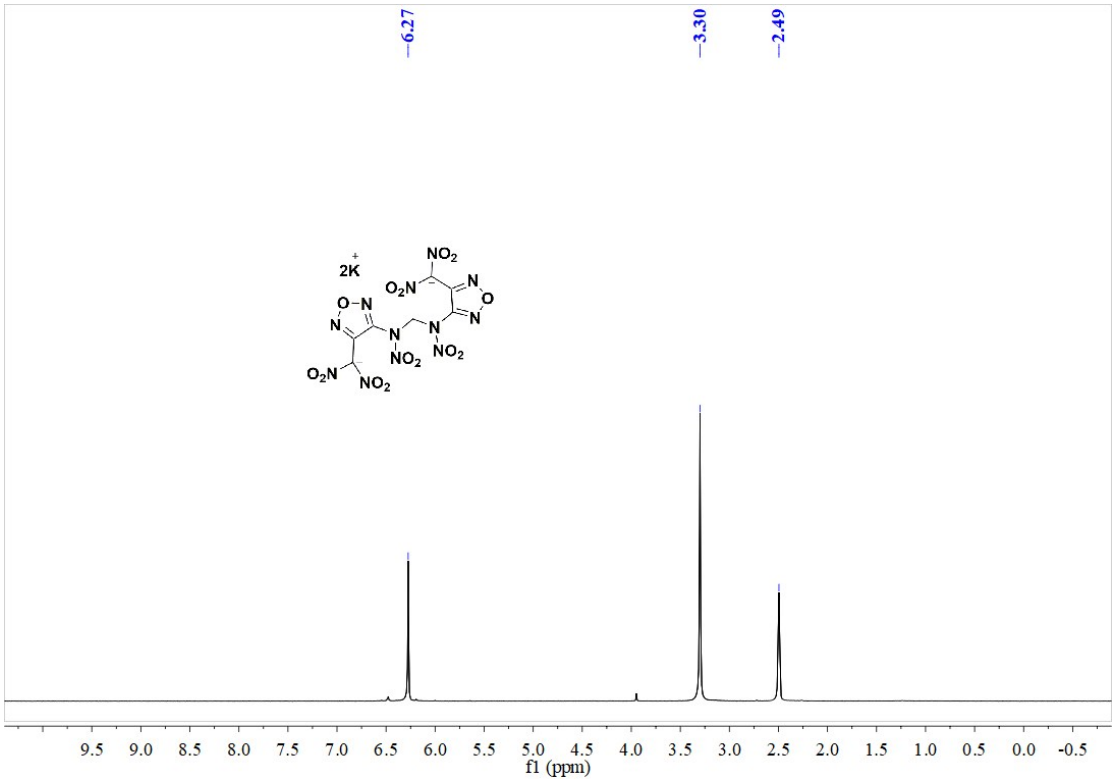


Fig S6 ^{1}H-NMR spectrum of **3** in d_6-DMSO.

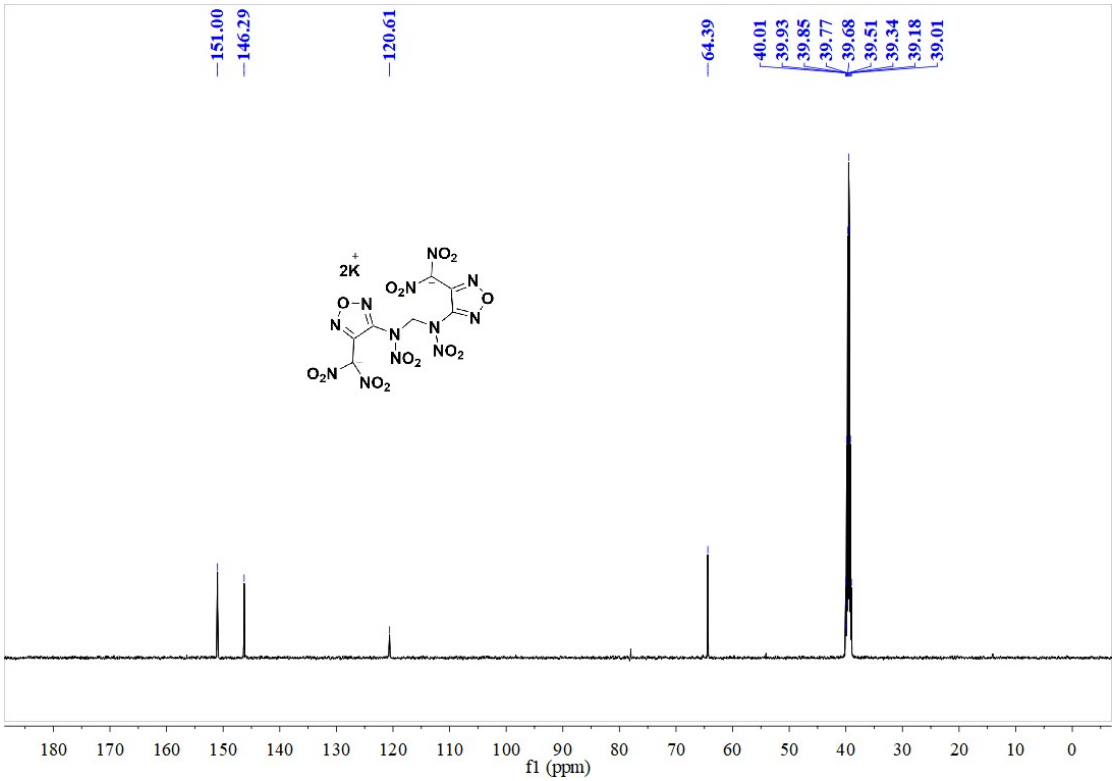


Fig S7 ^{13}C-NMR spectrum of **3** in d_6-DMSO.

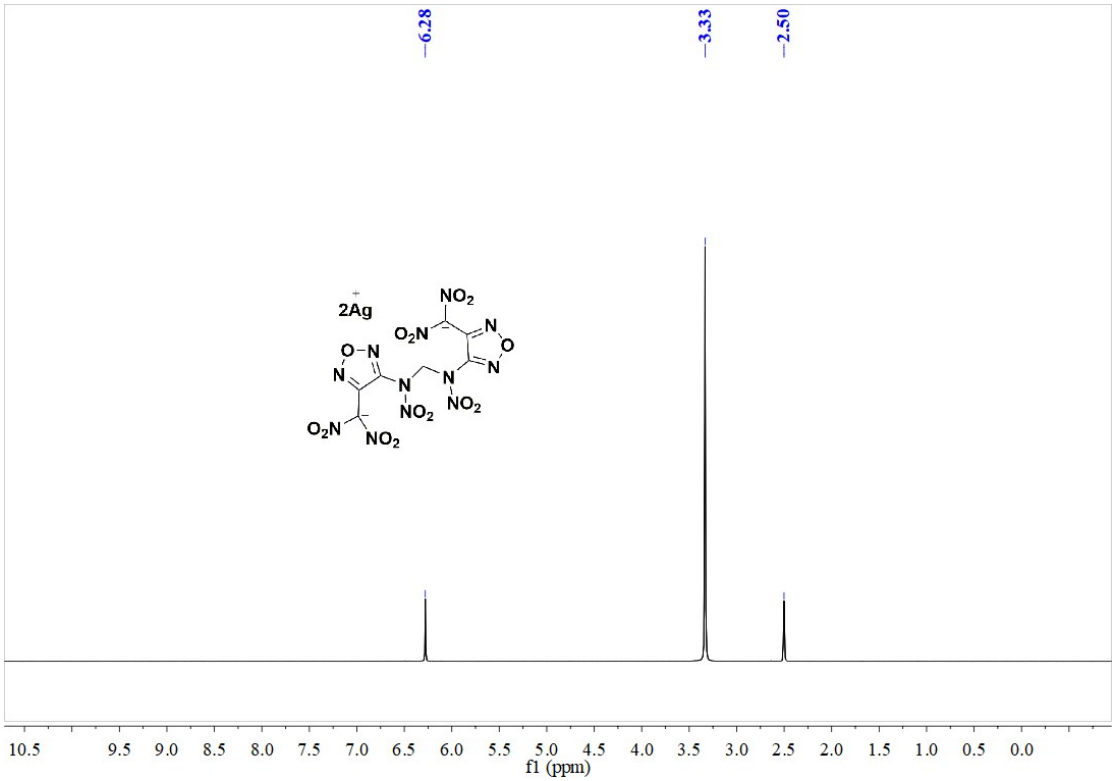


Fig S8 ^{1}H-NMR spectrum of **5** in d_6-DMSO.

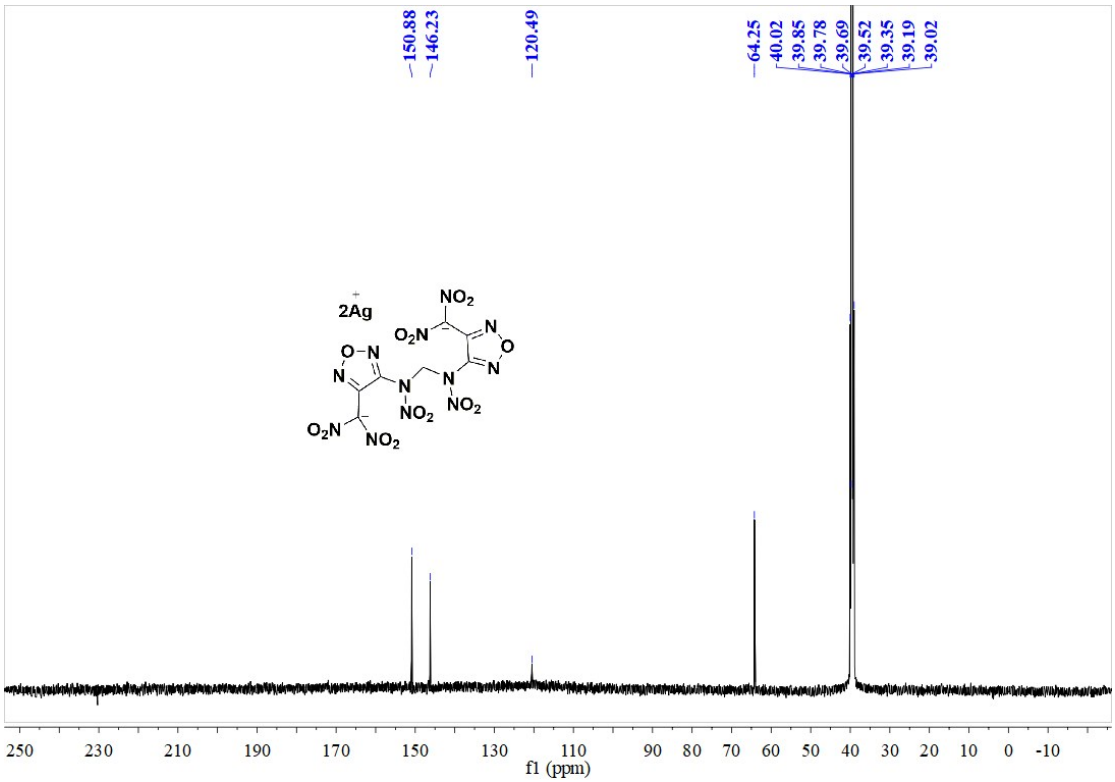


Fig S9 ^{13}C-NMR spectrum of **5** in d_6-DMSO.

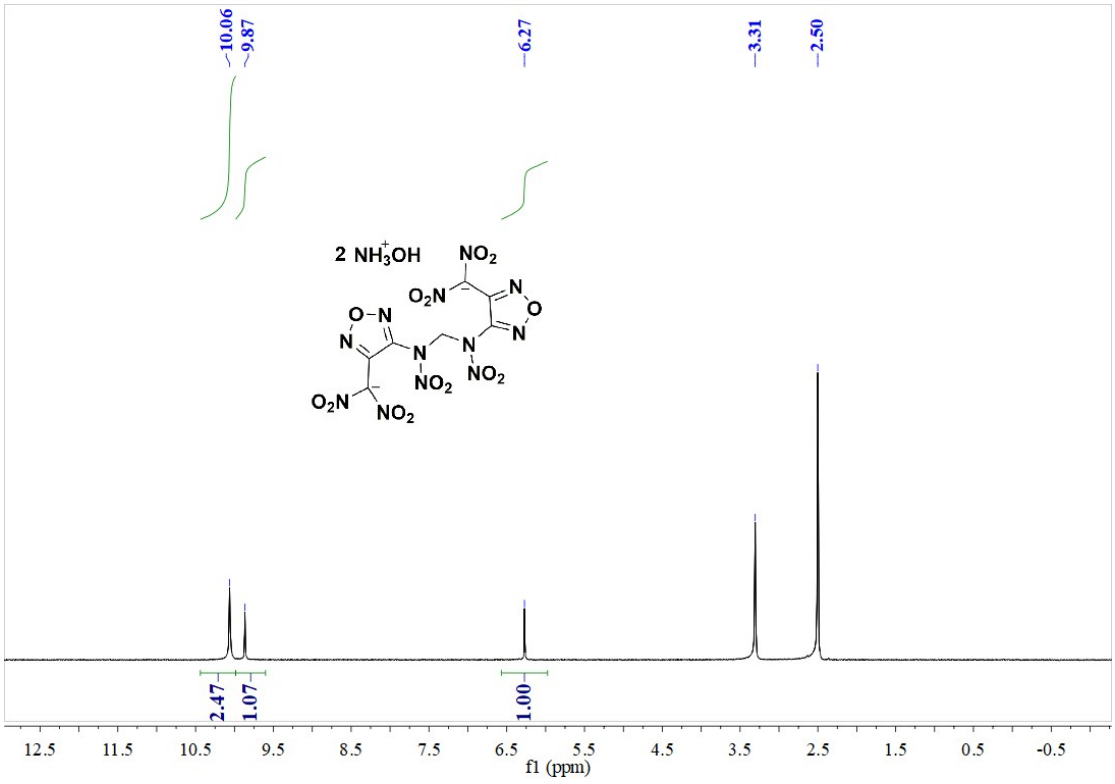


Fig S10 ^{1}H-NMR spectrum of **6** in d_6-DMSO.

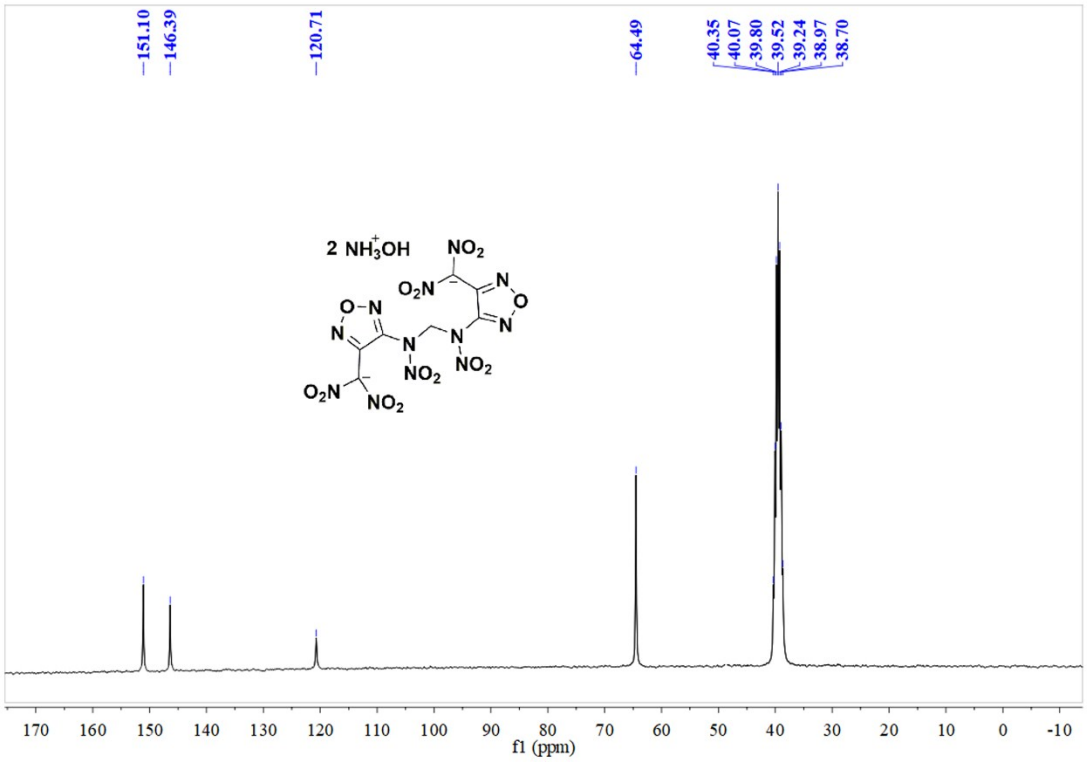


Fig S11 ^{13}C-NMR spectrum of **6** in d_6-DMSO.

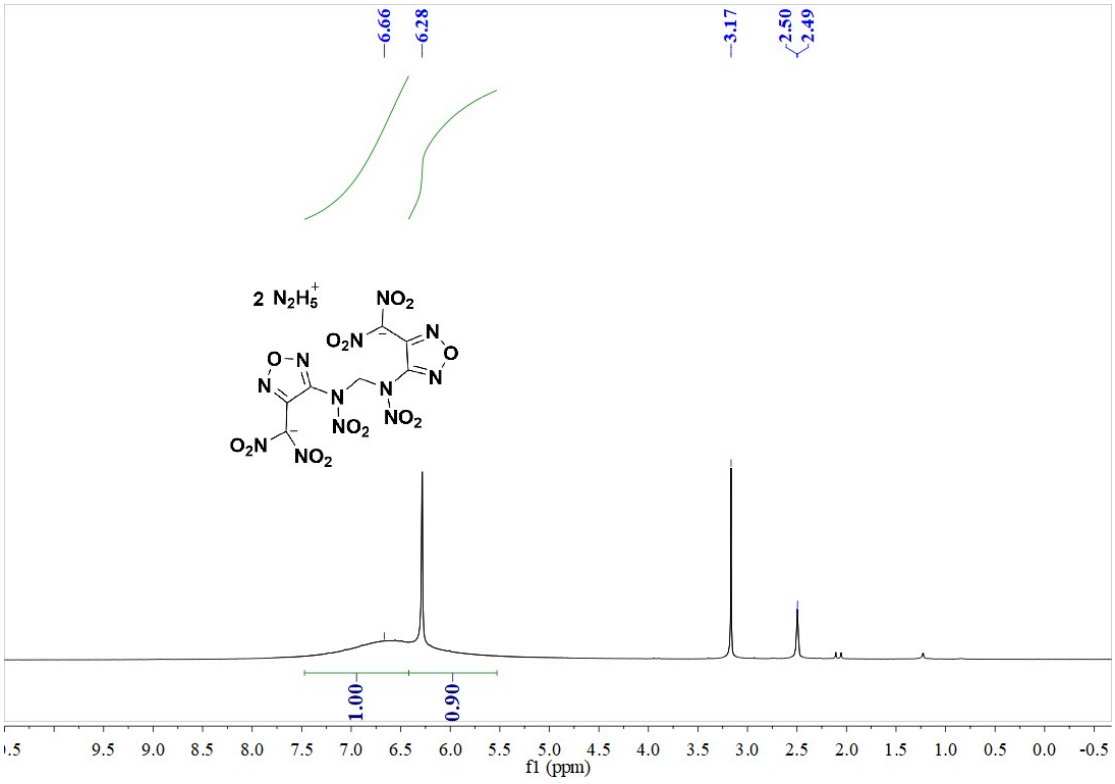


Fig S12 ^{1}H-NMR spectrum of **7** in d_6-DMSO.

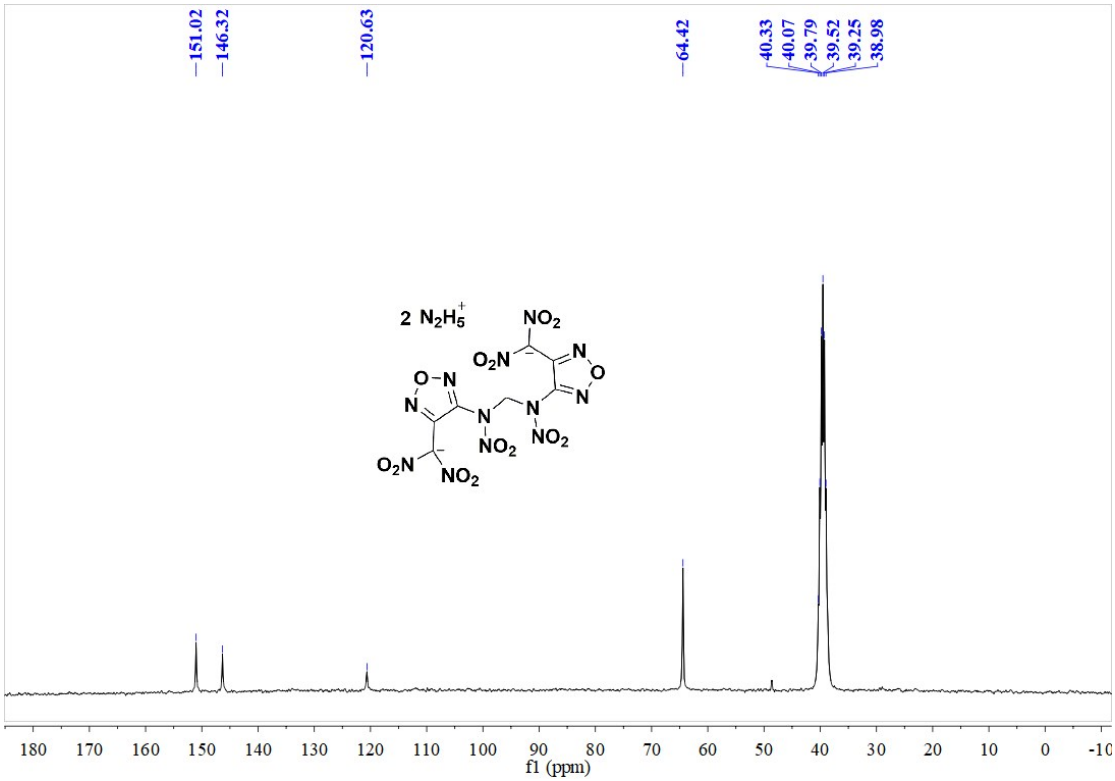


Fig S13 ^{13}C-NMR spectrum of **7** in d_6-DMSO.

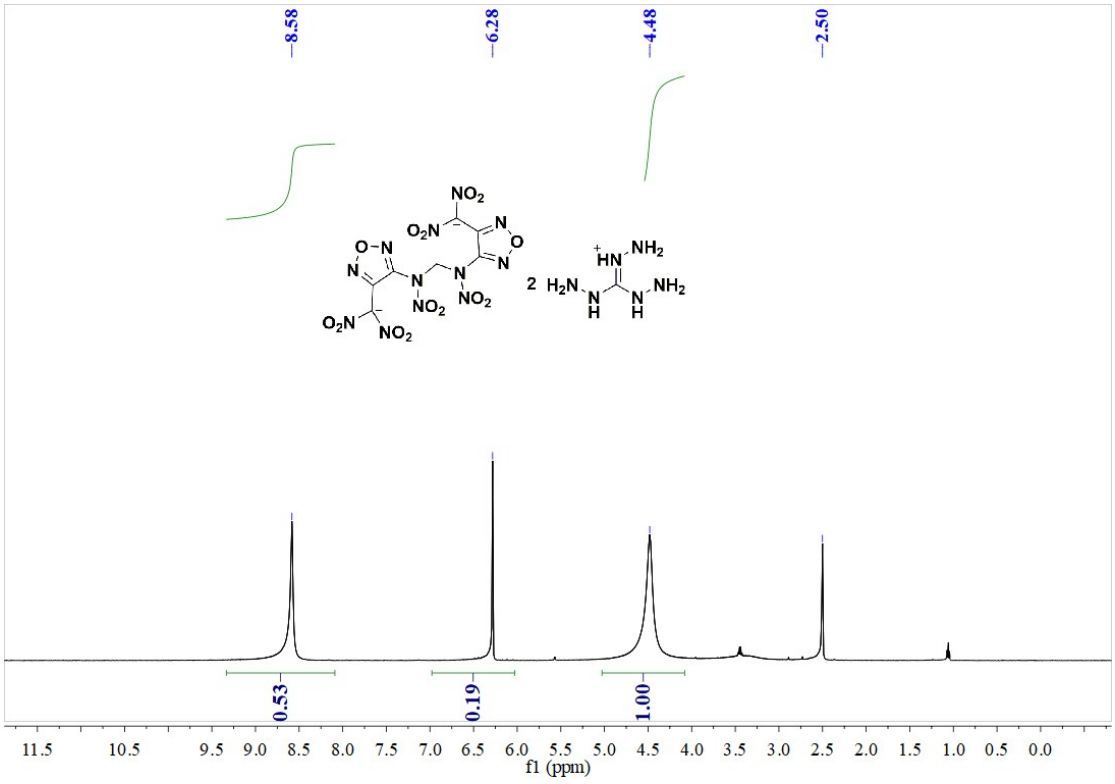


Fig S14 ^{1}H-NMR spectrum of **8** in d_6-DMSO.

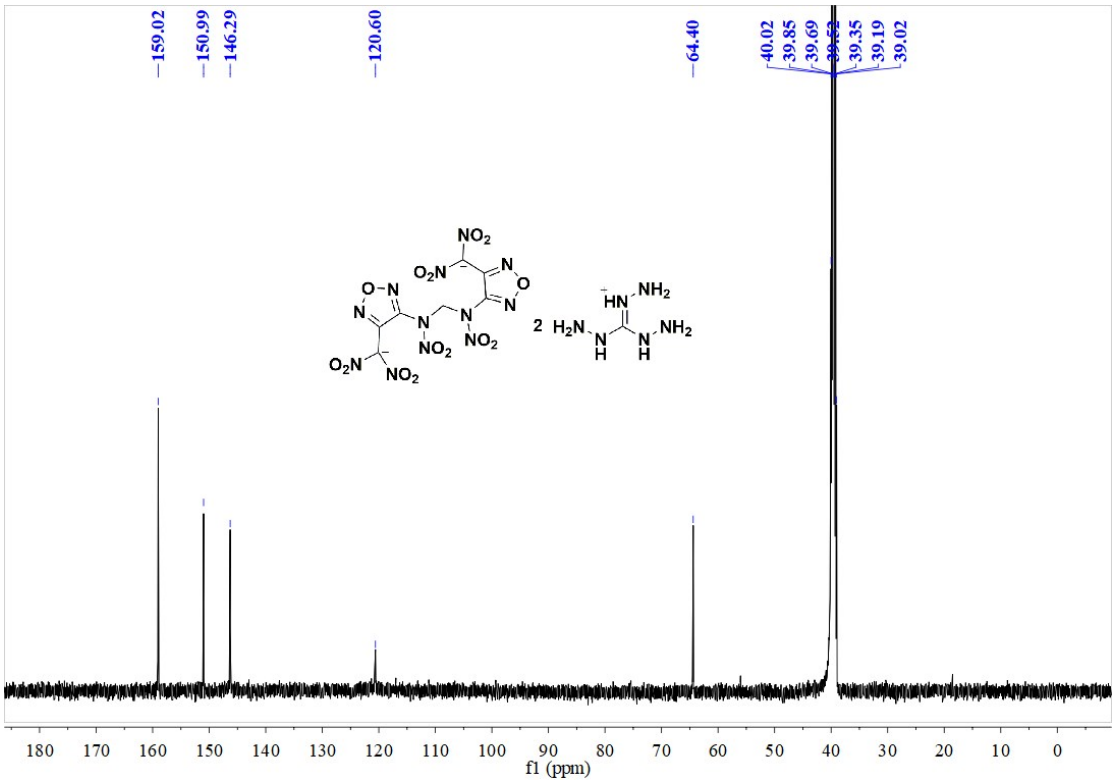


Fig S15 ^{13}C-NMR spectrum of **8** in d_6-DMSO.

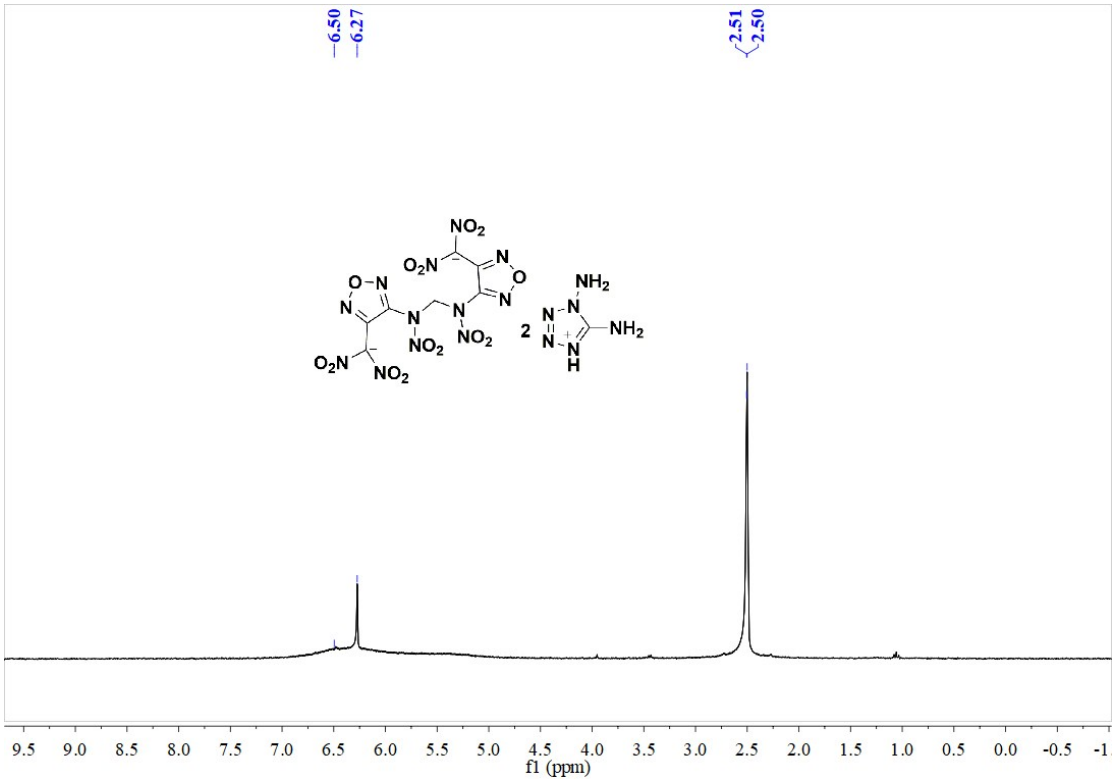


Fig S16 ^{1}H-NMR spectrum of **9** in d_6-DMSO.

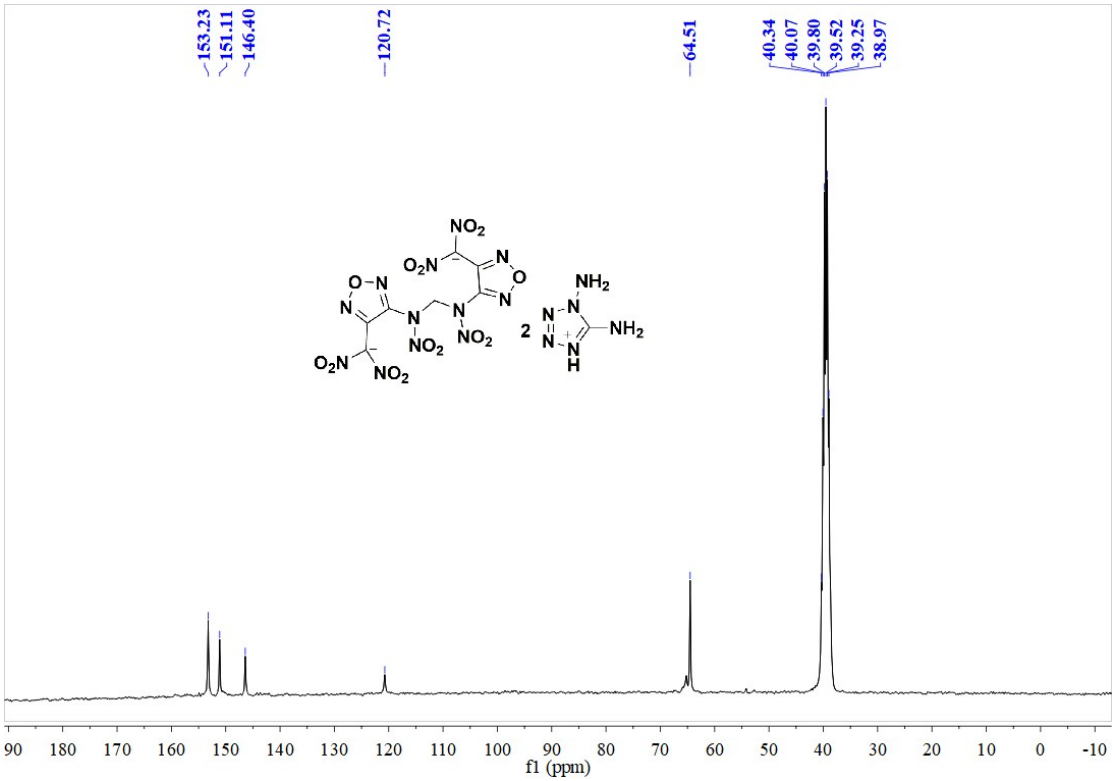


Fig S17 ^{13}C-NMR spectrum of **9** in d_6-DMSO.

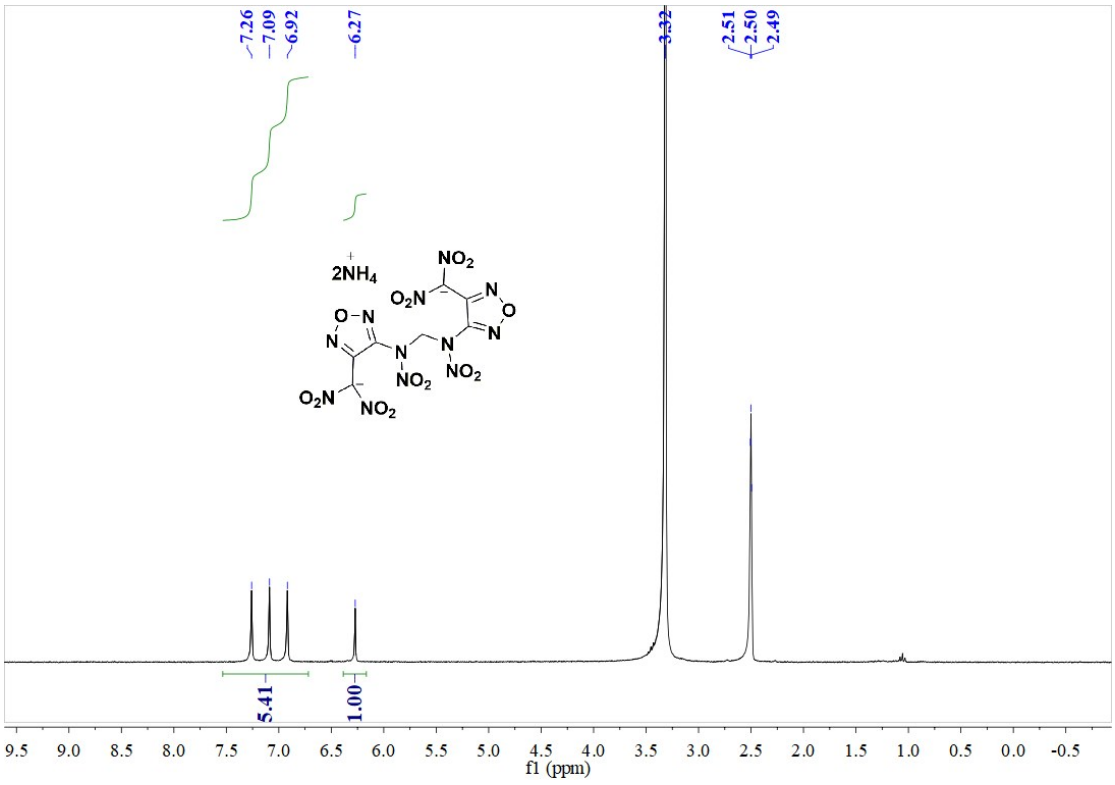


Fig S18 ^{1}H-NMR spectrum of **10** in d_6-DMSO.

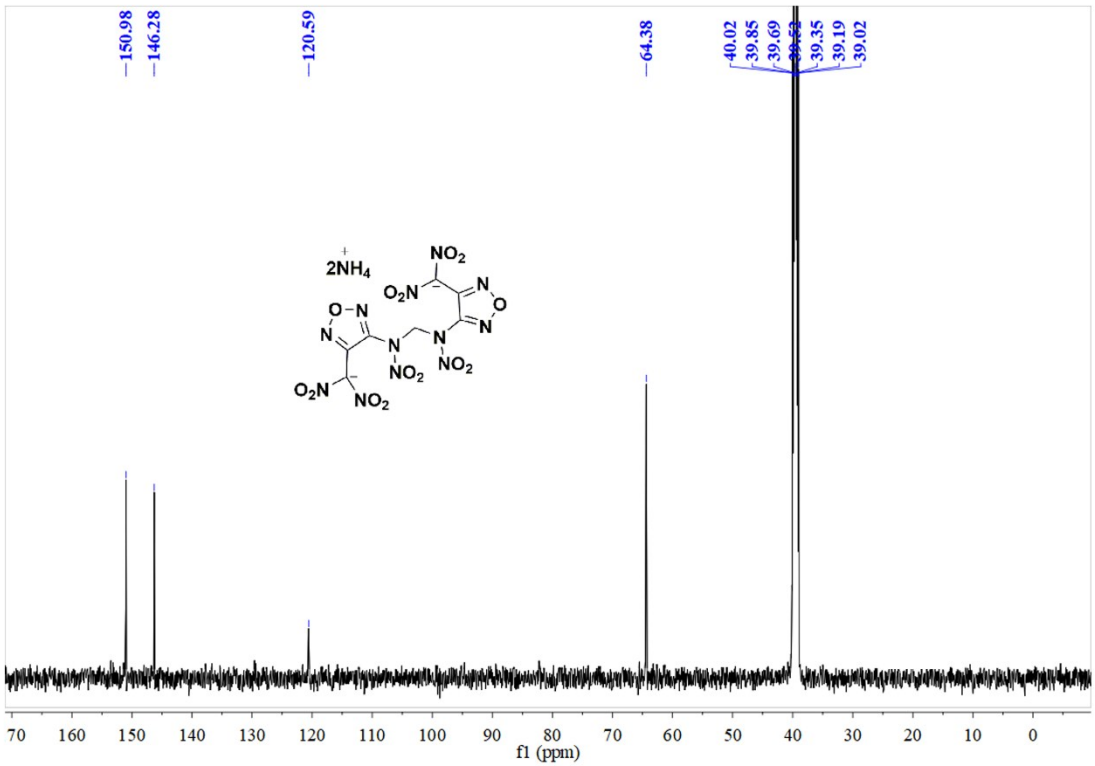


Fig S19 ^{13}C-NMR spectrum of **10** in d_6-DMSO.

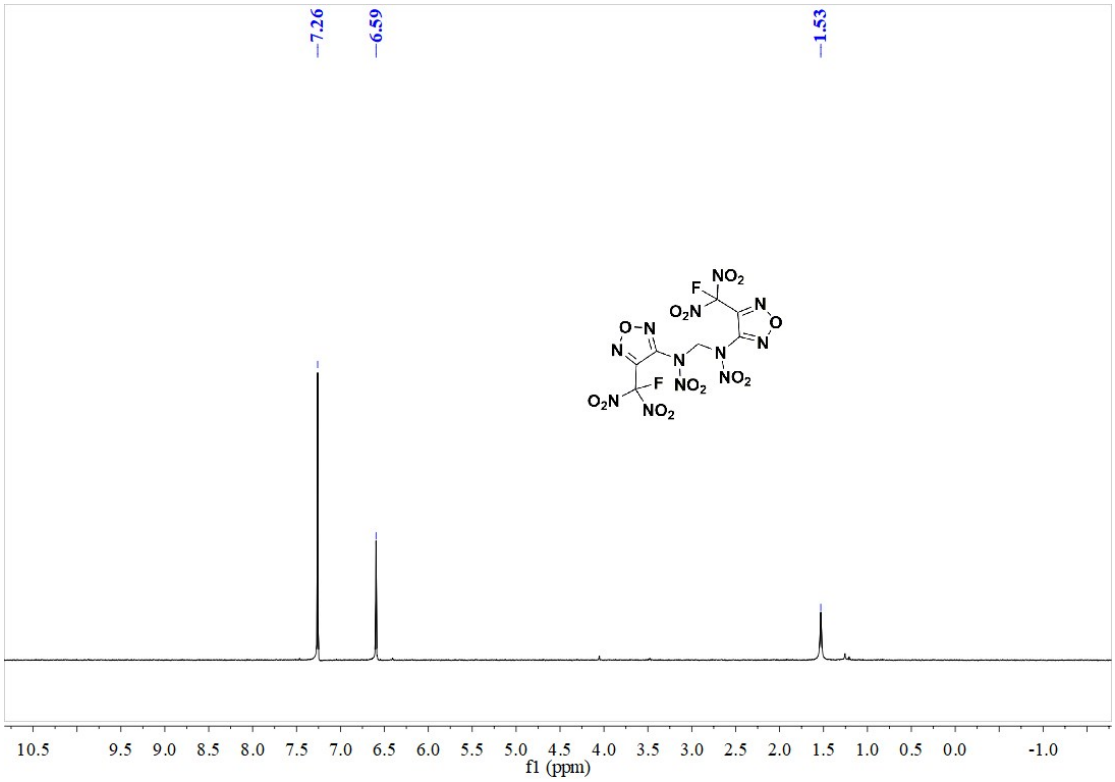


Fig S20 ^{1}H-NMR spectrum of **11** in d_6-DMSO.

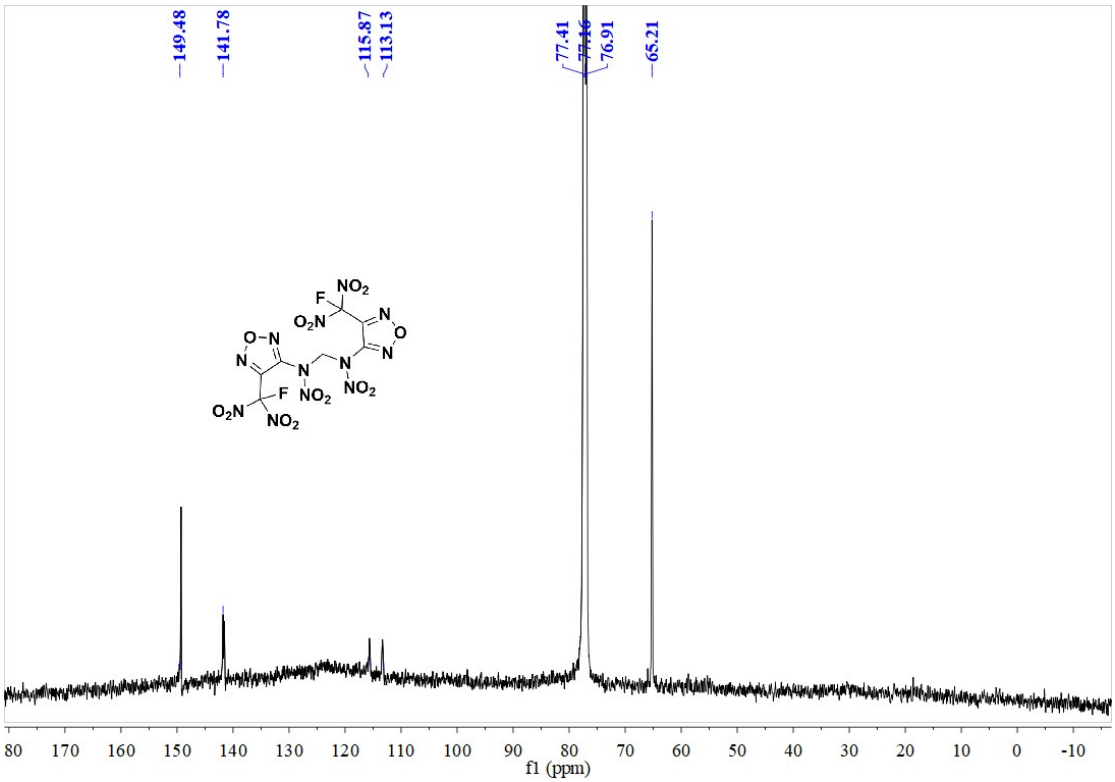


Fig S21 ^{13}C-NMR spectrum of **11** in d_6-DMSO.

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