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Supporting Information

A new family of nitrogen-rich salts based on oxy-bridged bis(dinitromethyl)furazan: syntheses, characterization and properties

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1. X-ray crystallography

Band angles and dihedral angles of the data collection and refinement are given in Table S1, S2, S3 and S4. The details of hydrogen bonds for **4**, **7** and **9** are gathered in Table S5, S6 and S7, respectively.

Table S1. Band angles and dihedral angles [°] for the structure of **2**.

C(2)-C(1)-N(2)	113.2(3)	N(2)-C(1)-C(2)-N(3)	-139.5(3)
C(2)-C(1)-N(1)	110.8(2)	N(1)-C(1)-C(2)-N(3)	100.3(4)
N(2)-C(1)-N(1)	107.0(3)	N(2)-C(1)-C(2)-C(3)	43.9(5)
C(2)-C(1)-H(2)	114(2)	N(1)-C(1)-C(2)-C(3)	-76.4(4)
N(2)-C(1)-H(2)	106(2)	N(3)-C(2)-C(3)-N(4)	0.4(4)
N(1)-C(1)-H(2)	104(2)	C(1)-C(2)-C(3)-N(4)	177.3(3)
N(3)-C(2)-C(3)	107.8(3)	N(3)-C(2)-C(3)-O(6)	-179.4(3)
N(3)-C(2)-C(1)	119.2(3)	C(1)-C(2)-C(3)-O(6)	-2.4(5)
C(3)-C(2)-C(1)	133.0(2)	N(5)-C(4)-C(5)-N(6)	0.0(3)
N(4)-C(3)-O(6)	126.5(3)	O(6)-C(4)-C(5)-N(6)	-179.8(3)
N(4)-C(3)-C(2)	110.7(2)	N(5)-C(4)-C(5)-C(6)	-179.2(3)
O(6)-C(3)-C(2)	122.8(2)	O(6)-C(4)-C(5)-C(6)	1.0(5)
N(5)-C(4)-O(6)	126.3(3)	N(6)-C(5)-C(6)-N(7)	-111.8(3)
N(5)-C(4)-C(5)	110.8(2)	C(4)-C(5)-C(6)-N(7)	67.4(4)
O(6)-C(4)-C(5)	122.9(2)	N(6)-C(5)-C(6)-N(8)	128.2(3)
N(6)-C(5)-C(4)	107.8(3)	C(4)-C(5)-C(6)-N(8)	-52.6(4)
N(6)-C(5)-C(6)	120.6(3)	N(16)-C(7)-C(8)-N(14)	131.2(3)
C(4)-C(5)-C(6)	131.6(2)	N(15)-C(7)-C(8)-N(14)	-109.4(3)
C(5)-C(6)-N(7)	112.4(2)	N(16)-C(7)-C(8)-C(9)	-50.8(4)
C(5)-C(6)-N(8)	109.5(2)	N(15)-C(7)-C(8)-C(9)	68.6(4)
N(7)-C(6)-N(8)	108.0(3)	N(14)-C(8)-C(9)-N(13)	-0.7(3)
C(5)-C(6)-H(1)	110.0(19)	C(7)-C(8)-C(9)-N(13)	-178.8(3)
N(7)-C(6)-H(1)	107.4(19)	N(14)-C(8)-C(9)-O(17)	-178.6(3)
N(8)-C(6)-H(1)	110(2)	C(7)-C(8)-C(9)-O(17)	3.3(5)
C(8)-C(7)-N(16)	112.1(2)	N(12)-C(10)-C(11)-N(11)	0.5(3)
C(8)-C(7)-N(15)	111.9(2)	O(17)-C(10)-C(11)-N(11)	-177.2(3)
N(16)-C(7)-N(15)	106.3(2)	N(12)-C(10)-C(11)-C(12)	-179.7(3)
C(8)-C(7)-H(4)	103(3)	O(17)-C(10)-C(11)-C(12)	2.6(5)
N(16)-C(7)-H(4)	109(3)	N(11)-C(11)-C(12)-N(10)	-125.8(3)
N(15)-C(7)-H(4)	114(3)	C(10)-C(11)-C(12)-N(10)	54.4(4)
N(14)-C(8)-C(9)	107.9(3)	N(11)-C(11)-C(12)-N(9)	113.6(3)
N(14)-C(8)-C(7)	119.6(2)	C(10)-C(11)-C(12)-N(9)	-66.2(4)
C(9)-C(8)-C(7)	132.5(2)	N(4)-C(3)-O(6)-C(4)	-9.1(5)
N(13)-C(9)-O(17)	126.3(2)	C(2)-C(3)-O(6)-C(4)	170.6(2)
N(13)-C(9)-C(8)	111.1(2)	N(5)-C(4)-O(6)-C(3)	8.3(4)
O(17)-C(9)-C(8)	122.6(2)	C(5)-C(4)-O(6)-C(3)	-172.0(3)

N(12)-C(10)-O(17)	126.2(3)	N(12)-C(10)-O(17)-C(9)	-0.2(4)
N(12)-C(10)-C(11)	111.6(2)	C(11)-C(10)-O(17)-C(9)	177.0(3)
O(17)-C(10)-C(11)	122.1(2)	N(13)-C(9)-O(17)-C(10)	8.9(5)
N(11)-C(11)-C(10)	107.2(3)	C(8)-C(9)-O(17)-C(10)	-173.5(3)
N(11)-C(11)-C(12)	120.0(3)	C(2)-C(1)-N(1)-O(2)	47.6(5)
C(10)-C(11)-C(12)	132.8(2)	N(2)-C(1)-N(1)-O(2)	-76.2(4)
C(11)-C(12)-N(10)	113.4(3)	C(2)-C(1)-N(1)-O(1)	-127.1(4)
C(11)-C(12)-N(9)	109.9(2)	N(2)-C(1)-N(1)-O(1)	109.0(4)
N(10)-C(12)-N(9)	107.7(3)	C(2)-C(1)-N(2)-O(4)	31.6(5)
C(11)-C(12)-H(3)	107(2)	N(1)-C(1)-N(2)-O(4)	153.9(3)
N(10)-C(12)-H(3)	104(2)	C(2)-C(1)-N(2)-O(3)	-151.3(4)
N(9)-C(12)-H(3)	114(2)	N(1)-C(1)-N(2)-O(3)	-28.9(5)
N(3)-O(5)-N(4)	111.1(2)	C(3)-C(2)-N(3)-O(5)	0.3(4)
C(3)-O(6)-C(4)	122.0(2)	C(1)-C(2)-N(3)-O(5)	-177.2(3)
N(6)-O(7)-N(5)	112.0(2)	N(4)-O(5)-N(3)-C(2)	-0.8(4)
N(14)-O(16)-N(13)	111.4(2)	O(6)-C(3)-N(4)-O(5)	178.9(3)
C(10)-O(17)-C(9)	121.9(2)	C(2)-C(3)-N(4)-O(5)	-0.8(4)
N(11)-O(18)-N(12)	112.0(2)	N(3)-O(5)-N(4)-C(3)	1.0(4)
O(2)-N(1)-O(1)	124.6(4)	O(6)-C(4)-N(5)-O(7)	179.6(3)
O(2)-N(1)-C(1)	116.9(3)	C(5)-C(4)-N(5)-O(7)	-0.2(3)
O(1)-N(1)-C(1)	118.3(4)	N(6)-O(7)-N(5)-C(4)	0.3(3)
O(4)-N(2)-O(3)	127.5(4)	C(4)-C(5)-N(6)-O(7)	0.1(3)
O(4)-N(2)-C(1)	115.8(3)	C(6)-C(5)-N(6)-O(7)	179.5(3)
O(3)-N(2)-C(1)	116.7(3)	N(5)-O(7)-N(6)-C(5)	-0.3(3)
C(2)-N(3)-O(5)	106.1(3)	C(5)-C(6)-N(7)-O(8)	-26.0(5)
C(3)-N(4)-O(5)	104.4(2)	N(8)-C(6)-N(7)-O(8)	94.9(4)
C(4)-N(5)-O(7)	103.4(2)	C(5)-C(6)-N(7)-O(11)	154.5(5)
C(5)-N(6)-O(7)	106.0(3)	N(8)-C(6)-N(7)-O(11)	-84.6(5)
O(8)-N(7)-O(11)	125.0(4)	C(5)-C(6)-N(8)-O(9)	-58.3(4)
O(8)-N(7)-C(6)	118.1(3)	N(7)-C(6)-N(8)-O(9)	179.0(3)
O(11)-N(7)-C(6)	116.9(3)	C(5)-C(6)-N(8)-O(10)	119.3(4)
O(9)-N(8)-O(10)	125.5(4)	N(7)-C(6)-N(8)-O(10)	-3.3(5)
O(9)-N(8)-C(6)	115.3(3)	C(11)-C(12)-N(9)-O(22)	-75.8(7)
O(10)-N(8)-C(6)	119.2(4)	N(10)-C(12)-N(9)-O(22)	160.2(7)
O(22)-N(9)-O(21)	125.9(5)	C(11)-C(12)-N(9)-O(21)	101.0(5)
O(22)-N(9)-C(12)	115.5(5)	N(10)-C(12)-N(9)-O(21)	-22.9(5)
O(21)-N(9)-C(12)	118.6(4)	C(11)-C(12)-N(10)-O(19)	-8.7(4)
O(19)-N(10)-O(20)	124.8(3)	N(9)-C(12)-N(10)-O(19)	113.2(4)
O(19)-N(10)-C(12)	118.5(3)	C(11)-C(12)-N(10)-O(20)	166.1(4)
O(20)-N(10)-C(12)	116.5(3)	N(9)-C(12)-N(10)-O(20)	-72.1(4)
C(11)-N(11)-O(18)	105.9(2)	C(10)-C(11)-N(11)-O(18)	-0.5(3)
C(10)-N(12)-O(18)	103.2(2)	C(12)-C(11)-N(11)-O(18)	179.6(3)
C(9)-N(13)-O(16)	103.7(2)	N(12)-O(18)-N(11)-C(11)	0.4(4)
C(8)-N(14)-O(16)	105.9(2)	O(17)-C(10)-N(12)-O(18)	177.3(3)

O(13)-N(15)-O(12)	127.6(3)	C(11)-C(10)-N(12)-O(18)	-0.2(3)
O(13)-N(15)-C(7)	116.5(2)	N(11)-O(18)-N(12)-C(10)	-0.1(3)
O(12)-N(15)-C(7)	115.8(3)	O(17)-C(9)-N(13)-O(16)	178.2(3)
O(15)-N(16)-O(14)	126.7(3)	C(8)-C(9)-N(13)-O(16)	0.4(3)
O(15)-N(16)-C(7)	115.6(3)	N(14)-O(16)-N(13)-C(9)	0.0(3)
O(14)-N(16)-C(7)	117.7(3)	C(9)-C(8)-N(14)-O(16)	0.6(3)
N(16)-C(7)-N(15)-O(12)	-97.4(3)	C(7)-C(8)-N(14)-O(16)	179.0(2)
C(8)-C(7)-N(16)-O(15)	-33.3(4)	N(13)-O(16)-N(14)-C(8)	-0.4(3)
N(15)-C(7)-N(16)-O(15)	-155.9(3)	C(8)-C(7)-N(15)-O(13)	-39.2(4)
C(8)-C(7)-N(16)-O(14)	148.4(3)	N(16)-C(7)-N(15)-O(13)	83.6(3)
N(15)-C(7)-N(16)-O(14)	25.8(4)	C(8)-C(7)-N(15)-O(12)	139.9(3)

Table S2. Band angles and dihedral angles [°] for the structure of **4**.

O(1)-N(1)-O(2)	122.50(16)	C(2)-N(3)-O(5)-N(4)	-0.5(2)
O(1)-N(1)-C(1)	122.11(17)	C(3)-N(4)-O(5)-N(3)	0.19(19)
O(2)-N(1)-C(1)	115.40(16)	C(5)-N(6)-O(7)-N(5)	0.3(2)
O(3)-N(2)-O(4)	120.74(16)	C(4)-N(5)-O(7)-N(6)	0.3(2)
O(3)-N(2)-C(1)	123.14(16)	O(3)-N(2)-C(1)-N(1)	5.1(3)
O(4)-N(2)-C(1)	116.10(16)	O(4)-N(2)-C(1)-N(1)	-173.45(16)
C(2)-N(3)-O(5)	105.77(16)	O(3)-N(2)-C(1)-C(2)	176.66(16)
C(3)-N(4)-O(5)	103.68(15)	O(4)-N(2)-C(1)-C(2)	-1.9(2)
C(4)-N(5)-O(7)	104.01(15)	O(1)-N(1)-C(1)-N(2)	-8.1(3)
C(5)-N(6)-O(7)	106.09(17)	O(2)-N(1)-C(1)-N(2)	171.70(17)
O(8)-N(7)-O(9)	121.74(16)	O(1)-N(1)-C(1)-C(2)	-179.72(16)
O(8)-N(7)-C(6)	123.71(16)	O(2)-N(1)-C(1)-C(2)	0.1(2)
O(9)-N(7)-C(6)	114.55(15)	O(5)-N(3)-C(2)-C(3)	0.6(2)
O(10)-N(8)-O(11)	120.09(16)	O(5)-N(3)-C(2)-C(1)	-175.90(16)
O(10)-N(8)-C(6)	122.98(16)	N(2)-C(1)-C(2)-N(3)	78.6(2)
O(11)-N(8)-C(6)	116.89(17)	N(1)-C(1)-C(2)-N(3)	-109.4(2)
H(9A)-N(9)-H(9B)	100(3)	N(2)-C(1)-C(2)-C(3)	-97.0(2)
H(9A)-N(9)-H(9C)	106(3)	N(1)-C(1)-C(2)-C(3)	75.0(2)
H(9B)-N(9)-H(9C)	115(3)	O(5)-N(4)-C(3)-O(6)	178.17(17)
H(9A)-N(9)-H(9D)	105(3)	O(5)-N(4)-C(3)-C(2)	0.19(19)
H(9C)-N(9)-H(9D)	111(3)	C(4)-O(6)-C(3)-N(4)	12.9(3)
H(10D)-N(10)-H(10C)	115(3)	C(4)-O(6)-C(3)-C(2)	-169.34(17)
H(10D)-N(10)-H(10B)	119(3)	N(3)-C(2)-C(3)-N(4)	-0.5(2)
H(10C)-N(10)-H(10B)	105(3)	C(1)-C(2)-C(3)-N(4)	175.62(18)
H(10D)-N(10)-H(10A)	110(5)	N(3)-C(2)-C(3)-O(6)	-178.61(17)
H(10C)-N(10)-H(10A)	115(4)	C(1)-C(2)-C(3)-O(6)	-2.5(3)
H(10B)-N(10)-H(1A)	90(4)	O(7)-N(5)-C(4)-O(6)	178.53(18)
N(3)-O(5)-N(4)	111.51(13)	O(7)-N(5)-C(4)-C(5)	-0.7(2)
C(4)-O(6)-C(3)	121.33(15)	C(3)-O(6)-C(4)-N(5)	5.6(3)
N(6)-O(7)-N(5)	111.37(15)	C(3)-O(6)-C(4)-C(5)	-175.27(17)
N(2)-C(1)-N(1)	123.02(17)	O(7)-N(6)-C(5)-C(4)	-0.7(2)

N(2)-C(1)-C(2)	118.48(16)	O(7)-N(6)-C(5)-C(6)	177.70(17)
N(1)-C(1)-C(2)	117.98(17)	N(5)-C(4)-C(5)-N(6)	0.9(2)
N(3)-C(2)-C(3)	107.59(17)	O(6)-C(4)-C(5)-N(6)	-178.35(18)
N(3)-C(2)-C(1)	122.35(17)	N(5)-C(4)-C(5)-C(6)	-177.32(19)
C(3)-C(2)-C(1)	129.95(16)	O(6)-C(4)-C(5)-C(6)	3.4(3)
N(4)-C(3)-O(6)	126.32(17)	O(10)-N(8)-C(6)-N(7)	1.1(3)
N(4)-C(3)-C(2)	111.45(16)	O(11)-N(8)-C(6)-N(7)	-176.62(16)
O(6)-C(3)-C(2)	122.20(16)	O(10)-N(8)-C(6)-C(5)	179.89(17)
N(5)-C(4)-O(6)	126.99(17)	O(11)-N(8)-C(6)-C(5)	2.2(3)
N(5)-C(4)-C(5)	111.07(17)	O(8)-N(7)-C(6)-N(8)	-7.0(3)
O(6)-C(4)-C(5)	121.93(16)	O(9)-N(7)-C(6)-N(8)	173.23(16)
N(6)-C(5)-C(4)	107.45(17)	O(8)-N(7)-C(6)-C(5)	174.22(17)
N(6)-C(5)-C(6)	122.59(17)	O(9)-N(7)-C(6)-C(5)	-5.6(2)
C(4)-C(5)-C(6)	129.93(17)	N(6)-C(5)-C(6)-N(8)	77.8(3)
N(8)-C(6)-N(7)	122.50(17)	C(4)-C(5)-C(6)-N(8)	-104.2(2)
N(8)-C(6)-C(5)	119.87(17)	N(6)-C(5)-C(6)-N(7)	-103.4(2)
N(7)-C(6)-C(5)	117.61(16)	C(4)-C(5)-C(6)-N(7)	74.6(3)

Table S3. Band angles and dihedral angles [°] for the structure of **7**.

O(2)-N(1)-O(1)	121.17(16)	C(2)-N(3)-O(5)-N(4)	0.2(3)
O(2)-N(1)-C(1)	117.46(16)	C(3)-N(4)-O(5)-N(3)	0.0(2)
O(1)-N(1)-C(1)	121.34(15)	C(5)-N(6)-O(7)-N(5)	0.80(19)
O(3)-N(2)-O(4)	121.69(16)	C(4)-N(5)-O(7)-N(6)	-0.76(19)
O(3)-N(2)-C(1)	122.44(16)	O(2)-N(1)-C(1)-N(2)	-176.74(18)
O(4)-N(2)-C(1)	115.87(15)	O(1)-N(1)-C(1)-N(2)	1.2(3)
C(2)-N(3)-O(5)	106.07(16)	O(2)-N(1)-C(1)-C(2)	5.1(3)
C(3)-N(4)-O(5)	103.34(15)	O(1)-N(1)-C(1)-C(2)	-176.97(18)
C(4)-N(5)-O(7)	103.26(14)	O(3)-N(2)-C(1)-N(1)	-20.3(3)
C(5)-N(6)-O(7)	106.02(14)	O(4)-N(2)-C(1)-N(1)	160.62(18)
O(8)-N(7)-O(9)	119.61(15)	O(3)-N(2)-C(1)-C(2)	157.96(19)
O(8)-N(7)-C(6)	123.39(15)	O(4)-N(2)-C(1)-C(2)	-21.1(3)
O(9)-N(7)-C(6)	116.98(14)	O(5)-N(3)-C(2)-C(3)	-0.3(2)
O(11)-N(8)-O(10)	120.54(16)	O(5)-N(3)-C(2)-C(1)	177.77(19)
O(11)-N(8)-C(6)	117.16(15)	N(1)-C(1)-C(2)-N(3)	-44.3(3)
O(10)-N(8)-C(6)	122.31(15)	N(2)-C(1)-C(2)-N(3)	137.5(2)
C(7)-N(9)-H(9A)	120.0	N(1)-C(1)-C(2)-C(3)	133.4(2)
C(7)-N(9)-H(9B)	120.0	N(2)-C(1)-C(2)-C(3)	-44.8(3)
H(9A)-N(9)-H(9B)	120.0	O(5)-N(4)-C(3)-O(6)	-175.8(2)
C(7)-N(10)-H(10A)	120.0	O(5)-N(4)-C(3)-C(2)	-0.2(2)
C(7)-N(10)-H(10B)	120.0	C(4)-O(6)-C(3)-N(4)	-25.6(3)
H(10A)-N(10)-H(10B)	120.0	C(4)-O(6)-C(3)-C(2)	159.13(19)
C(7)-N(11)-H(11A)	120.0	N(3)-C(2)-C(3)-N(4)	0.3(2)
C(7)-N(11)-H(11B)	120.0	C(1)-C(2)-C(3)-N(4)	-177.76(18)
H(11A)-N(11)-H(11B)	120.0	N(3)-C(2)-C(3)-O(6)	176.30(19)

C(8)-N(12)-H(12A)	120.0	C(1)-C(2)-C(3)-O(6)	-1.8(3)
C(8)-N(12)-H(12B)	120.0	O(7)-N(5)-C(4)-O(6)	179.55(18)
H(12A)-N(12)-H(12B)	120.0	O(7)-N(5)-C(4)-C(5)	0.4(2)
C(8)-N(13)-H(13A)	120.0	C(3)-O(6)-C(4)-N(5)	21.4(3)
C(8)-N(13)-H(13B)	120.0	C(3)-O(6)-C(4)-C(5)	-159.60(18)
H(13A)-N(13)-H(13B)	120.0	O(7)-N(6)-C(5)-C(4)	-0.49(19)
C(8)-N(14)-H(14A)	120.0	O(7)-N(6)-C(5)-C(6)	177.56(15)
C(8)-N(14)-H(14B)	120.0	N(5)-C(4)-C(5)-N(6)	0.0(2)
H(14A)-N(14)-H(14B)	120.0	O(6)-C(4)-C(5)-N(6)	-179.14(18)
N(3)-O(5)-N(4)	111.58(14)	N(5)-C(4)-C(5)-C(6)	-177.95(17)
C(3)-O(6)-C(4)	124.64(14)	O(6)-C(4)-C(5)-C(6)	2.9(3)
N(6)-O(7)-N(5)	111.49(12)	O(8)-N(7)-C(6)-N(8)	-5.4(3)
N(1)-C(1)-N(2)	121.19(15)	O(9)-N(7)-C(6)-N(8)	173.45(16)
N(1)-C(1)-C(2)	121.61(15)	O(8)-N(7)-C(6)-C(5)	176.56(16)
N(2)-C(1)-C(2)	117.17(15)	O(9)-N(7)-C(6)-C(5)	-4.6(2)
N(3)-C(2)-C(3)	107.11(16)	O(11)-N(8)-C(6)-N(7)	-173.03(17)
N(3)-C(2)-C(1)	126.85(17)	O(10)-N(8)-C(6)-N(7)	7.6(3)
C(3)-C(2)-C(1)	126.01(16)	O(11)-N(8)-C(6)-C(5)	5.0(3)
N(4)-C(3)-O(6)	128.07(17)	O(10)-N(8)-C(6)-C(5)	-174.39(17)
N(4)-C(3)-C(2)	111.90(16)	N(6)-C(5)-C(6)-N(7)	131.43(19)
O(6)-C(3)-C(2)	119.89(15)	C(4)-C(5)-C(6)-N(7)	-50.9(3)
N(5)-C(4)-O(6)	126.76(16)	N(6)-C(5)-C(6)-N(8)	-46.6(3)
N(5)-C(4)-C(5)	111.87(16)	C(4)-C(5)-C(6)-N(8)	131.02(19)
O(6)-C(4)-C(5)	121.37(15)	N(8)-C(6)-C(5)	120.18(15)
N(6)-C(5)-C(4)	107.36(16)	N(11)-C(7)-N(9)	120.03(18)
N(6)-C(5)-C(6)	124.84(16)	N(11)-C(7)-N(10)	120.34(19)
C(4)-C(5)-C(6)	127.77(15)	N(9)-C(7)-N(10)	119.64(19)
N(7)-C(6)-N(8)	121.02(15)	N(13)-C(8)-N(14)	120.31(16)
N(7)-C(6)-C(5)	118.77(15)	N(13)-C(8)-N(12)	119.85(16)
N(14)-C(8)-N(12)	119.84(16)		

Table S4. Band angles and dihedral angles [°] for the structure of **9**.

O(2)-N(1)-O(1)	120.5(3)	C(2)-N(3)-O(5)-N(4)	0.5(4)
O(2)-N(1)-C(1)	123.3(3)	C(3)-N(4)-O(5)-N(3)	-0.5(4)
O(1)-N(1)-C(1)	116.2(3)	O(2)-N(1)-C(1)-N(2)	-8.8(4)
O(3)-N(2)-O(4)	121.0(3)	O(1)-N(1)-C(1)-N(2)	173.7(3)
O(3)-N(2)-C(1)	121.5(3)	O(2)-N(1)-C(1)-C(2)	168.1(3)
O(4)-N(2)-C(1)	117.5(3)	O(1)-N(1)-C(1)-C(2)	-9.5(4)
C(2)-N(3)-O(5)	106.4(3)	O(3)-N(2)-C(1)-N(1)	-17.9(4)
C(3)-N(4)-O(5)	104.6(3)	O(4)-N(2)-C(1)-N(1)	163.4(3)
C(4)-N(5)-H(5A)	120.0	O(3)-N(2)-C(1)-C(2)	165.3(3)
C(4)-N(5)-H(5B)	120.0	O(4)-N(2)-C(1)-C(2)	-13.5(4)
H(5A)-N(5)-H(5B)	120.0	O(5)-N(3)-C(2)-C(3)	-0.2(4)
C(4)-N(6)-H(6A)	120.0	O(5)-N(3)-C(2)-C(1)	177.4(3)

C(4)-N(6)-H(6B)	120.0	N(1)-C(1)-C(2)-N(3)	135.1(3)
H(6A)-N(6)-H(6B)	120.0	N(2)-C(1)-C(2)-N(3)	-48.0(4)
C(4)-N(7)-C(5)	125.3(3)	N(1)-C(1)-C(2)-C(3)	-47.9(5)
C(5)-N(8)-H(8A)	120.0	O(5)-N(4)-C(3)-C(2)	0.4(4)
C(5)-N(8)-H(8B)	120.0	C(3)#1-O(6)-C(3)-N(4)	8.9(3)
H(8A)-N(8)-H(8B)	120.0	C(3)#1-O(6)-C(3)-C(2)	-171.1(4)
C(5)-N(9)-H(9A)	120.0	N(3)-C(2)-C(3)-N(4)	-0.1(4)
C(5)-N(9)-H(9B)	120.0	C(1)-C(2)-C(3)-N(4)	-177.4(3)
H(9A)-N(9)-H(9B)	120.0	N(3)-C(2)-C(3)-O(6)	179.9(3)
N(3)-O(5)-N(4)	111.2(2)	C(1)-C(2)-C(3)-O(6)	2.6(6)
C(3)-O(6)-C(3)#1	121.0(3)	C(5)-N(7)-C(4)-N(6)	-152.2(3)
N(1)-C(1)-N(2)	121.6(3)	C(5)-N(7)-C(4)-N(5)	31.1(5)
N(1)-C(1)-C(2)	119.0(3)	C(4)-N(7)-C(5)-N(8)	-165.1(3)
N(2)-C(1)-C(2)	119.3(3)	C(4)-N(7)-C(5)-N(9)	18.0(5)
N(3)-C(2)-C(3)	107.7(3)	N(6)-C(4)-N(5)	117.9(3)
N(3)-C(2)-C(1)	121.0(3)	N(6)-C(4)-N(7)	116.9(3)
C(3)-C(2)-C(1)	131.2(3)	N(5)-C(4)-N(7)	125.2(3)
N(4)-C(3)-O(6)	125.9(3)	N(8)-C(5)-N(9)	118.6(3)
N(4)-C(3)-C(2)	110.1(3)	N(8)-C(5)-N(7)	117.0(3)
O(6)-C(3)-C(2)	124.0(3)	N(9)-C(5)-N(7)	124.3(3)

Table S5. Hydrogen bonds present in **4**

D-H	d(D-H) [nm]	d(H..A) [nm]	<DHA [°]	d(D..A) [nm]	A	Symmetry code
N9-H9A	0.0930	0.2146	148.99	0.2981	O10	-
N9-H9A	0.0930	0.2443	136.61	0.3184	O11	-
N9-H9A	0.0930	0.2631	150.63	0.3471	N8	-
N9-H9B	0.0945	0.1963	162.56	0.2879	O4	-x+1,-y+2, -z+1
N9-H9C	0.0919	0.2155	151.07	0.2993	O8	-x, -y+1, -z+1
N9-H9C	0.0919	0.2237	135.48	0.2963	O10	-x, -y+1, -z+1
N9-H9D	0.0965	0.2189	153.46	0.3083	O3	x, y-1, z
N9-H9D	0.0965	0.2208	120.31	0.2820	O2	-x+1, -y+1, -z+1
N10-H10D	0.1014	0.2028	152.21	0.2963	O1	-x+1, -y+1, -z+1
N10-H10D	0.1014	0.2545	120.13	0.3177	O9	x, y-1, z
N10-H10C	0.0881	0.2327	146.67	0.3101	N5	-x+1, -y+1, -z
N10-H10C	0.0881	0.2531	118.14	0.3047	N4	-x+1, -y+1, -z
N10-H10B	0.0979	0.1903	172.36	0.2876	O11	-
N10-H10A	0.0810	0.2209	160.16	0.2984	O9	-x, -y+1, -z
N10-H10A	0.0810	0.2376	121.88	0.2887	O5	x-1, y-1, z

Table S6. Hydrogen bonds present in **7**

D-H	d(D-H) [nm]	d(H..A) [nm]	<DHA [°]	d(D..A) [nm]	A	Symmetry code
N9-H9A	0.0860	0.2085	152.56	0.2876	O3	-x,-y+1,-z+1

N9-H9B	0.0860	0.2292	146.97	0.3049	O10	-
N9-H9B	0.0860	0.2389	152.84	0.3179	O11	-
N9-H9B	0.0860	0.2688	164.19	0.3523	N8	-
N10-H10A	0.0860	0.2238	173.34	0.3094	O9	x,y-1,z
N10-H10B	0.0860	0.2461	149.62	0.3232	O11	-
N10-H10B	0.0860	0.2550	113.46	0.2998	O5	-x+1,-y+1,-z
N11-H11A	0.0860	0.2225	145.74	0.2975	O1	-x,-y+1,-z+1
N11-H11A	0.0860	0.2283	144.36	0.3024	O3	-x,-y+1,-z+1
N11-H11B	0.0860	0.2060	165.18	0.2900	O8	x,y-1,z
N12-H12A	0.0860	0.2358	138.83	0.3058	O10	-x+1,-y+1,-z+1
N12-H12A	0.0860	0.2482	135.04	0.3150	O9	-
N12-H12B	0.0860	0.2305	145.53	0.3053	N3	-x+1,-y+2,-z
N12-H12B	0.0860	0.2628	130.80	0.3256	O4	x+1,y,z
N13-H13A	0.0860	0.2147	146.24	0.2902	O1	x+1,y-1,z
N13-H13B	0.0860	0.2195	149.67	0.2969	O8	-x+1,-y+1,-z+1
N13-H13B	0.0860	0.2288	140.71	0.3003	O10	-x+1,-y+1,-z+1
N14-H14A	0.0860	0.2321	151.60	0.3105	O2	x+1,y-1,z
N14-H14A	0.0860	0.2663	117.04	0.3149	N5	-x+2,-y+1,-z
N14-H14B	0.0860	0.2378	136.28	0.3058	O4	x+1,y,z
N14-H14B	0.0860	0.2597	130.54	0.3223	O2	-x+1,-y+2,-z
N14-H14B	0.0860	0.2656	118.72	0.3161	O7	-x+2,-y+1,-z

Table S7. Hydrogen bonds present in **9**

D-H	d(D-H) [nm]	d(H..A) [nm]	<DHA [°]	d(D..A) [nm]	A	Symmetry code
N5-H5A	0.0860	0.2460	148.83	0.3227	O2	-x+1/2, -y+3/2, z+1/2
N5-H5B	0.0860	0.2363	157.11	0.3173	N4	-x+1/2, -y+1/2, z+1/2
N5-H5B	0.0860	0.2539	110.45	0.2952	N9	
N5-H5B	0.0860	0.2576	146.86	0.3329	O5	-x+1/2, -y+1/2, z+1/2
N6-H6A	0.0860	0.2279	149.64	0.3052	O1	-x+1/2, -y+3/2, z+1/2
N6-H6A	0.0860	0.2340	153.91	0.3135	O2	-x+1/2, -y+3/2, z+1/2
N6-H6A	0.0860	0.2648	174.87	0.3506	N1	-x+1/2, -y+3/2, z+1/2
N6-H6B	0.0860	0.2253	130.50	0.2887	O4	-x+1/2, y-1/2, z+1
N8-H8A	0.0860	0.2169	147.81	0.2933	O3	-x+1/2, y-3/2, z+1
N8-H8A	0.0860	0.2243	137.67	0.2937	O2	-x+1/2, y-3/2, z+1
N8-H8B	0.0860	0.2100	177.55	0.2959	N7	-x, -y, -z+2
N9-H9A	0.0860	0.2629	134.47	0.3289	O3	-x+1/2, y-3/2, z+1
N9-H9B	0.0860	0.2245	153.33	0.3039	O1	x, -y+1, z+1/2
N9-H9B	0.0860	0.2475	115.70	0.2952	N5	

2. Theoretical study

Computations were performed with the Gaussian 09 (Revision B. 01) suite of programs.[1] The geometric optimization of the structures and frequency analyses were carried out using B3LYP functional with the 6-31+G** basis set, and single-point energies were calculated at the

MP2(full)/6-311++G** level. All of the optimized structures were characterized to be true local energy minima on the potential-energy surface without imaginary frequencies.

Geometry coordinates

The optimized structure of the following structure

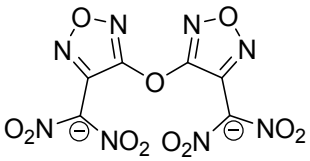
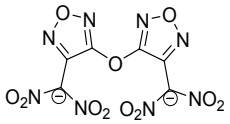
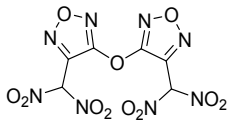
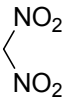


Table S8. Geometry coordinates of oxy-bridged bis(dinitromethyl)furazan anion.

O	2.26116500	2.53437400	1.55649100
C	1.05729700	1.12729900	0.52088100
C	2.41752900	0.65082500	0.52192300
O	-2.26169000	2.53472000	-1.55585000
C	-2.41764600	0.65087700	-0.52174600
C	-1.05743000	1.12739400	-0.52103900
N	-0.96858200	2.26195700	-1.15184600
N	-3.13319100	1.53953300	-1.16360200
N	0.96818000	2.26168000	1.15197200
N	3.13282000	1.53932000	1.16427800
O	0.00005700	0.45089600	-0.00038500
C	3.01205700	-0.55974800	-0.05684700
C	-3.01193400	-0.55991700	0.05681600
N	3.23395300	-1.65136700	0.78448100
O	2.78375900	-1.53601800	1.95793900
O	3.83696700	-2.67247800	0.40510600
N	3.38285900	-0.51281100	-1.39987200
O	3.09648500	0.56192400	-2.00164300
O	3.95220200	-1.45886700	-1.97414800
N	-3.23380400	-1.65133700	-0.78476900
O	-2.78375400	-1.53562200	-1.95825200
O	-3.83665000	-2.67262100	-0.40559200
N	-3.38262200	-0.51333200	1.39988300
O	-3.95190400	-1.45954200	1.97397700
O	-3.09620500	0.56124800	2.00190300

Table S9. Ab Initio computional data.

结构	E_0(hartree)	H_{corr}	ZPE	HOF ^{Exp}(kJ/mol)	HOF ^{Calcd} (kJ/mol)

	-1490.9129728	0.137177	0.115531	-	-11.3
	-1492.0131986	0.163808	0.141541	-	240.3
CH_4	-40.397464	0.048605	0.044793	-74.9 [2]	-
CH_3OCH_3	-154.6771595	0.084916	0.079632	-184.1 [2]	-
	-261.5324524	0.050116	0.045698	-	196 [3]
	-448.1640608	0.046603	0.039724	-	-222.8 [3]
	-448.7003763	0.060215	0.052849	-58.9 [2]	-
CH_3CH_3	-79.6068548	0.079041	0.074611	-84 [2]	

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2. NIST Chemistry WebBook .
3. L. Liang, D. Cao, J. Song, H. Huang, K. Wang, C. Bian, X. Dong and Z. Zhou. *J. Mater. Chem. A*, 2013, **1**, 8857-8865.

3. ^{1}H and ^{13}C NMR spectra of compounds 2-9.

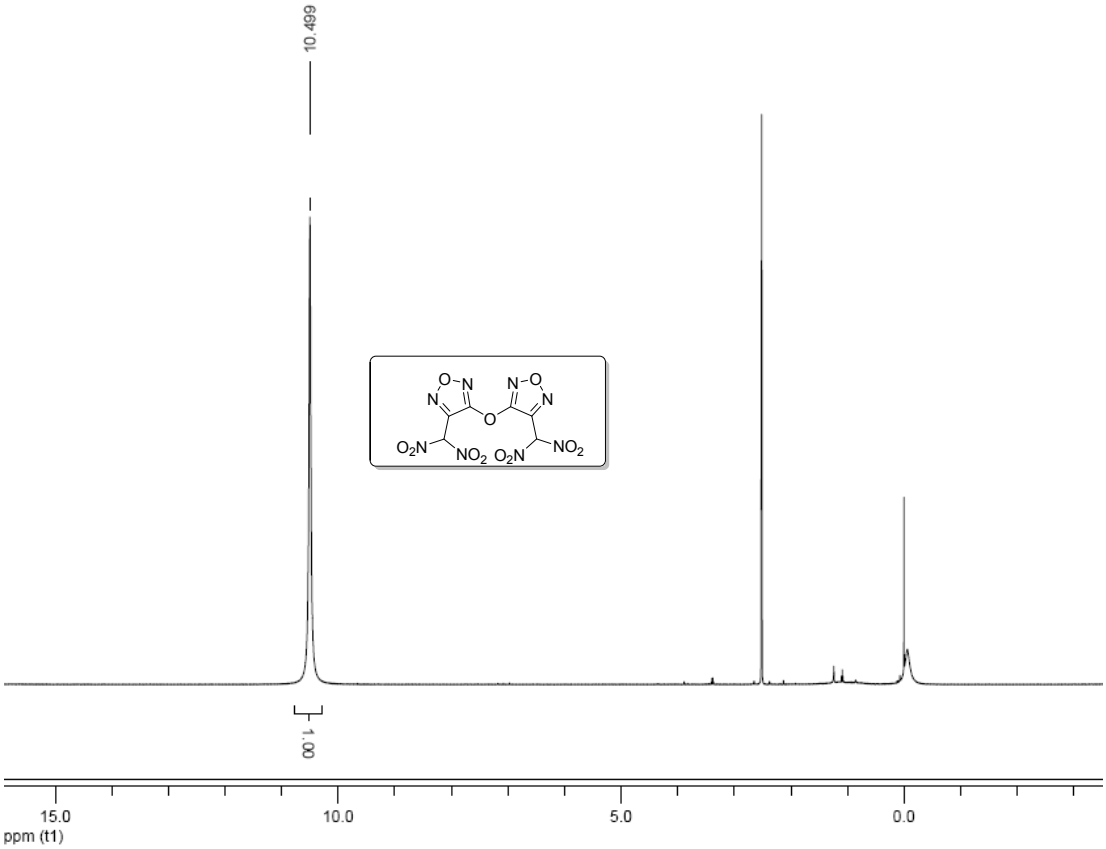

Fig. S1 ^{1}H NMR spectrum of **2** in DMSO-*d6*

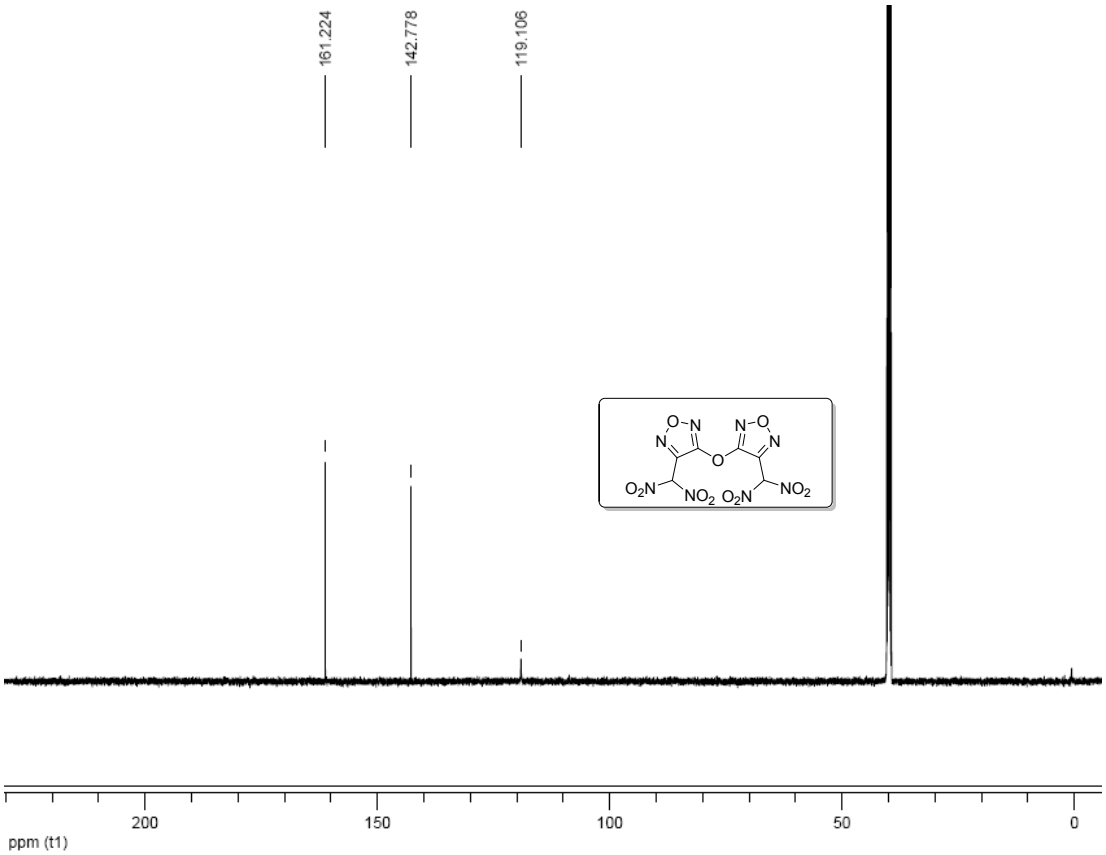

Fig. S2 ^{13}C NMR spectrum of **2** in DMSO-*d6*

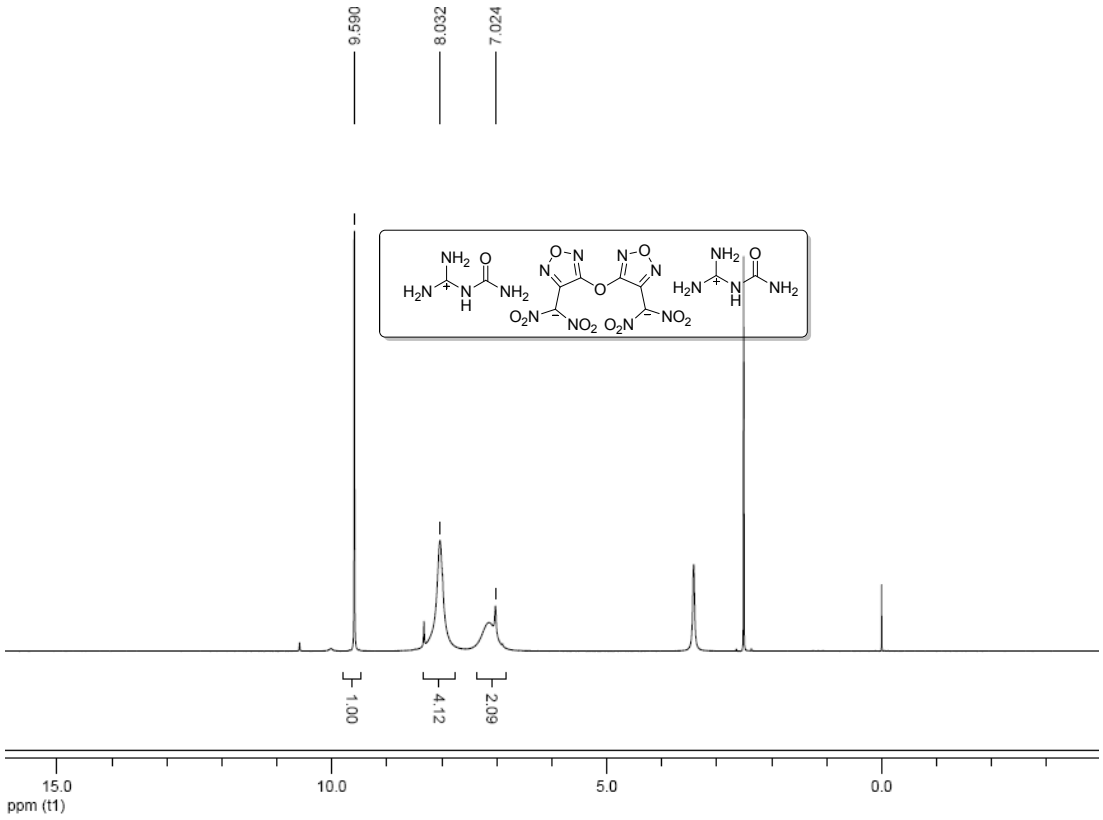

Fig. S3 ^{1}H NMR spectrum of **3** in DMSO-*d6*

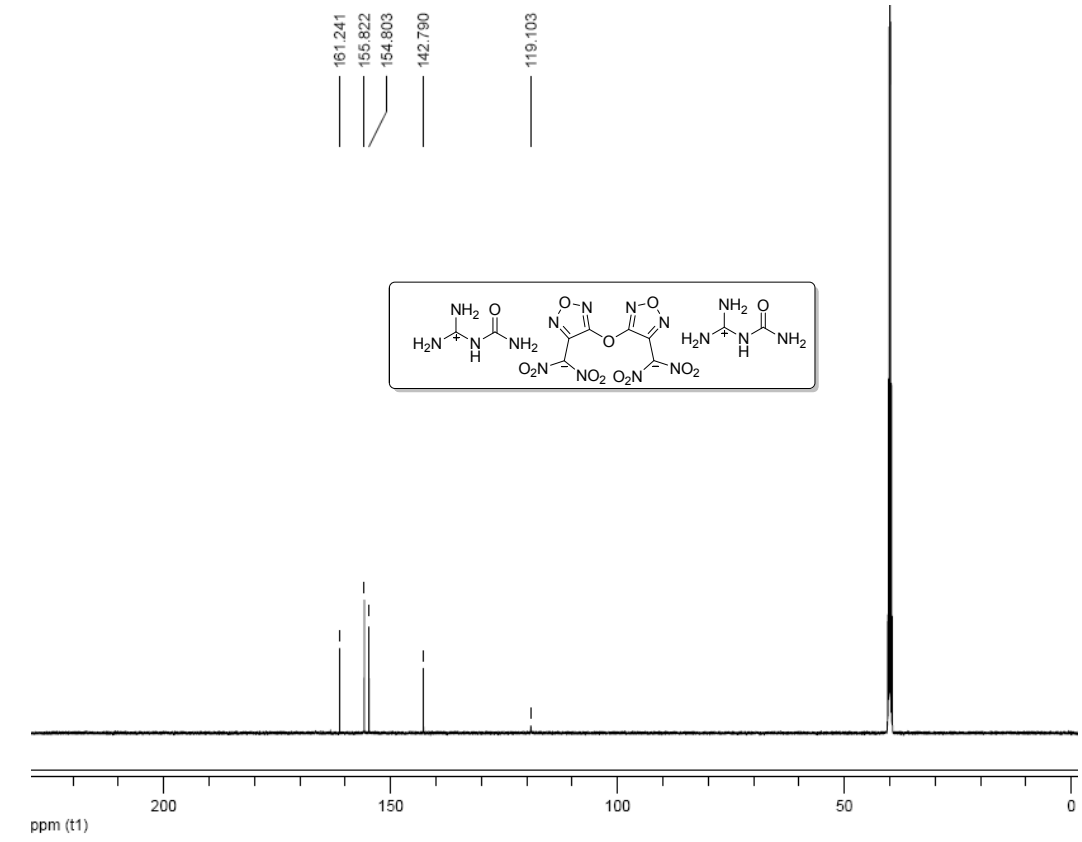

Fig. S4 ^{13}C NMR spectrum of **3** in DMSO-*d6*

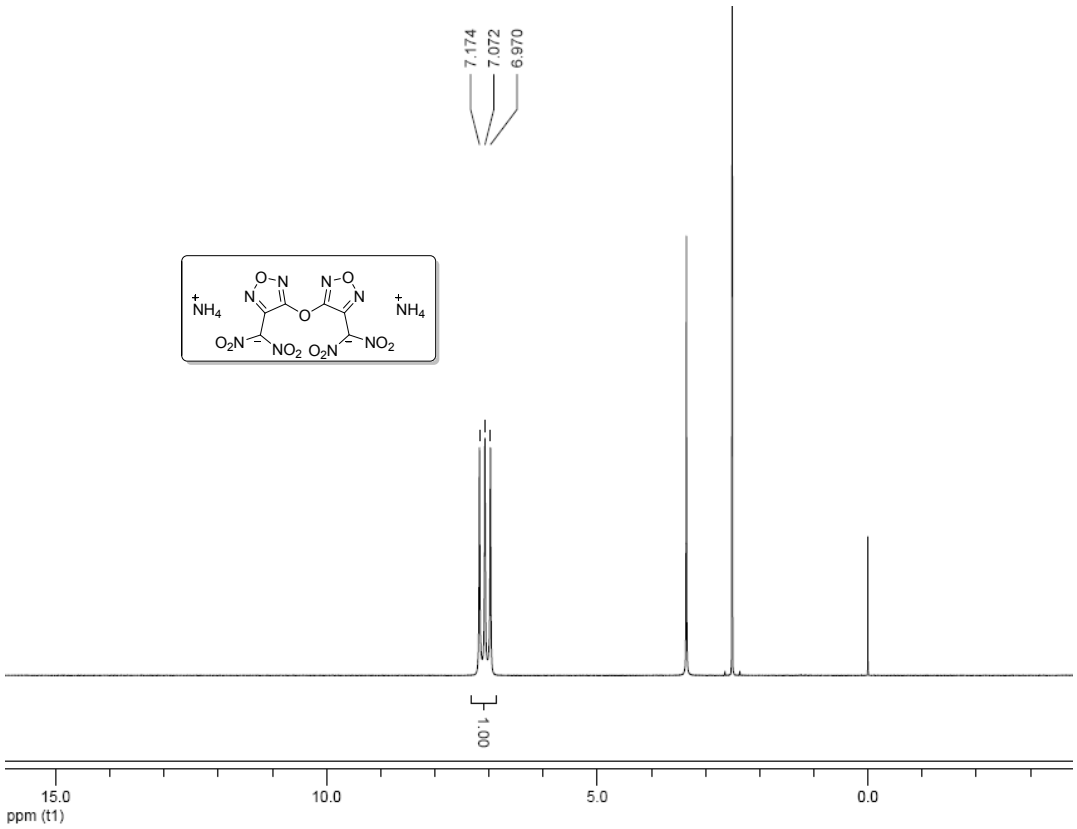

Fig. S5 ^{1}H NMR spectrum of **4** in DMSO-*d6*

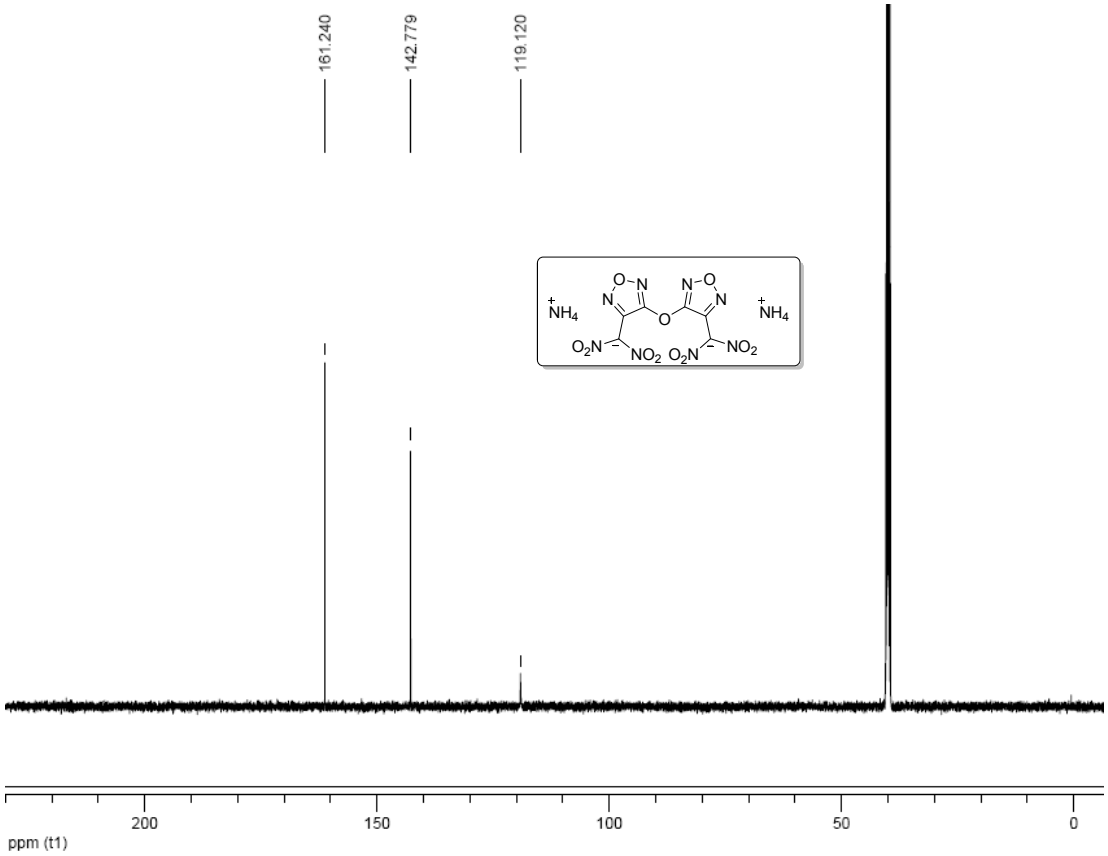

Fig. S6 ^{13}C NMR spectrum of **4** in DMSO-*d6*

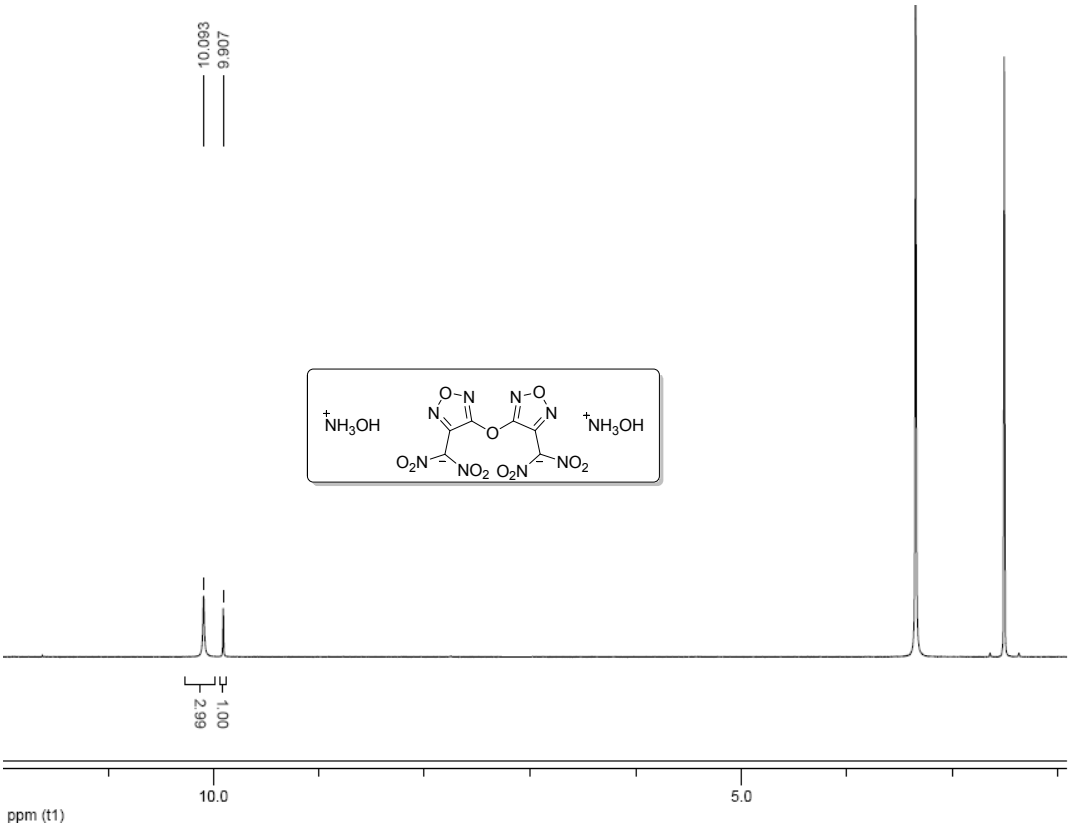

Fig. S7 ^{1}H NMR spectrum of **5** in DMSO-*d6*

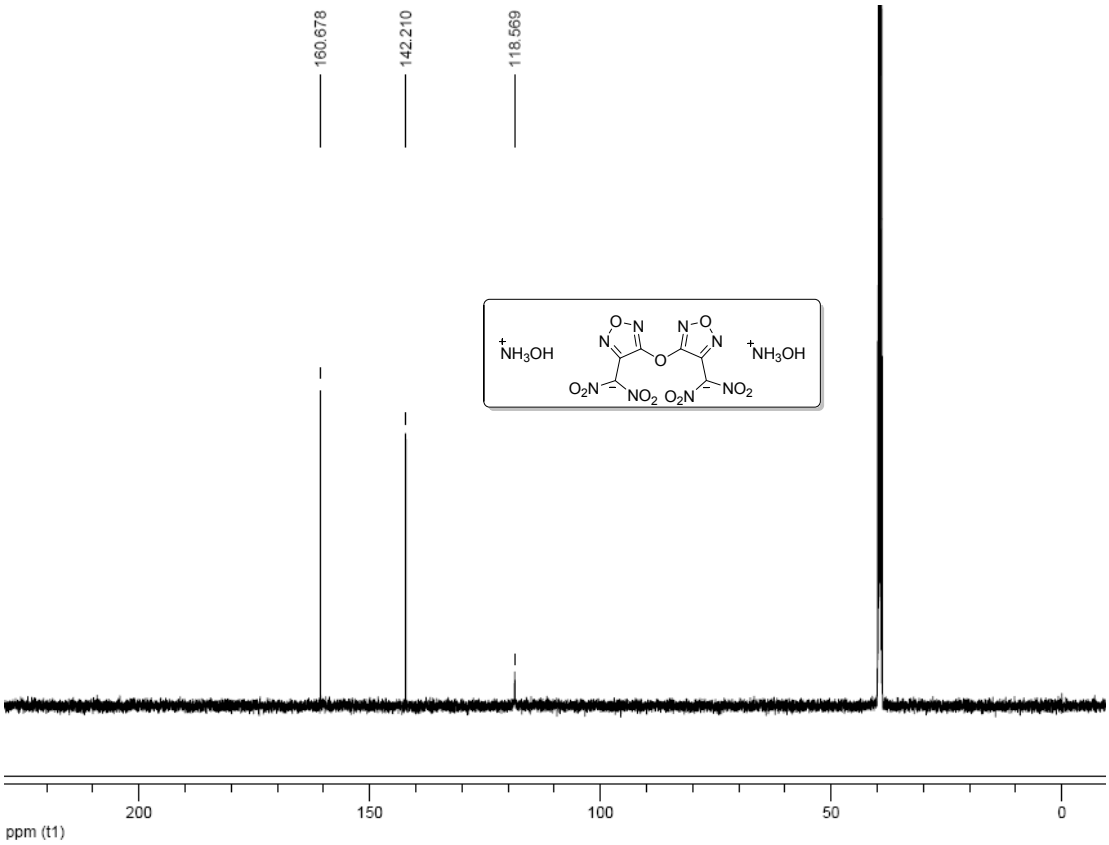

Fig. S8 ^{13}C NMR spectrum of **5** in DMSO-*d6*

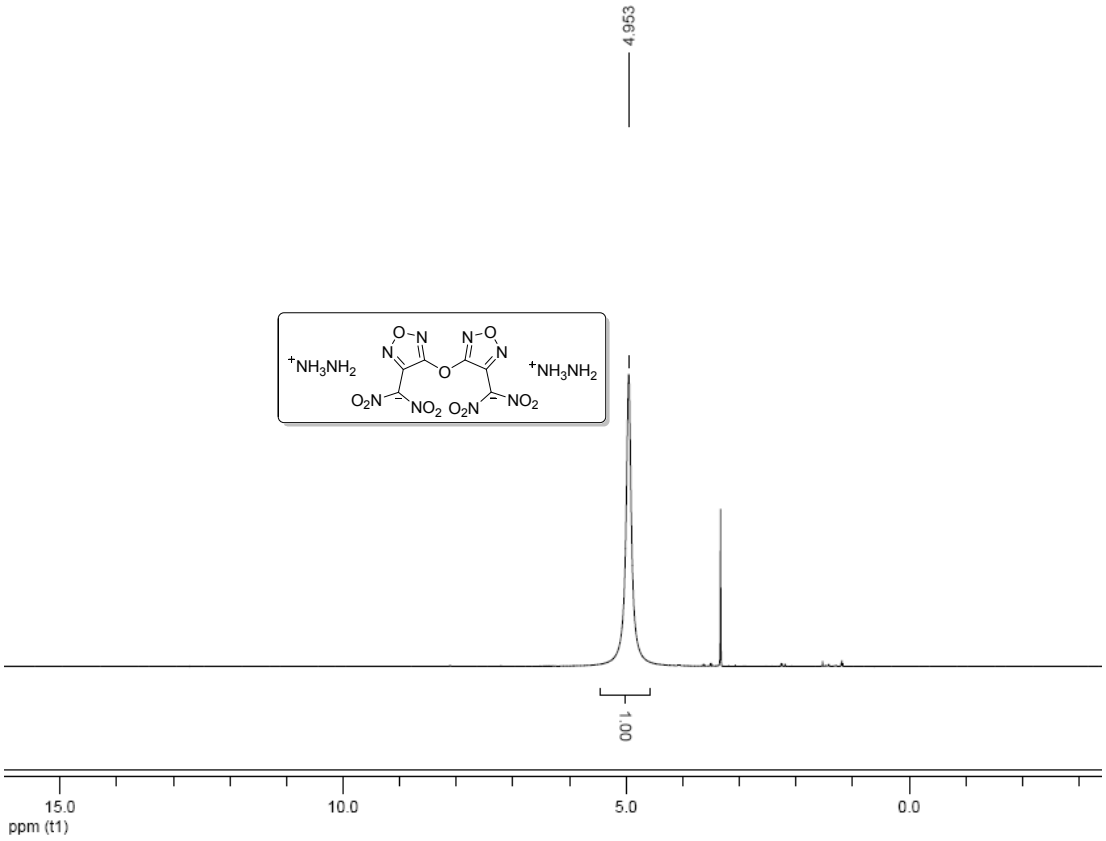

Fig. S9 ^{1}H NMR spectrum of **6** in CD_3OD

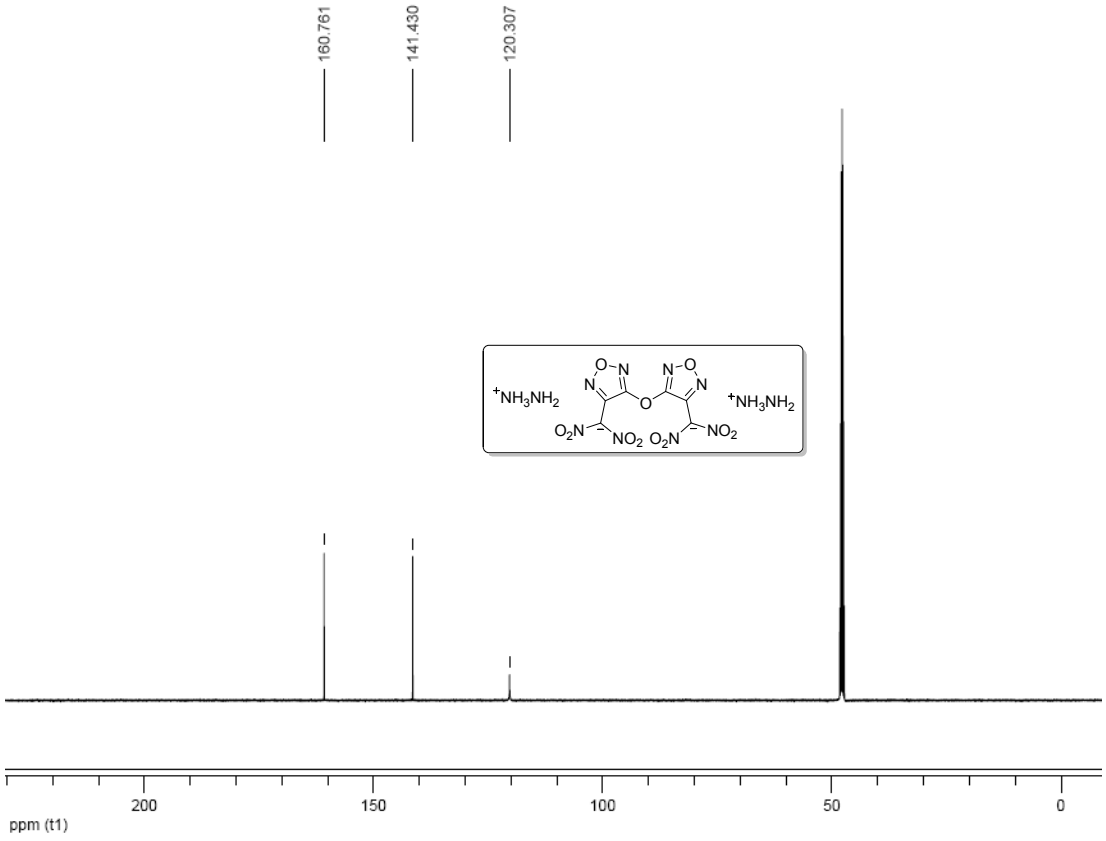

Fig. S10 ^{13}C NMR spectrum of **6** in CD_3OD

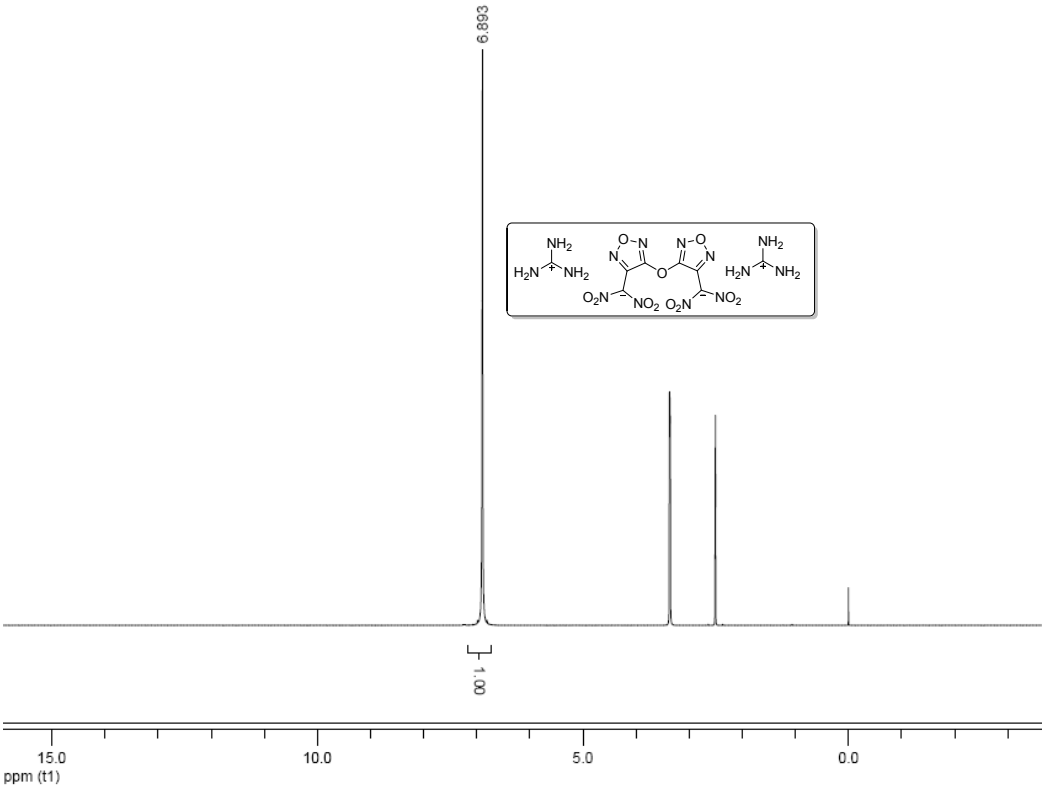

Fig. S11 ^{1}H NMR spectrum of **7** in DMSO-*d6*

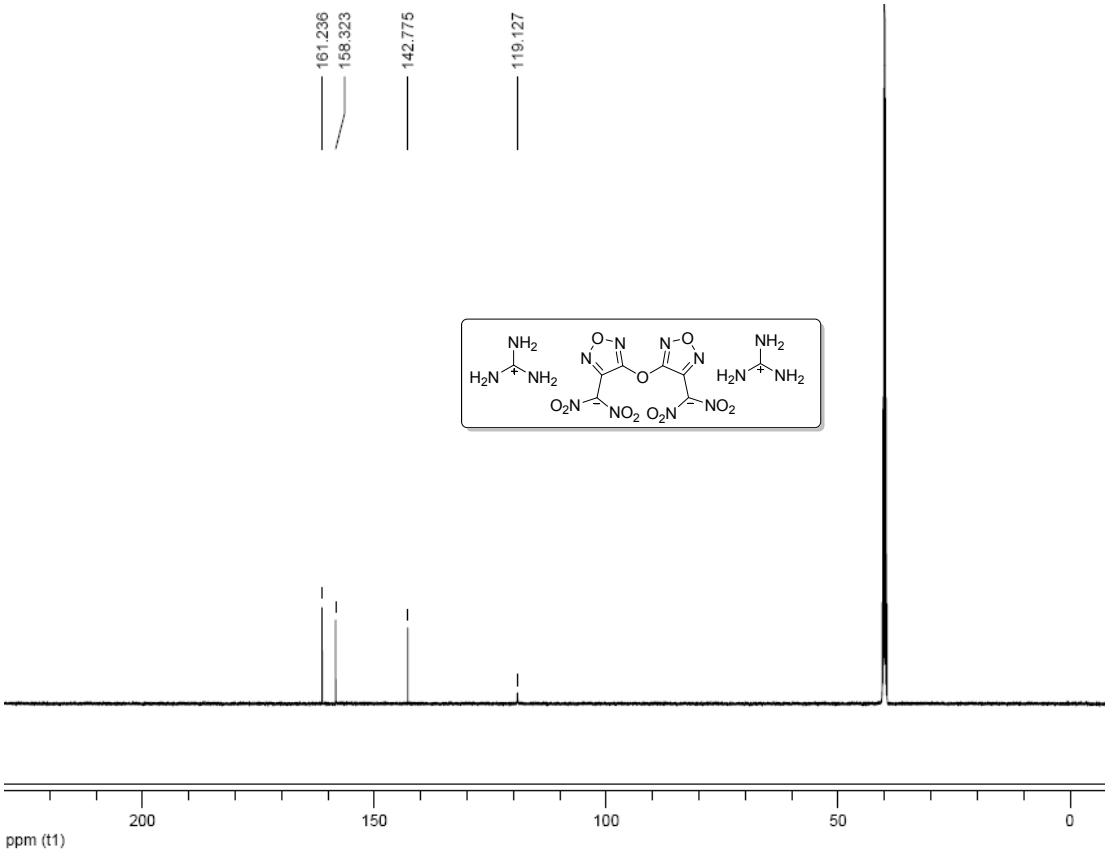

Fig. S12 ^{13}C NMR spectrum of **7** in DMSO-*d6*

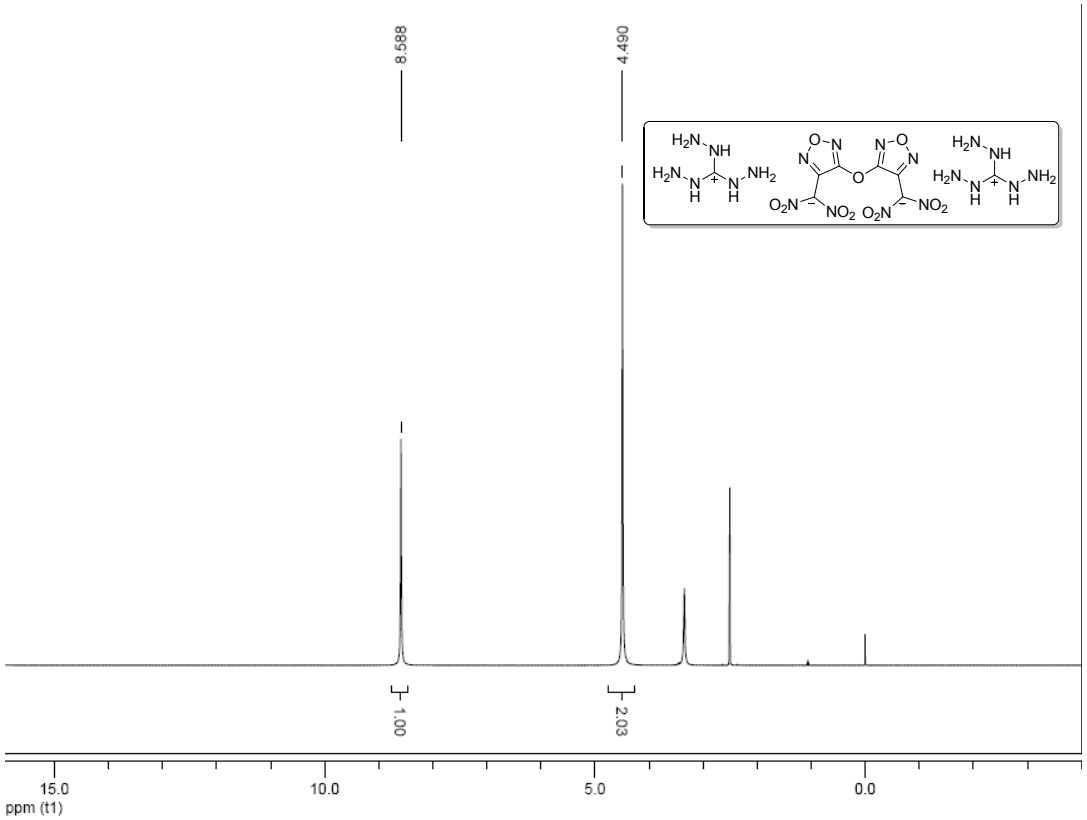

Fig. S13 ^{1}H NMR spectrum of **8** in DMSO-*d6*

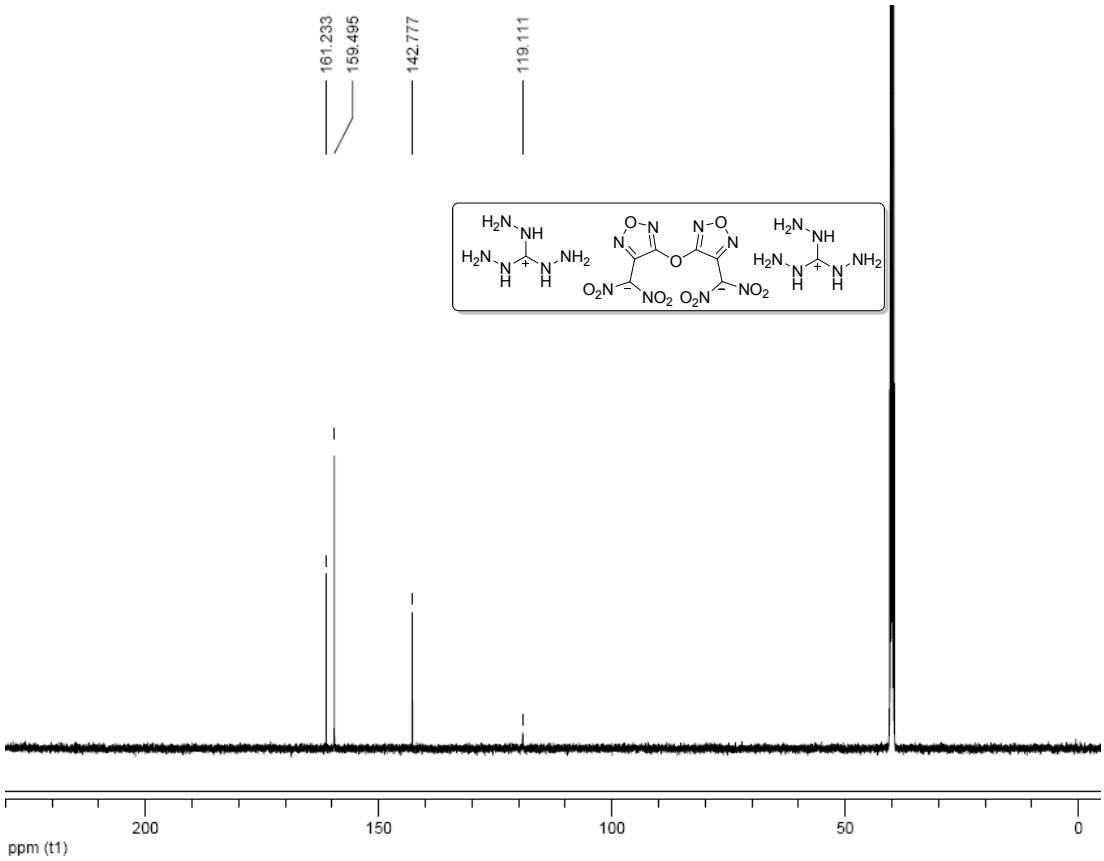

Fig. S14 ^{13}C NMR spectrum of **8** in DMSO-*d6*

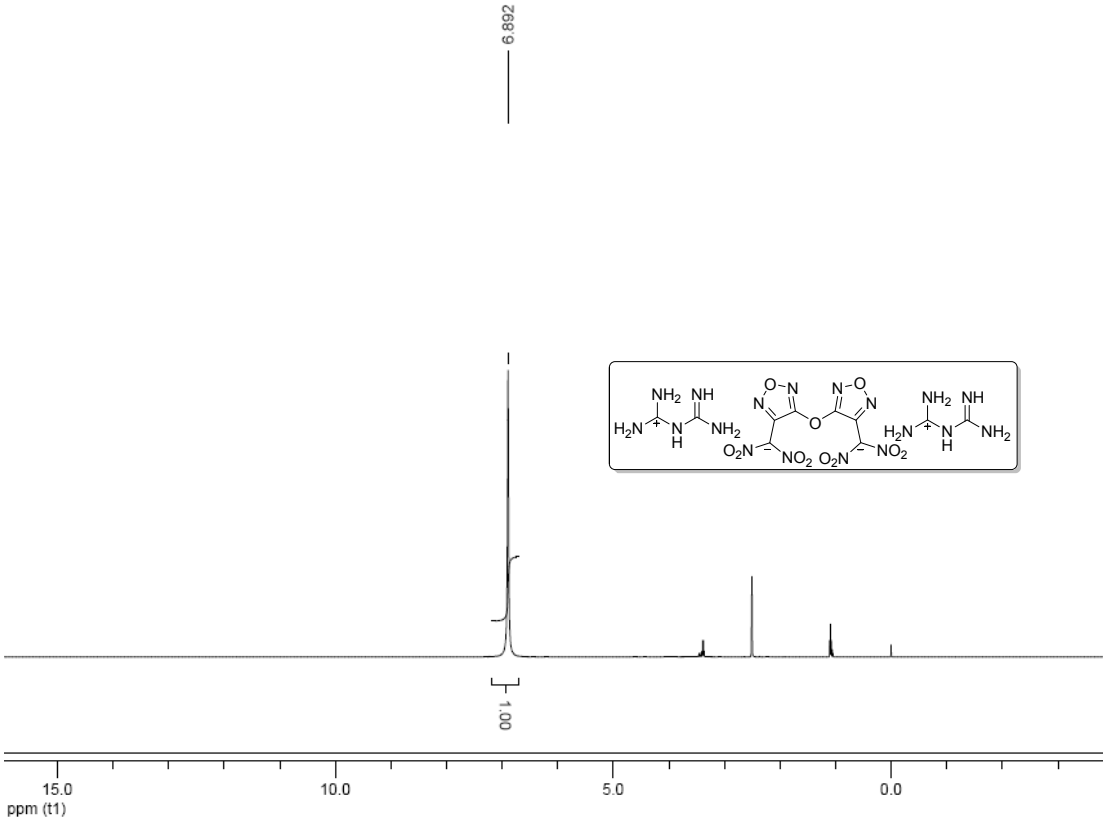

Fig. S15 ^{1}H NMR spectrum of **9** in DMSO-*d6*

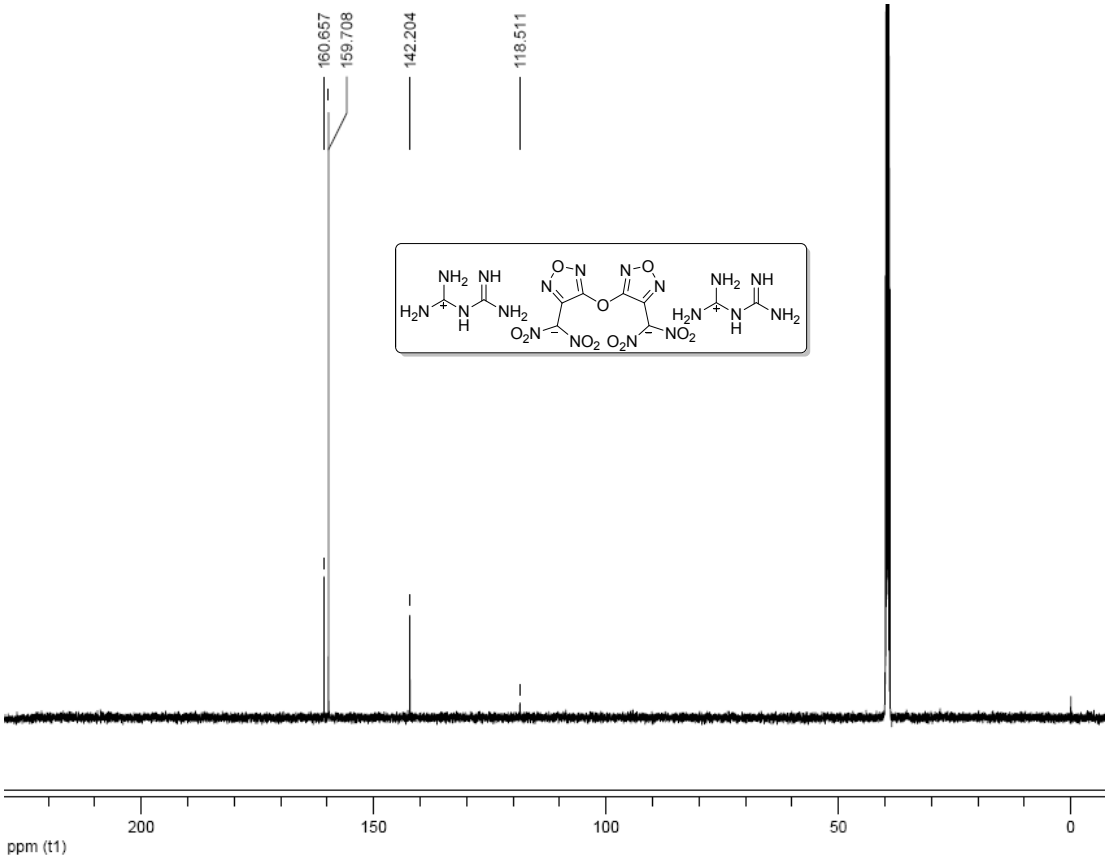

Fig. S16 ^{13}C NMR spectrum of **9** in DMSO-*d6*

4. DSC curves of compounds 3-9

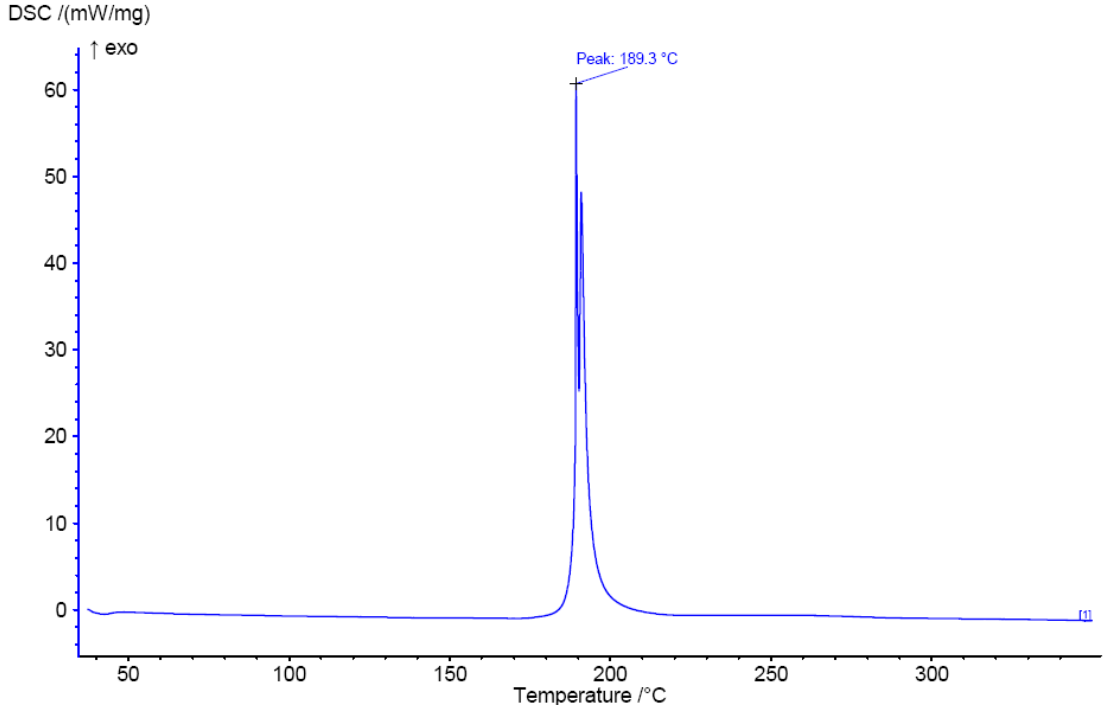

Fig. S17 DSC curve of **3**

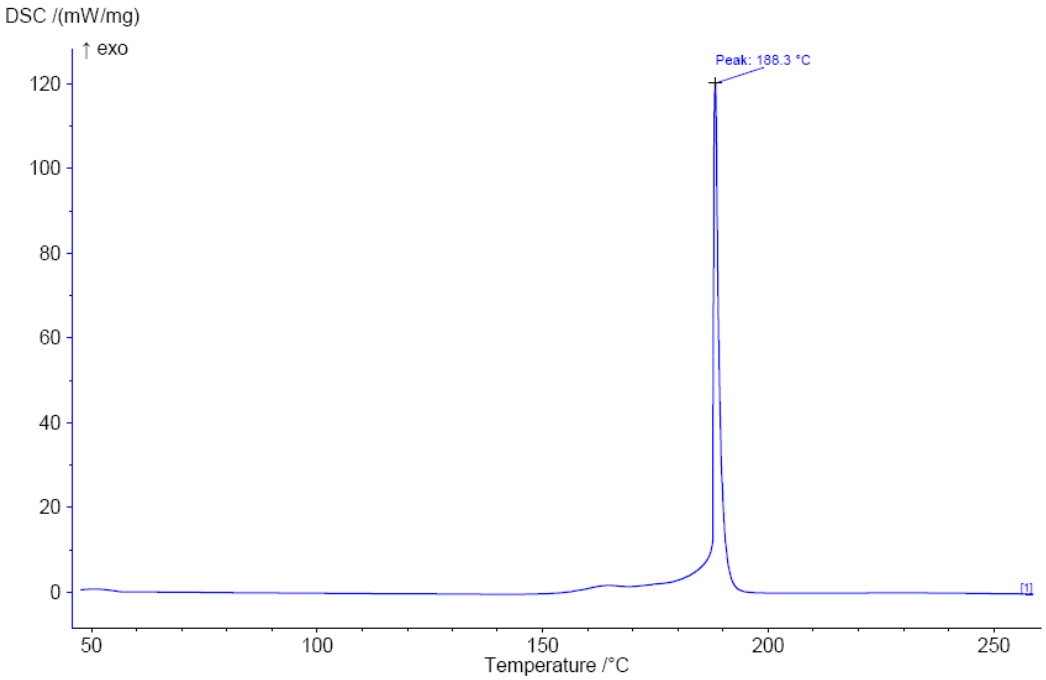

Fig. S18 DSC curve of **4**

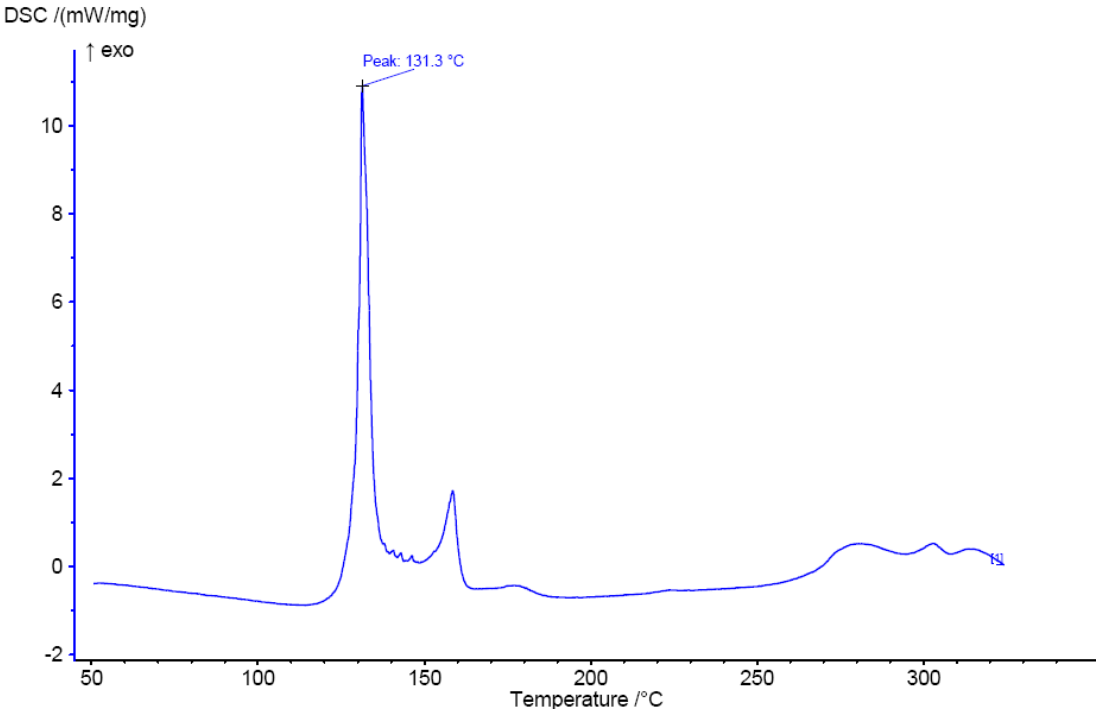

Fig. S19 DSC curve of **5**

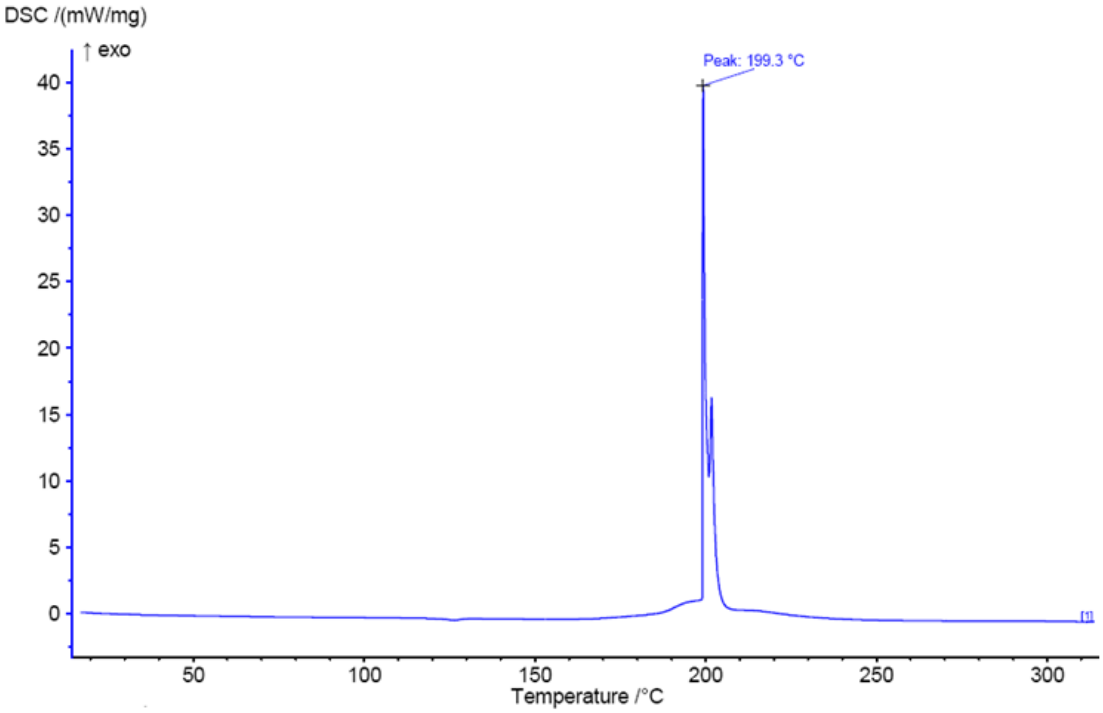

Fig. S20 DSC curve of **6**

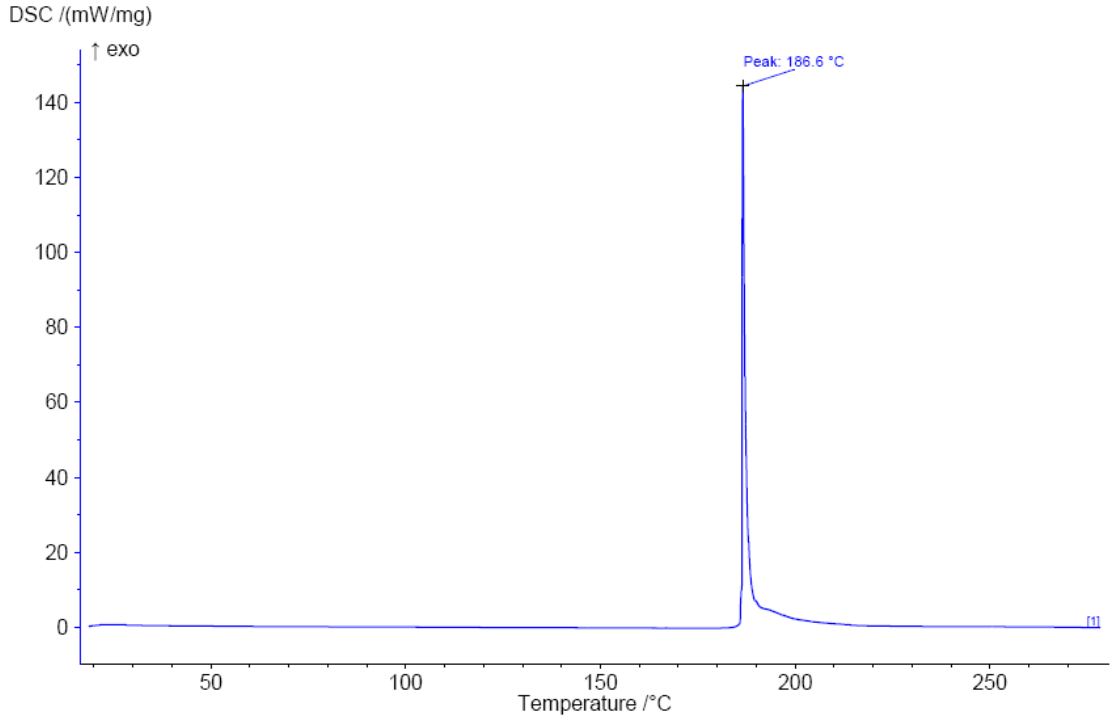

Fig. S21 DSC curve of **7**

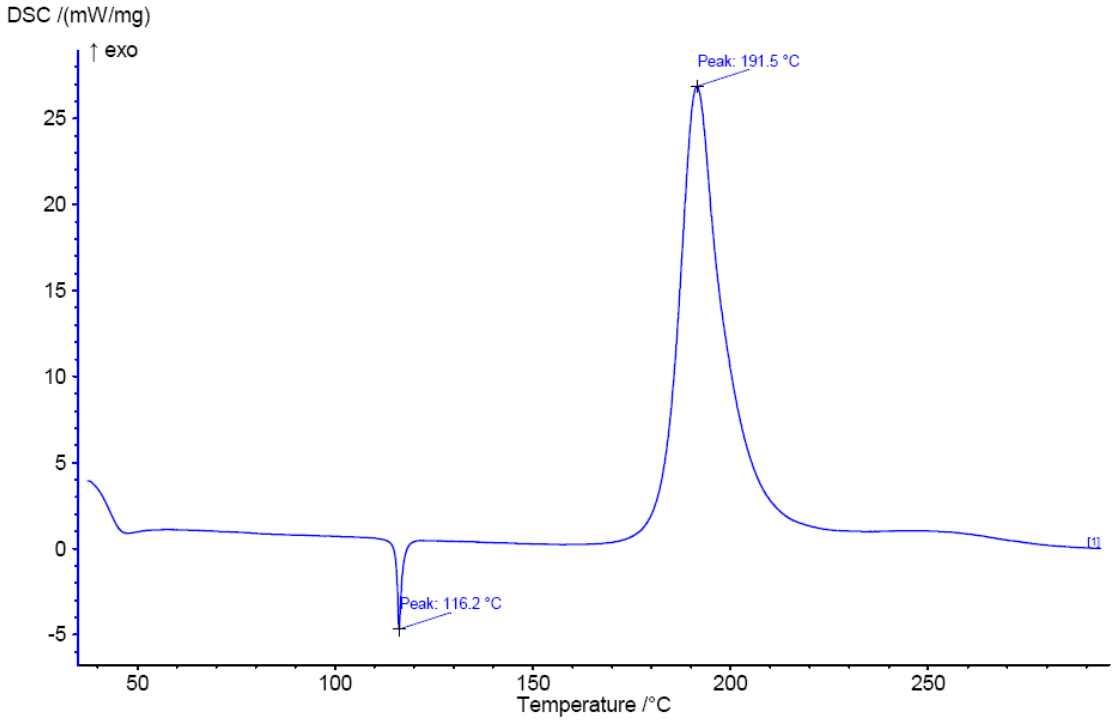

Fig. S22 DSC curve of **8**

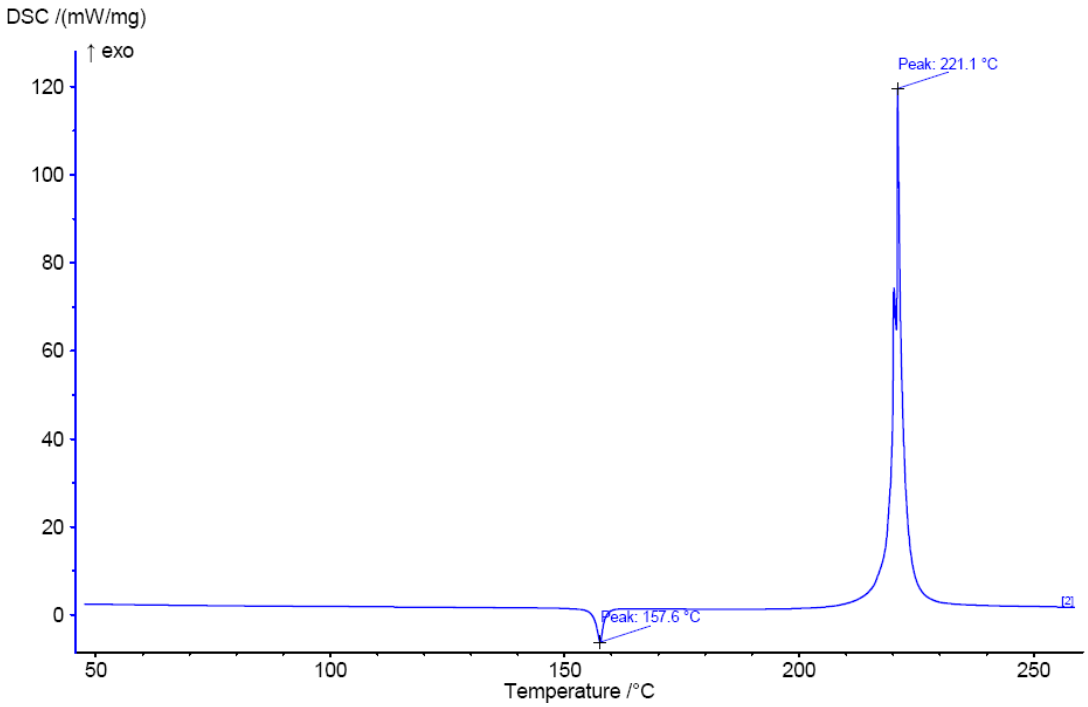

Fig. S23 DSC curve of **9.**