Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Synthesis, single crystal structure of fully-substituted polynitrobenzene derivatives for high-energy materials

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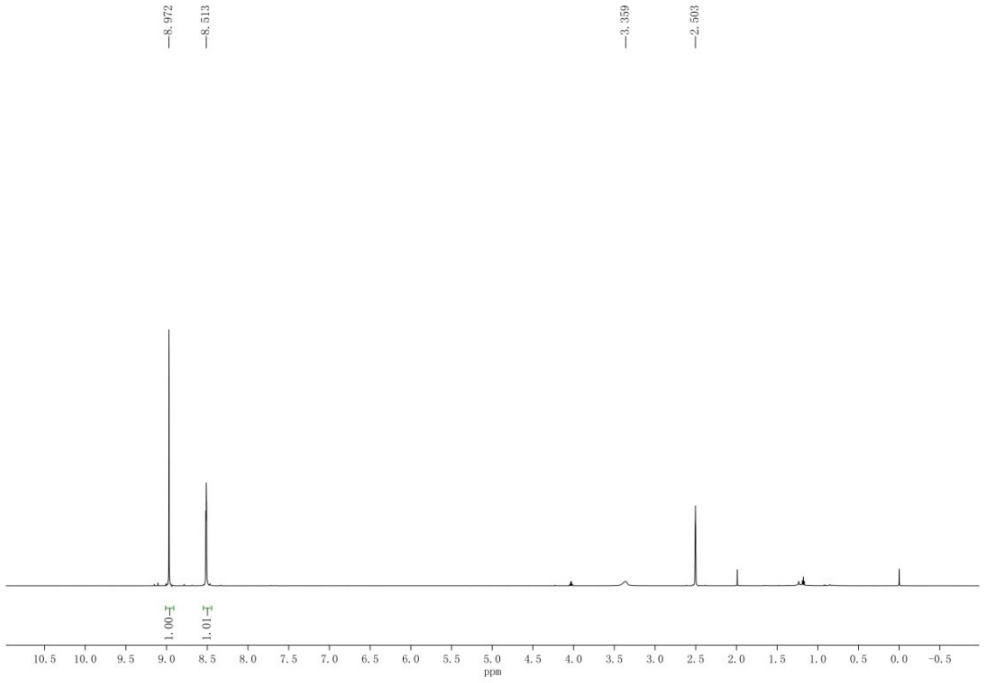

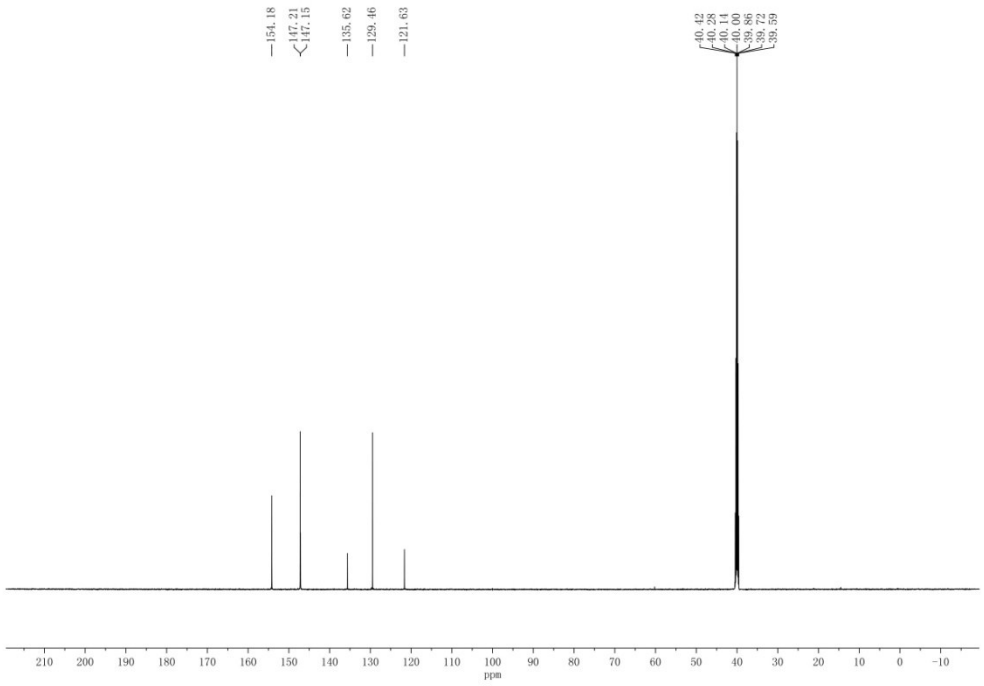

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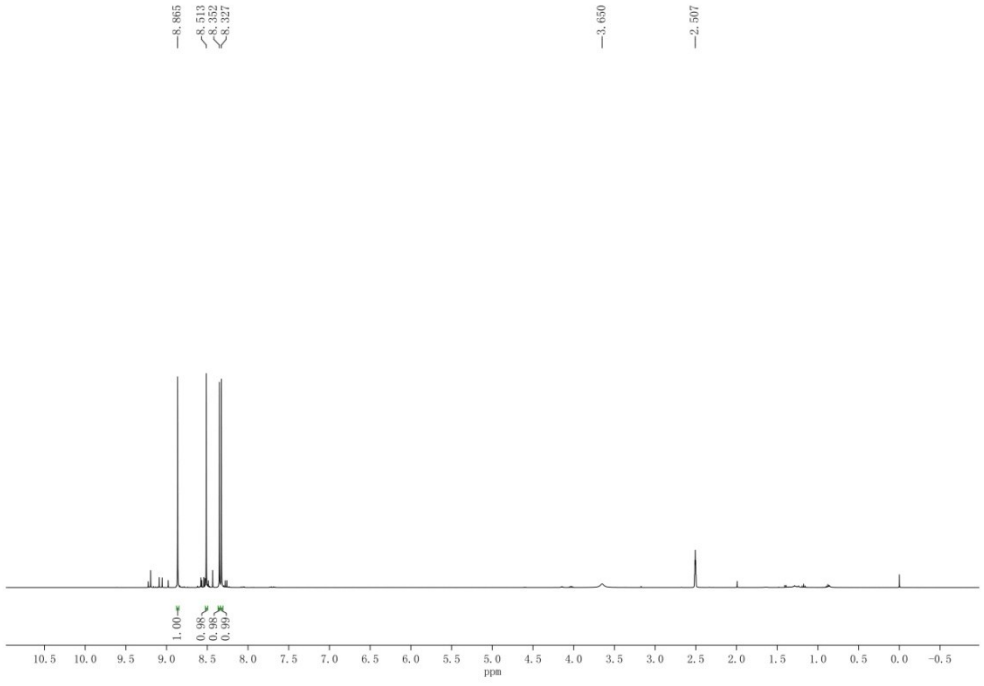

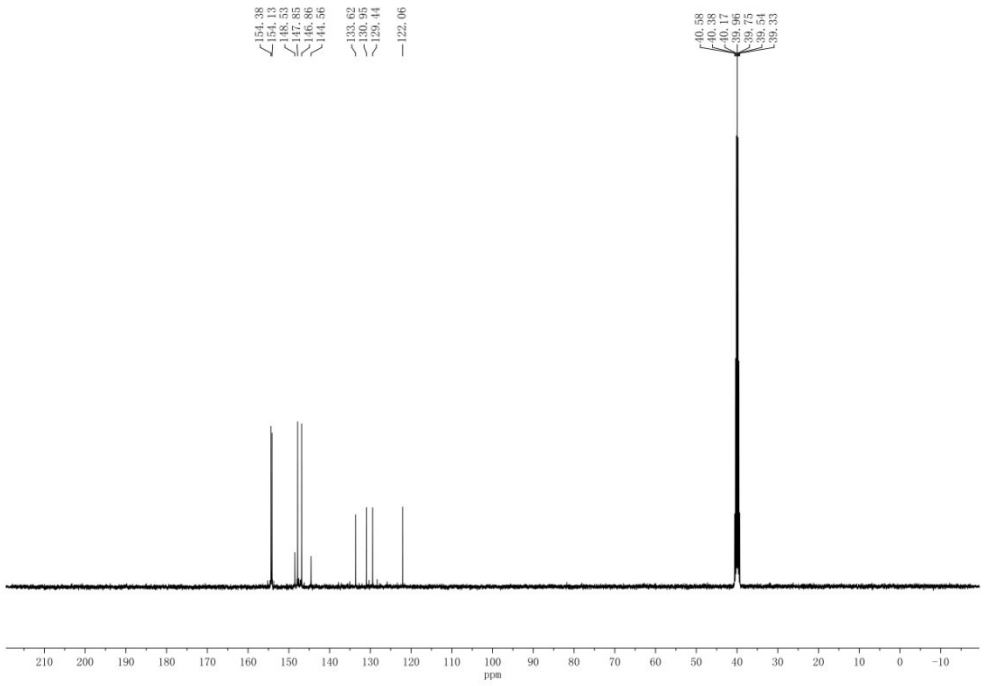

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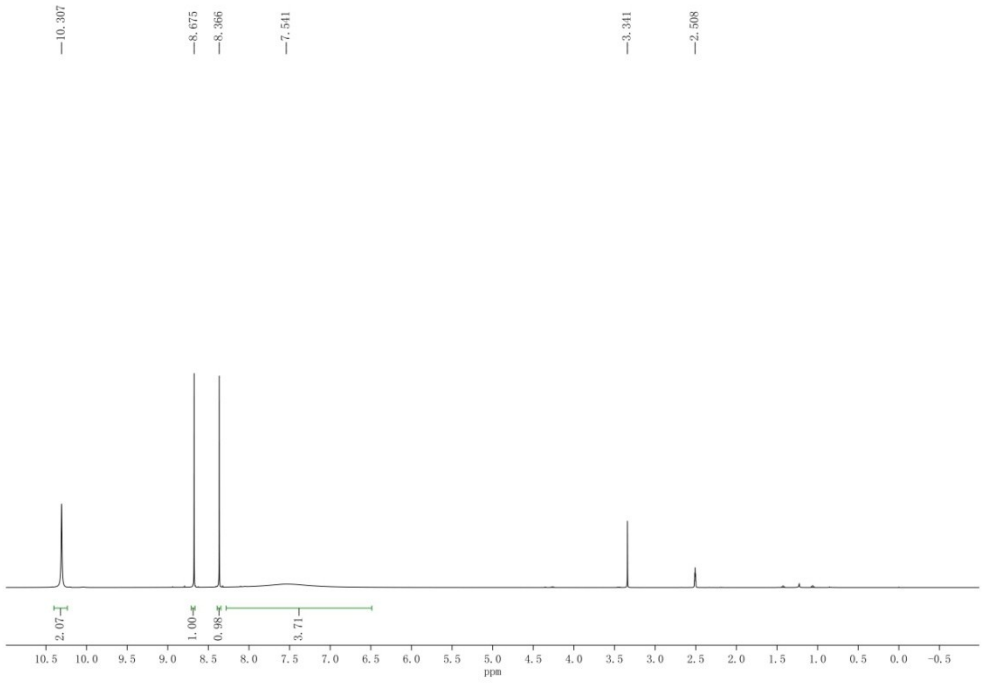

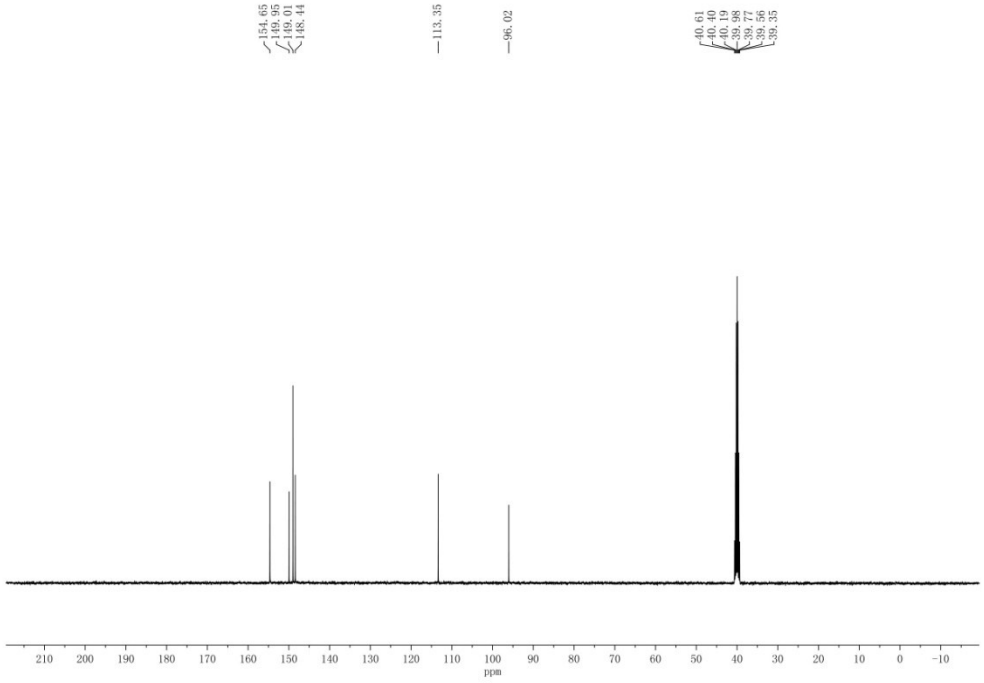

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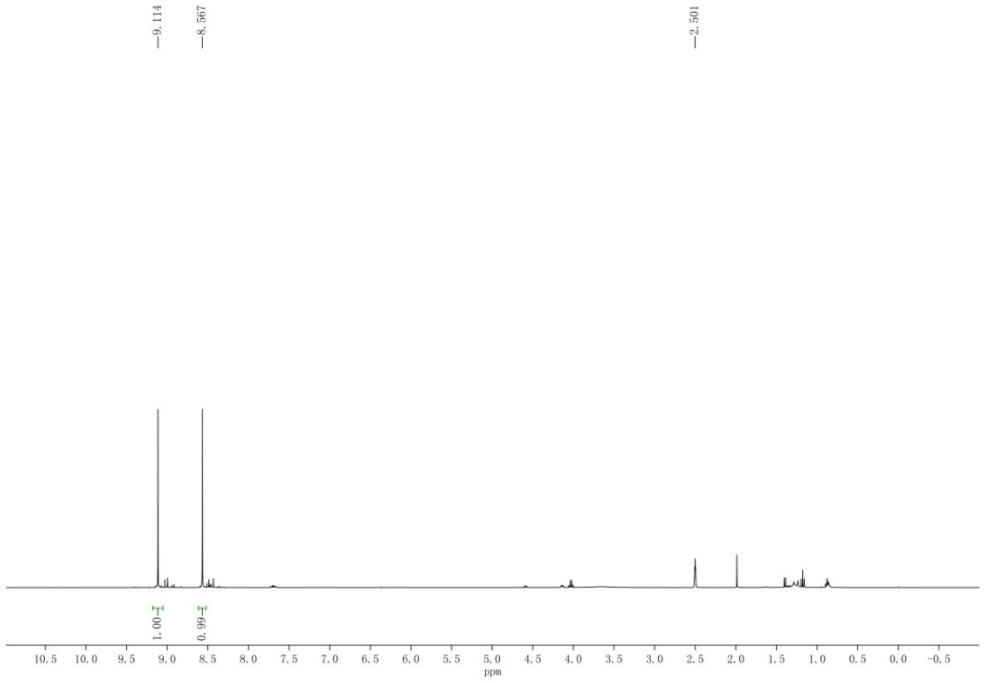

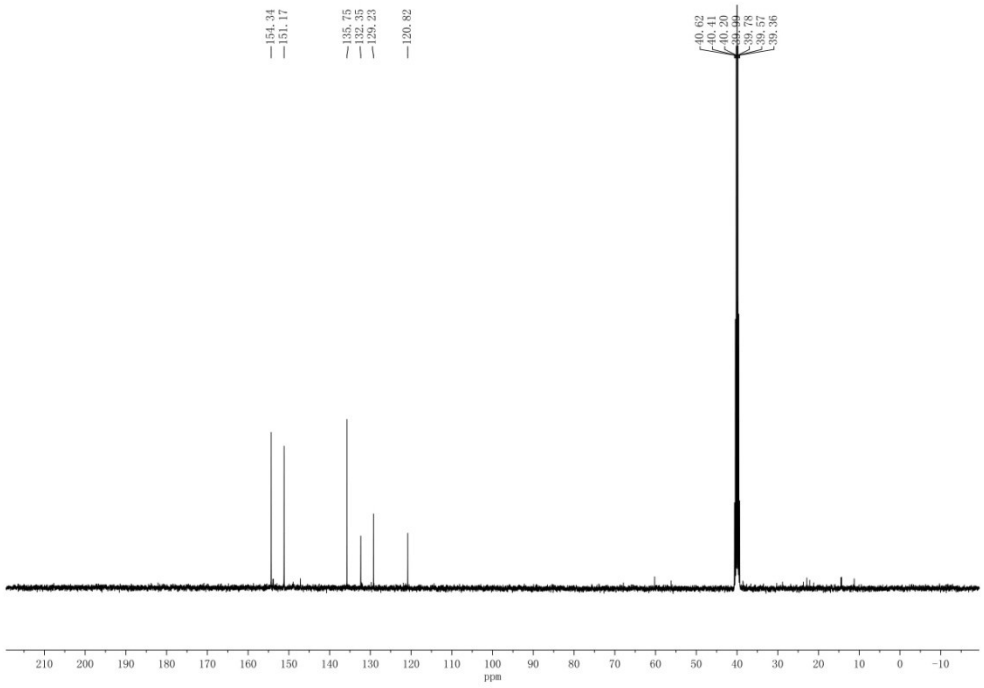

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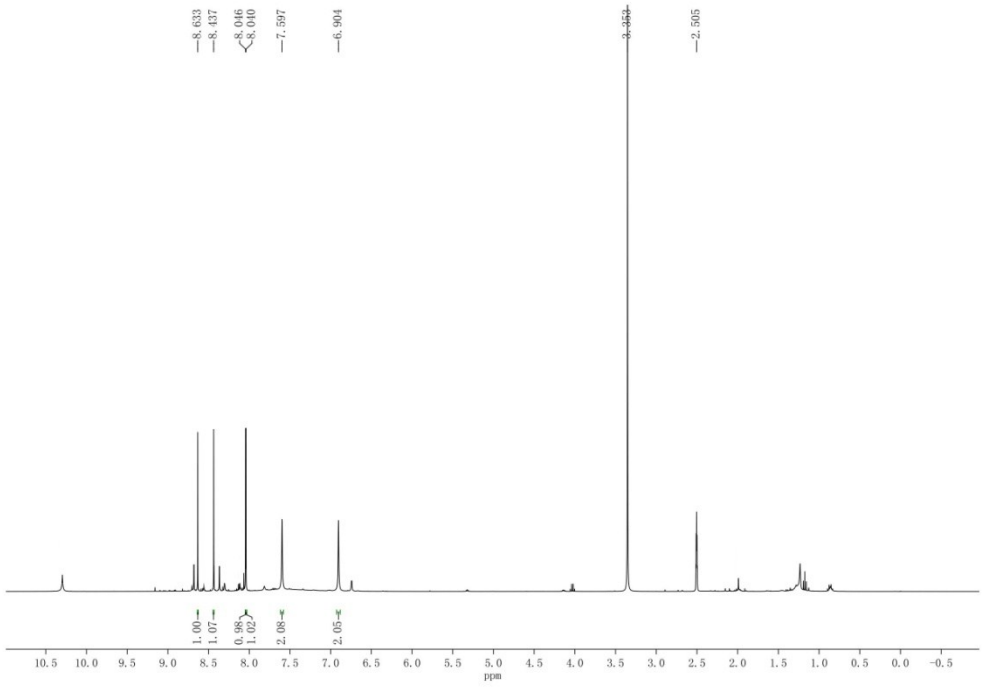

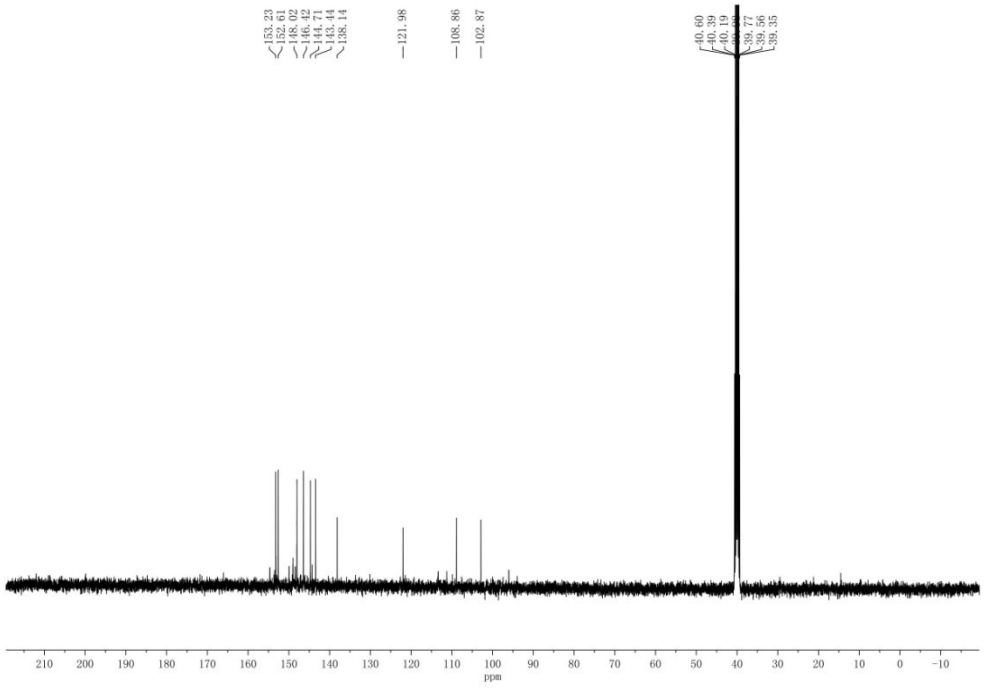

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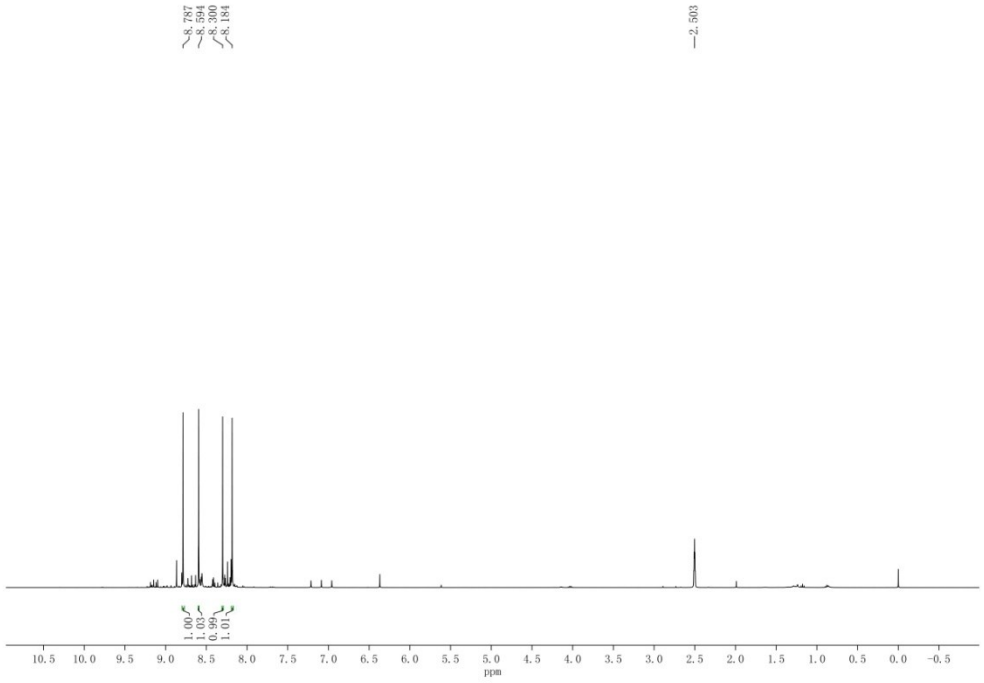
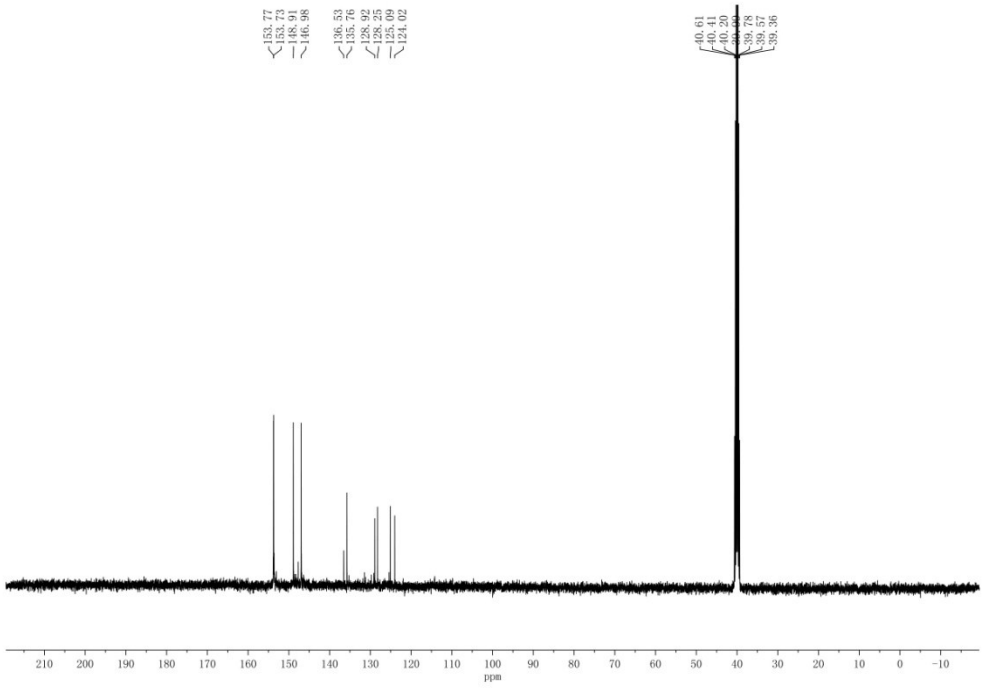
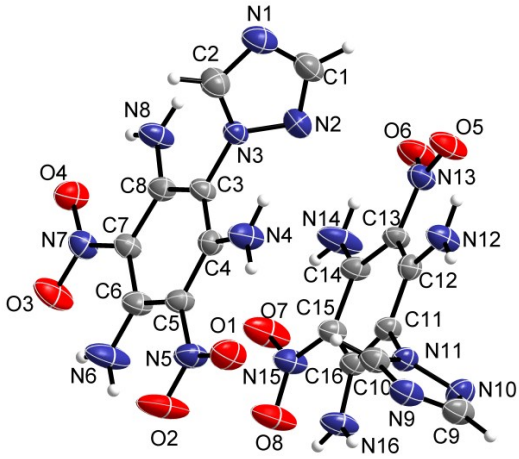
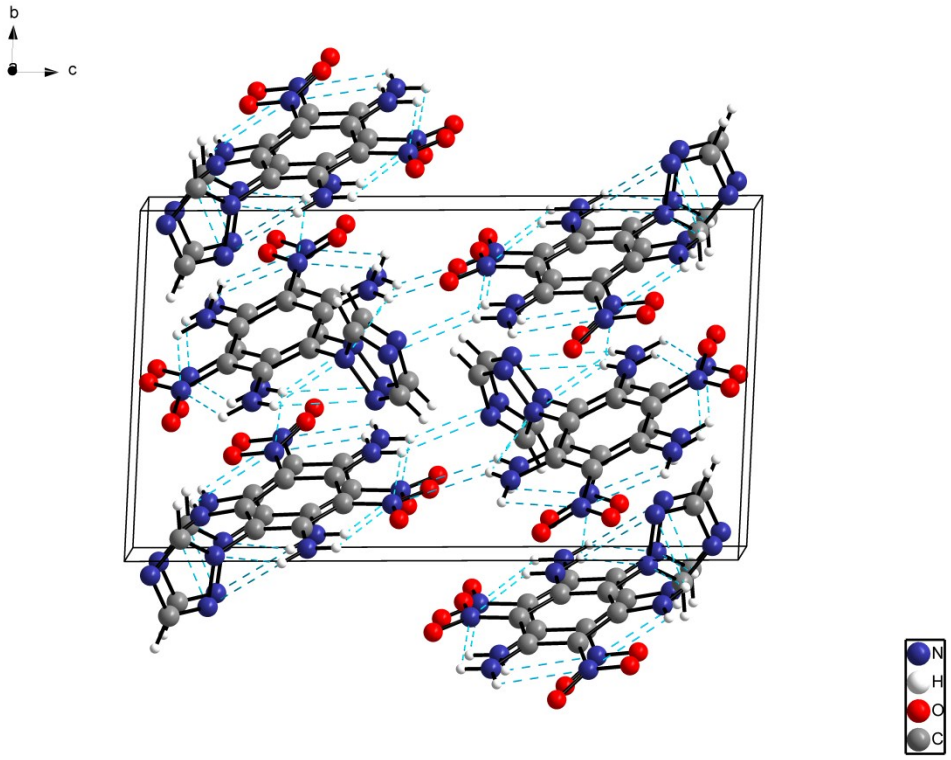




Crystal structures and crystalline parameters

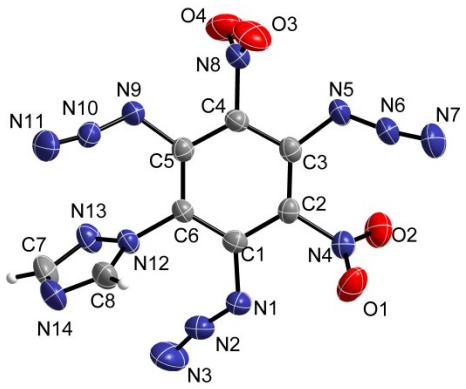


(a)

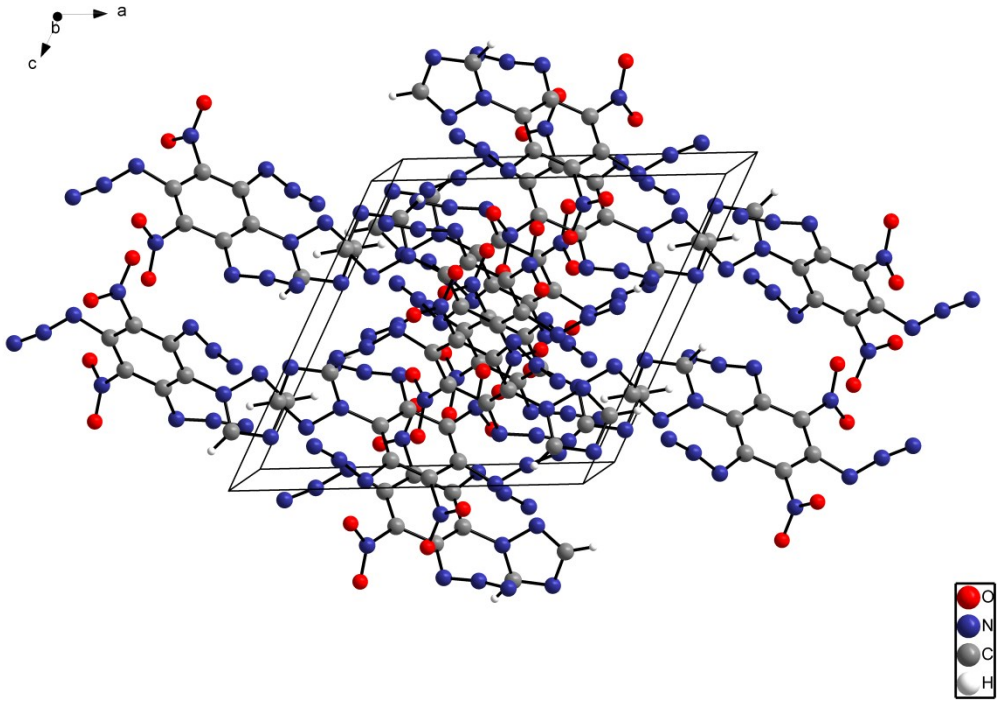


(b)

Fig. S1 (a) Thermal ellipsoid plot (50%) and labelling scheme of **6**. (b) Ball-and-stick packing diagram of **6** viewed down the *a* axis. Dashed lines indicate strong hydrogen bonding.



(a)



(b)

Fig.S2 (a) Thermal ellipsoid plot (50%) and labelling scheme of **7**. (b) Ball-and-stick packing diagram of **7** viewed down the *b* axis. Dashed lines indicate strong hydrogen bonding.

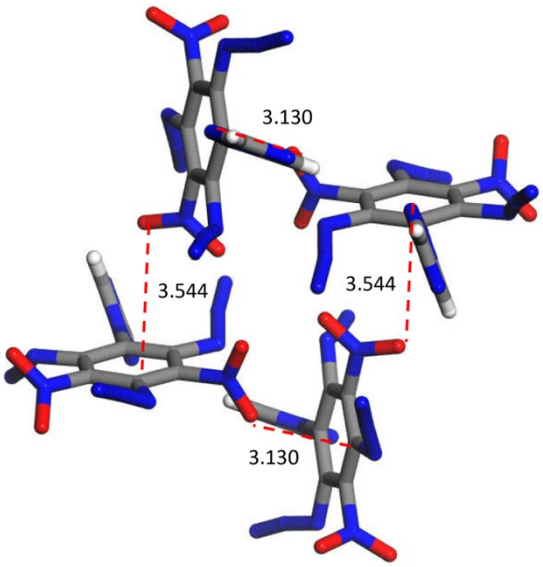
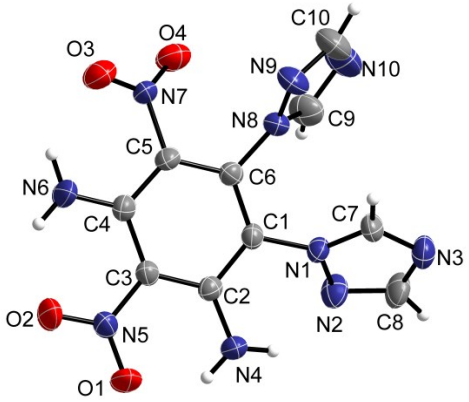
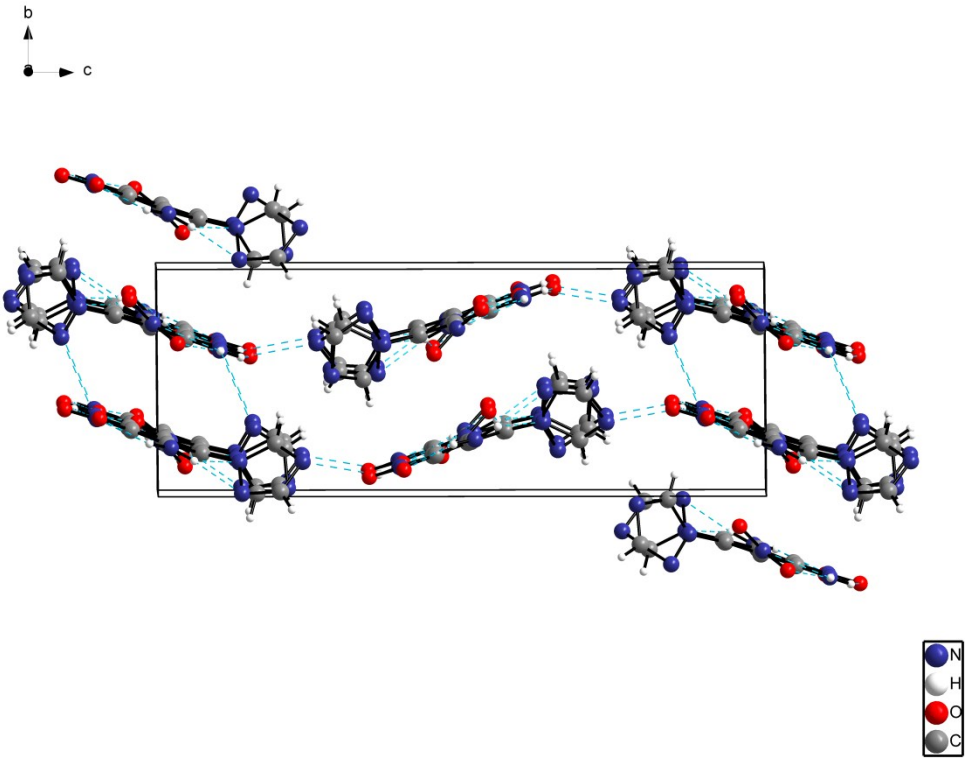


Fig.S3 Figure showing the nitro-π interactions (dashed red lines between nitro oxygen atoms and ring centroids) for each molecule of **7**



(a)



(b)

Fig.S4 (a) Thermal ellipsoid plot (50%) and labelling scheme of **8**. (b) Ball-and-stick packing diagram of **8** viewed down the *a* axis. Dashed lines indicate strong hydrogen bonding.

Table S1. Crystal data and structure refinement details for **4**, **5**, **6**, **7** and **8**

	4	**5**	**6**	**7**	**8**
Formula	$C_8H_2Cl_3N_5O_4$	$C_{20}H_8Cl_4N_{16}O_8$	$C_{16}H_{16}N_{16}O_8$	$C_8H_2N_{14}O_4$	$C_{10}H_8N_{10}O_4$
Molecular weight [g mol^{-1}]	338.50	742.22	560.45	358.24	332.26
T [K]	273(2)	293(2)	293(2)	293(2)	293(2)
Crystal size [mm^3]	0.21×0.16×0.13	0.22×0.17×0.13	0.20×0.17×0.11	0.18×0.16×0.13	0.17×0.13×0.07
Crystal system	Monoclinic	Monoclinic	Triclinic	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/c$	P-1	$P2_1/c$	$P2_1/c$
a [Å]	8.8432(19)	16.424(3)	7.4815(11)	11.5557(18)	8.941(3)
b [Å]	17.400(4)	10.270(2)	9.2466(13)	11.6416(19)	7.445(3)
c [Å]	16.430(4)	17.559(3)	16.151(3)	11.1129(17)	20.759(7)
α [˚]	90	90	87.286(4)	90	90
β [˚]	91.832(4)	92.886(4)	87.725(3)	116.222(3)	106.328(15)
γ [˚]	90	90	89.891(3)	90	90
V [Å^3]	2526.9(9)	2958.0(10)	1115.2(3)	1341.1(4)	1326.1(8)
Z	8	4	2	4	4
λ [Å]	0.71073	0.71073	0.71073	0.71073	0.71073
ρ_{calc} [g cm^{-3}]	1.780	1.667	1.669	1.774	1.664
μ [mm^{-1}]	0.746	0.476	0.138	0.148	0.135
F (000)	1344	1488	576	720	680
ϑ range [˚]	1.705-25.999	1.241-24.997	2.489-25.498	1.964-25.496	2.045-25.499
Reflections collected	14977 / 4970	15478 / 5161	6451 / 4134	7543 / 2497	7331 / 2456
Index ranges	-10≤h≤9 -21≤k≤21 -20≤l≤19	-19≤h≤19 -11≤k≤12 -15≤l≤20	-8≤h≤9 -11≤k≤6 -17≤l≤19	-13≤h≤13 -13≤k≤14 -12≤l≤13	-7≤h≤10 -8≤k≤9 -25≤l≤24
R_{int}	0.0357	0.0433	0.0212	0.0334	0.0749
Data / restraints / parameters	4970 / 0 / 361	5161 / 13 / 433	4134 / 0 / 361	2497 / 0 / 235	2456 / 0 / 225
Final R index [$I > 2\sigma(I)$]	R1=0.0413, wR2=0.1040	R1=0.0788, wR2=0.2088	R1=0.0486, wR2=0.1219	R1=0.0468, wR2=0.1089	R1=0.0522, wR2=0.1137
Final R index [all data]	R1=0.0582, wR2=0.1139	R1=0.0965, wR2=0.2193	R1=0.0647, wR2=0.1331	R1=0.0620, wR2=0.1174	R1=0.1012, wR2=0.1328
GOF on F^2	1.020	1.118	1.034	1.039	0.974
CCDC number	1552452	1552455	1552453	1552454	1552456

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

	x	y	z	U(eq)
Cl(1)	10196(1)	3609(1)	-250(1)	67(1)
Cl(2)	4189(1)	3562(1)	-821(1)	60(1)
Cl(3)	6435(1)	4385(1)	2116(1)	62(1)
Cl(4)	7644(1)	637(1)	-1834(1)	67(1)
Cl(5)	4029(1)	1439(1)	571(1)	68(1)
Cl(6)	10048(1)	1495(1)	1070(1)	64(1)
N(1)	7397(2)	3377(1)	-1263(1)	42(1)
N(2)	7305(3)	2637(1)	-1491(1)	69(1)
N(3)	7592(3)	3402(1)	-2571(1)	63(1)
N(4)	3973(2)	4043(1)	905(1)	53(1)
N(5)	9470(2)	4125(2)	1427(1)	57(1)

N(6)	6870(2)	1664(1)	1551(1)	41(1)
N(7)	6885(3)	2408(1)	1775(1)	65(1)
N(8)	6722(3)	1645(1)	2862(1)	60(1)
N(9)	4682(2)	909(1)	-1104(1)	53(1)
N(10)	10194(2)	1019(2)	-674(1)	59(1)
O(1)	3371(2)	3490(1)	1172(2)	96(1)
O(2)	3413(2)	4663(1)	835(2)	102(1)
O(3)	10066(2)	3567(2)	1725(1)	87(1)
O(4)	9823(3)	4774(2)	1548(2)	103(1)
O(5)	4166(2)	1448(1)	-1468(1)	88(1)
O(6)	4204(3)	265(1)	-1138(2)	90(1)
O(7)	10673(3)	391(2)	-779(2)	108(1)
O(8)	10849(3)	1603(2)	-817(2)	97(1)
C(1)	8407(2)	3738(1)	78(1)	40(1)
C(2)	7179(2)	3600(1)	-444(1)	38(1)
C(3)	5718(2)	3702(1)	-177(1)	41(1)
C(4)	5519(2)	3944(1)	611(1)	40(1)
C(5)	6727(2)	4095(1)	1139(1)	40(1)
C(6)	8164(2)	3985(1)	861(1)	41(1)
C(7)	7565(3)	3811(2)	-1916(2)	62(1)
C(8)	7437(4)	2692(2)	-2277(2)	70(1)
C(9)	7431(3)	939(1)	-856(1)	41(1)
C(10)	6013(2)	1053(1)	-560(1)	40(1)
C(11)	5806(2)	1310(1)	220(1)	41(1)
C(12)	7063(2)	1441(1)	731(1)	38(1)
C(13)	8497(2)	1344(1)	438(1)	41(1)
C(14)	8664(2)	1096(1)	-352(1)	42(1)
C(15)	6760(3)	1228(2)	2210(2)	59(1)
C(16)	6796(3)	2350(2)	2566(2)	65(1)

Table S3. Bond lengths [Å] and angles [°] for **4**.

Cl(1)-C(1)	1.703(2)
Cl(2)-C(3)	1.708(2)
Cl(3)-C(5)	1.710(2)
Cl(4)-C(9)	1.707(2)
Cl(5)-C(11)	1.706(2)
Cl(6)-C(13)	1.714(2)
N(1)-C(7)	1.323(3)

N(1)-N(2)	1.343(3)
N(1)-C(2)	1.419(3)
N(2)-C(8)	1.305(3)
N(3)-C(7)	1.291(3)
N(3)-C(8)	1.334(4)
N(4)-O(1)	1.191(3)
N(4)-O(2)	1.191(3)
N(4)-C(4)	1.474(3)
N(5)-O(4)	1.187(3)
N(5)-O(3)	1.201(3)
N(5)-C(6)	1.480(3)
N(6)-C(15)	1.328(3)
N(6)-N(7)	1.346(3)
N(6)-C(12)	1.417(3)
N(7)-C(16)	1.309(3)
N(7)-O(1)	3.739(4)
N(8)-C(15)	1.296(3)
N(8)-C(16)	1.323(3)
N(9)-O(5)	1.194(3)
N(9)-O(6)	1.199(3)
N(9)-C(10)	1.477(3)
N(10)-O(7)	1.187(3)
N(10)-O(8)	1.197(3)
N(10)-C(14)	1.474(3)
C(1)-C(6)	1.380(3)
C(1)-C(2)	1.383(3)
C(2)-C(3)	1.390(3)
C(3)-C(4)	1.378(3)
C(4)-C(5)	1.379(3)
C(5)-C(6)	1.378(3)
C(7)-C(8)	2.038(4)
C(7)-H(7)	0.9300
C(8)-H(8)	0.9300
C(9)-C(10)	1.373(3)
C(9)-C(14)	1.375(3)
C(10)-C(11)	1.375(3)
C(11)-C(12)	1.391(3)
C(12)-C(13)	1.381(3)

C(13)-C(14)	1.381(3)
C(15)-C(16)	2.039(4)
C(15)-H(15)	0.9300
C(16)-H(16)	0.9300

C(7)-N(1)-N(2)	109.2(2)
C(7)-N(1)-C(2)	129.4(2)
N(2)-N(1)-C(2)	121.10(18)
C(8)-N(2)-N(1)	101.5(2)
C(7)-N(3)-C(8)	101.8(2)
O(1)-N(4)-O(2)	125.3(2)
O(1)-N(4)-C(4)	117.1(2)
O(2)-N(4)-C(4)	117.5(2)
O(4)-N(5)-O(3)	126.2(2)
O(4)-N(5)-C(6)	117.2(2)
O(3)-N(5)-C(6)	116.6(2)
C(15)-N(6)-N(7)	109.1(2)
C(15)-N(6)-C(12)	129.3(2)
N(7)-N(6)-C(12)	121.46(18)
C(16)-N(7)-N(6)	101.4(2)
C(16)-N(7)-O(1)	103.04(19)
N(6)-N(7)-O(1)	114.26(16)
C(15)-N(8)-C(16)	102.3(2)
O(5)-N(9)-O(6)	125.6(2)
O(5)-N(9)-C(10)	117.0(2)
O(6)-N(9)-C(10)	117.4(2)
O(7)-N(10)-O(8)	125.2(2)
O(7)-N(10)-C(14)	118.1(2)
O(8)-N(10)-C(14)	116.7(2)
N(4)-O(1)-N(7)	97.31(16)
C(6)-C(1)-C(2)	119.35(19)
C(6)-C(1)-Cl(1)	120.66(17)
C(2)-C(1)-Cl(1)	119.99(17)
C(1)-C(2)-C(3)	120.0(2)
C(1)-C(2)-N(1)	120.54(19)
C(3)-C(2)-N(1)	119.39(19)
C(4)-C(3)-C(2)	119.0(2)
C(4)-C(3)-Cl(2)	120.24(17)

C(2)-C(3)-Cl(2)	120.76(17)
C(3)-C(4)-C(5)	121.98(19)
C(3)-C(4)-N(4)	119.40(19)
C(5)-C(4)-N(4)	118.6(2)
C(6)-C(5)-C(4)	117.9(2)
C(6)-C(5)-Cl(3)	121.41(17)
C(4)-C(5)-Cl(3)	120.64(17)
C(5)-C(6)-C(1)	121.7(2)
C(5)-C(6)-N(5)	118.6(2)
C(1)-C(6)-N(5)	119.68(19)
N(3)-C(7)-N(1)	111.5(2)
N(3)-C(7)-C(8)	39.85(15)
N(1)-C(7)-C(8)	71.62(16)
N(3)-C(7)-H(7)	124.3
N(1)-C(7)-H(7)	124.3
C(8)-C(7)-H(7)	164.1
N(2)-C(8)-N(3)	116.0(2)
N(2)-C(8)-C(7)	77.71(17)
N(3)-C(8)-C(7)	38.33(14)
N(2)-C(8)-H(8)	122.0
N(3)-C(8)-H(8)	122.0
C(7)-C(8)-H(8)	160.3
C(10)-C(9)-C(14)	118.3(2)
C(10)-C(9)-Cl(4)	120.49(17)
C(14)-C(9)-Cl(4)	121.18(17)
C(9)-C(10)-C(11)	121.8(2)
C(9)-C(10)-N(9)	118.7(2)
C(11)-C(10)-N(9)	119.47(19)
C(10)-C(11)-C(12)	119.23(19)
C(10)-C(11)-Cl(5)	120.65(17)
C(12)-C(11)-Cl(5)	120.09(17)
C(13)-C(12)-C(11)	119.6(2)
C(13)-C(12)-N(6)	120.33(19)
C(11)-C(12)-N(6)	120.04(19)
C(14)-C(13)-C(12)	119.6(2)
C(14)-C(13)-Cl(6)	120.68(17)
C(12)-C(13)-Cl(6)	119.71(17)
C(9)-C(14)-C(13)	121.4(2)

C(9)-C(14)-N(10)	119.1(2)
C(13)-C(14)-N(10)	119.5(2)
N(8)-C(15)-N(6)	111.0(2)
N(8)-C(15)-C(16)	39.34(15)
N(6)-C(15)-C(16)	71.69(16)
N(8)-C(15)-H(15)	124.5
N(6)-C(15)-H(15)	124.5
C(16)-C(15)-H(15)	163.8
N(7)-C(16)-N(8)	116.2(2)
N(7)-C(16)-C(15)	77.83(17)
N(8)-C(16)-C(15)	38.38(13)
N(7)-C(16)-H(16)	121.9
N(8)-C(16)-H(16)	121.9
C(15)-C(16)-H(16)	160.3

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	38(1)	110(1)	54(1)	-10(1)	9(1)	3(1)
Cl(2)	43(1)	91(1)	44(1)	-6(1)	-9(1)	-3(1)
Cl(3)	67(1)	83(1)	35(1)	-14(1)	8(1)	-3(1)
Cl(4)	71(1)	94(1)	35(1)	-16(1)	6(1)	10(1)
Cl(5)	39(1)	112(1)	52(1)	-12(1)	8(1)	8(1)
Cl(6)	42(1)	97(1)	50(1)	-9(1)	-10(1)	-5(1)
N(1)	49(1)	46(1)	30(1)	-2(1)	3(1)	0(1)
N(2)	116(2)	49(1)	44(1)	-8(1)	4(1)	-2(1)
N(3)	74(2)	82(2)	32(1)	-4(1)	5(1)	2(1)
N(4)	40(1)	72(2)	47(1)	0(1)	7(1)	0(1)
N(5)	46(1)	83(2)	42(1)	-6(1)	-2(1)	-9(1)
N(6)	48(1)	44(1)	30(1)	-3(1)	1(1)	1(1)
N(7)	104(2)	49(1)	44(1)	-5(1)	5(1)	-2(1)
N(8)	73(2)	73(2)	32(1)	-4(1)	0(1)	-5(1)
N(9)	45(1)	76(2)	38(1)	-4(1)	-3(1)	0(1)
N(10)	44(1)	87(2)	48(1)	6(1)	9(1)	4(1)
O(1)	60(1)	115(2)	114(2)	44(2)	32(1)	-2(1)
O(2)	67(1)	76(2)	165(3)	-6(2)	32(2)	25(1)
O(3)	64(1)	121(2)	75(2)	19(1)	-26(1)	5(1)

O(4)	92(2)	95(2)	121(2)	-26(2)	-33(2)	-27(1)
O(5)	65(1)	119(2)	76(2)	28(1)	-28(1)	-1(1)
O(6)	84(2)	82(2)	103(2)	-20(1)	-30(1)	-20(1)
O(7)	79(2)	106(2)	143(3)	0(2)	47(2)	38(1)
O(8)	63(1)	121(2)	109(2)	23(2)	32(1)	-11(1)
C(1)	36(1)	48(1)	37(1)	1(1)	4(1)	0(1)
C(2)	43(1)	42(1)	28(1)	2(1)	1(1)	-1(1)
C(3)	38(1)	47(1)	37(1)	1(1)	-3(1)	-3(1)
C(4)	38(1)	46(1)	35(1)	4(1)	6(1)	0(1)
C(5)	45(1)	44(1)	30(1)	0(1)	4(1)	-3(1)
C(6)	38(1)	49(1)	34(1)	0(1)	-4(1)	-4(1)
C(7)	90(2)	57(2)	38(1)	3(1)	11(1)	-4(1)
C(8)	97(2)	68(2)	44(2)	-19(1)	1(2)	5(2)
C(9)	47(1)	48(1)	29(1)	0(1)	3(1)	5(1)
C(10)	42(1)	47(1)	32(1)	1(1)	-4(1)	1(1)
C(11)	37(1)	49(1)	36(1)	1(1)	4(1)	4(1)
C(12)	43(1)	41(1)	29(1)	0(1)	0(1)	3(1)
C(13)	39(1)	49(1)	35(1)	2(1)	-3(1)	0(1)
C(14)	35(1)	53(1)	39(1)	4(1)	3(1)	6(1)
C(15)	88(2)	54(2)	35(1)	4(1)	-2(1)	-3(1)
C(16)	87(2)	64(2)	43(2)	-17(1)	0(1)	0(1)

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

	x	y	z	U(eq)
H(7)	76524344	-190474		
H(8)	74242262	-261384		
H(15)	6716694	220471		
H(16)	67842781	290278		

Table S6. Torsion angles [°] for **4**.

C(7)-N(1)-N(2)-C(8)	0.3(3)
C(2)-N(1)-N(2)-C(8)	174.7(2)
C(15)-N(6)-N(7)-C(16)	0.6(3)
C(12)-N(6)-N(7)-C(16)	-175.2(2)
C(15)-N(6)-N(7)-O(1)	-109.48(19)
C(12)-N(6)-N(7)-O(1)	74.8(2)
O(2)-N(4)-O(1)-N(7)	-157.5(3)

C(4)-N(4)-O(1)-N(7)	24.8(2)
C(6)-C(1)-C(2)-C(3)	-0.7(3)
Cl(1)-C(1)-C(2)-C(3)	179.73(17)
C(6)-C(1)-C(2)-N(1)	177.2(2)
Cl(1)-C(1)-C(2)-N(1)	-2.3(3)
C(7)-N(1)-C(2)-C(1)	-87.8(3)
N(2)-N(1)-C(2)-C(1)	99.1(3)
C(7)-N(1)-C(2)-C(3)	90.1(3)
N(2)-N(1)-C(2)-C(3)	-83.0(3)
C(1)-C(2)-C(3)-C(4)	0.2(3)
N(1)-C(2)-C(3)-C(4)	-177.7(2)
C(1)-C(2)-C(3)-Cl(2)	177.97(17)
N(1)-C(2)-C(3)-Cl(2)	0.0(3)
C(2)-C(3)-C(4)-C(5)	0.6(3)
Cl(2)-C(3)-C(4)-C(5)	-177.12(17)
C(2)-C(3)-C(4)-N(4)	-179.1(2)
Cl(2)-C(3)-C(4)-N(4)	3.1(3)
O(1)-N(4)-C(4)-C(3)	86.1(3)
O(2)-N(4)-C(4)-C(3)	-91.9(3)
O(1)-N(4)-C(4)-C(5)	-93.7(3)
O(2)-N(4)-C(4)-C(5)	88.4(3)
C(3)-C(4)-C(5)-C(6)	-1.0(3)
N(4)-C(4)-C(5)-C(6)	178.8(2)
C(3)-C(4)-C(5)-Cl(3)	-179.28(18)
N(4)-C(4)-C(5)-Cl(3)	0.5(3)
C(4)-C(5)-C(6)-C(1)	0.5(3)
Cl(3)-C(5)-C(6)-C(1)	178.78(18)
C(4)-C(5)-C(6)-N(5)	-178.4(2)
Cl(3)-C(5)-C(6)-N(5)	-0.1(3)
C(2)-C(1)-C(6)-C(5)	0.3(3)
Cl(1)-C(1)-C(6)-C(5)	179.89(18)
C(2)-C(1)-C(6)-N(5)	179.2(2)
Cl(1)-C(1)-C(6)-N(5)	-1.3(3)
O(4)-N(5)-C(6)-C(5)	-77.7(3)
O(3)-N(5)-C(6)-C(5)	101.7(3)
O(4)-N(5)-C(6)-C(1)	103.4(3)
O(3)-N(5)-C(6)-C(1)	-77.2(3)
C(8)-N(3)-C(7)-N(1)	-0.3(3)

N(2)-N(1)-C(7)-N(3)	0.0(3)
C(2)-N(1)-C(7)-N(3)	-173.8(2)
N(2)-N(1)-C(7)-C(8)	-0.2(2)
C(2)-N(1)-C(7)-C(8)	-174.0(2)
N(1)-N(2)-C(8)-N(3)	-0.5(4)
N(1)-N(2)-C(8)-C(7)	-0.20(19)
C(7)-N(3)-C(8)-N(2)	0.5(4)
C(14)-C(9)-C(10)-C(11)	-0.5(3)
Cl(4)-C(9)-C(10)-C(11)	-178.71(18)
C(14)-C(9)-C(10)-N(9)	178.1(2)
Cl(4)-C(9)-C(10)-N(9)	-0.1(3)
O(5)-N(9)-C(10)-C(9)	-94.1(3)
O(6)-N(9)-C(10)-C(9)	86.6(3)
O(5)-N(9)-C(10)-C(11)	84.6(3)
O(6)-N(9)-C(10)-C(11)	-94.8(3)
C(9)-C(10)-C(11)-C(12)	-1.6(3)
N(9)-C(10)-C(11)-C(12)	179.7(2)
C(9)-C(10)-C(11)-Cl(5)	-179.60(18)
N(9)-C(10)-C(11)-Cl(5)	1.8(3)
C(10)-C(11)-C(12)-C(13)	2.8(3)
Cl(5)-C(11)-C(12)-C(13)	-179.26(17)
C(10)-C(11)-C(12)-N(6)	-176.3(2)
Cl(5)-C(11)-C(12)-N(6)	1.6(3)
C(15)-N(6)-C(12)-C(13)	-88.8(3)
N(7)-N(6)-C(12)-C(13)	86.0(3)
C(15)-N(6)-C(12)-C(11)	90.3(3)
N(7)-N(6)-C(12)-C(11)	-94.9(3)
C(11)-C(12)-C(13)-C(14)	-1.7(3)
N(6)-C(12)-C(13)-C(14)	177.3(2)
C(11)-C(12)-C(13)-Cl(6)	-179.33(17)
N(6)-C(12)-C(13)-Cl(6)	-0.2(3)
C(10)-C(9)-C(14)-C(13)	1.6(3)
Cl(4)-C(9)-C(14)-C(13)	179.74(18)
C(10)-C(9)-C(14)-N(10)	-176.6(2)
Cl(4)-C(9)-C(14)-N(10)	1.5(3)
C(12)-C(13)-C(14)-C(9)	-0.4(3)
Cl(6)-C(13)-C(14)-C(9)	177.11(18)
C(12)-C(13)-C(14)-N(10)	177.8(2)

Cl(6)-C(13)-C(14)-N(10)	-4.7(3)
O(7)-N(10)-C(14)-C(9)	-73.5(3)
O(8)-N(10)-C(14)-C(9)	105.7(3)
O(7)-N(10)-C(14)-C(13)	108.2(3)
O(8)-N(10)-C(14)-C(13)	-72.5(3)
C(16)-N(8)-C(15)-N(6)	0.7(3)
N(7)-N(6)-C(15)-N(8)	-0.9(3)
C(12)-N(6)-C(15)-N(8)	174.5(2)
N(7)-N(6)-C(15)-C(16)	-0.40(19)
C(12)-N(6)-C(15)-C(16)	174.9(2)
N(6)-N(7)-C(16)-N(8)	-0.2(3)
O(1)-N(7)-C(16)-N(8)	118.3(2)
N(6)-N(7)-C(16)-C(15)	-0.38(18)
O(1)-N(7)-C(16)-C(15)	118.10(13)
C(15)-N(8)-C(16)-N(7)	-0.3(4)

Symmetry transformations used to generate equivalent atoms:

Table S7. Hydrogen bonds for **4** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(7)-H(7)...O(2)#1	0.93	2.66	3.323(4)	129.1
C(8)-H(8)...O(1)#2	0.93	2.55	3.396(4)	151.6
C(15)-H(15)...O(6)#3	0.93	2.53	3.237(3)	132.6
C(16)-H(16)...O(8)#4	0.93	2.52	3.348(4)	147.7

Symmetry transformations used to generate equivalent atoms:

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

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

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	8688(1)	9094(2)	2716(1)	65(1)
Cl(2)	11001(1)	6901(2)	1115(1)	62(1)
Cl(3)	6554(1)	547(2)	7501(1)	67(1)
Cl(4)	4189(1)	3308(2)	6054(1)	58(1)
N(1)	10231(3)	7638(6)	2532(3)	54(1)
N(2)	9990(3)	7643(5)	-258(2)	45(1)
N(3)	8521(2)	9081(4)	-211(2)	42(1)
N(4)	8913(3)	9584(5)	-807(3)	54(1)

N(5)	7589(3)	9256(9)	-1126(4)	101(3)
N(6)	7897(2)	9796(4)	1214(3)	40(1)
N(7)	7201(3)	9116(5)	1310(4)	63(2)
N(8)	6953(3)	11239(5)	1227(4)	78(2)
N(9)	5050(3)	2180(6)	7417(3)	54(1)
N(10)	4981(3)	2572(5)	4623(3)	50(1)
N(11)	6412(3)	1060(4)	4594(3)	44(1)
N(12)	6356(4)	-109(6)	4272(4)	82(2)
N(13)	7157(4)	1156(8)	3609(3)	85(2)
N(14)	7201(2)	201(4)	5944(3)	43(1)
N(15)	7858(3)	854(5)	5703(4)	64(2)
N(16)	8194(3)	-1189(5)	6032(5)	89(2)
O(1)	10768(3)	8341(7)	2775(3)	101(2)
O(2)	10038(4)	6608(5)	2786(3)	86(2)
O(3)	9619(3)	6760(5)	-568(3)	72(1)
O(4)	10603(3)	8148(5)	-470(2)	67(1)
O(5)	5293(4)	3156(6)	7711(3)	97(2)
O(6)	4551(4)	1484(7)	7622(3)	113(2)
O(7)	4459(3)	1955(6)	4321(3)	92(2)
O(8)	5242(4)	3588(5)	4398(3)	104(2)
C(1)	9072(3)	8739(5)	1848(3)	36(1)
C(2)	9786(3)	8063(5)	1815(3)	38(1)
C(3)	10106(3)	7738(5)	1128(3)	36(1)
C(4)	9679(3)	8095(5)	472(3)	32(1)
C(5)	8954(3)	8776(4)	480(3)	32(1)
C(6)	8651(3)	9123(4)	1185(3)	34(1)
C(7)	7740(4)	11049(5)	1179(4)	61(2)
C(8)	6658(4)	10034(6)	1304(4)	67(2)
C(9)	7739(4)	8880(9)	-412(4)	82(3)
C(10)	8322(4)	9653(8)	-1333(4)	72(2)
C(11)	6098(3)	1102(5)	6661(3)	37(1)
C(12)	5410(3)	1854(5)	6675(3)	38(1)
C(13)	5039(3)	2348(5)	6016(3)	38(1)
C(14)	5375(3)	2056(5)	5333(3)	36(1)
C(15)	6073(3)	1323(4)	5304(3)	34(1)
C(16)	6448(3)	850(4)	5971(3)	35(1)
C(17)	7415(4)	-1013(6)	6128(4)	66(2)
C(18)	8422(4)	-10(6)	5775(5)	81(2)

C(19)	6877(4)	1825(7)	4170(4)	75(2)
C(20)	6808(5)	15(8)	3688(4)	82(2)

Table S9. Bond lengths [Å] and angles [°] for **5**.

Cl(1)-C(1)	1.717(5)
Cl(2)-C(3)	1.704(5)
Cl(3)-C(11)	1.717(5)
Cl(4)-C(13)	1.713(5)
N(1)-O(2)	1.196(7)
N(1)-O(1)	1.201(7)
N(1)-C(2)	1.489(7)
N(2)-O(3)	1.207(6)
N(2)-O(4)	1.208(6)
N(2)-C(4)	1.478(6)
N(3)-C(9)	1.331(7)
N(3)-N(4)	1.359(6)
N(3)-C(5)	1.410(6)
N(4)-C(10)	1.306(8)
N(5)-C(9)	1.322(8)
N(5)-C(10)	1.339(8)
N(6)-C(7)	1.313(7)
N(6)-N(7)	1.356(6)
N(6)-C(6)	1.421(6)
N(7)-C(8)	1.297(7)
N(8)-C(7)	1.315(7)
N(8)-C(8)	1.338(8)
N(9)-O(6)	1.158(7)
N(9)-O(5)	1.187(7)
N(9)-C(12)	1.495(7)
N(10)-O(7)	1.172(6)
N(10)-O(8)	1.203(7)
N(10)-C(14)	1.474(7)
N(11)-N(12)	1.328(7)
N(11)-C(19)	1.346(8)
N(11)-C(15)	1.417(6)
N(12)-C(20)	1.302(8)
N(13)-C(19)	1.303(9)
N(13)-C(20)	1.316(10)

N(14)-C(17)	1.331(7)
N(14)-N(15)	1.356(6)
N(14)-C(16)	1.408(6)
N(15)-C(18)	1.284(8)
N(16)-C(17)	1.310(8)
N(16)-C(18)	1.352(9)
C(1)-C(2)	1.366(7)
C(1)-C(6)	1.382(7)
C(2)-C(3)	1.381(7)
C(3)-C(4)	1.367(7)
C(4)-C(5)	1.382(6)
C(5)-C(6)	1.402(7)
C(7)-H(7)	0.9300
C(8)-H(8)	0.9300
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
C(11)-C(12)	1.371(7)
C(11)-C(16)	1.390(7)
C(12)-C(13)	1.377(7)
C(13)-C(14)	1.377(7)
C(14)-C(15)	1.375(7)
C(15)-C(16)	1.384(7)
C(17)-H(17)	0.9300
C(18)-H(18)	0.9300
C(19)-C(20)	2.043(10)
C(19)-H(19)	0.9300
C(20)-H(20)	0.9300

O(2)-N(1)-O(1)	127.1(6)
O(2)-N(1)-C(2)	116.4(5)
O(1)-N(1)-C(2)	116.4(5)
O(3)-N(2)-O(4)	126.4(5)
O(3)-N(2)-C(4)	116.0(4)
O(4)-N(2)-C(4)	117.5(5)
C(9)-N(3)-N(4)	110.0(5)
C(9)-N(3)-C(5)	129.2(5)
N(4)-N(3)-C(5)	120.7(4)
C(10)-N(4)-N(3)	101.6(4)

C(9)-N(5)-C(10)	102.6(5)
C(7)-N(6)-N(7)	110.2(4)
C(7)-N(6)-C(6)	130.0(4)
N(7)-N(6)-C(6)	119.7(4)
C(8)-N(7)-N(6)	102.0(5)
C(7)-N(8)-C(8)	103.4(5)
O(6)-N(9)-O(5)	127.9(6)
O(6)-N(9)-C(12)	116.7(5)
O(5)-N(9)-C(12)	115.4(5)
O(7)-N(10)-O(8)	125.8(6)
O(7)-N(10)-C(14)	118.0(5)
O(8)-N(10)-C(14)	116.2(5)
N(12)-N(11)-C(19)	108.7(5)
N(12)-N(11)-C(15)	121.7(4)
C(19)-N(11)-C(15)	129.4(5)
C(20)-N(12)-N(11)	102.5(6)
C(19)-N(13)-C(20)	102.6(6)
C(17)-N(14)-N(15)	109.5(5)
C(17)-N(14)-C(16)	131.0(5)
N(15)-N(14)-C(16)	119.5(4)
C(18)-N(15)-N(14)	102.0(5)
C(17)-N(16)-C(18)	102.0(5)
C(2)-C(1)-C(6)	120.2(4)
C(2)-C(1)-Cl(1)	120.0(4)
C(6)-C(1)-Cl(1)	119.8(4)
C(1)-C(2)-C(3)	121.6(4)
C(1)-C(2)-N(1)	119.9(4)
C(3)-C(2)-N(1)	118.4(4)
C(4)-C(3)-C(2)	118.0(4)
C(4)-C(3)-Cl(2)	122.0(4)
C(2)-C(3)-Cl(2)	120.0(4)
C(3)-C(4)-C(5)	122.1(4)
C(3)-C(4)-N(2)	117.5(4)
C(5)-C(4)-N(2)	120.2(4)
C(4)-C(5)-C(6)	118.8(4)
C(4)-C(5)-N(3)	120.0(4)
C(6)-C(5)-N(3)	121.1(4)
C(1)-C(6)-C(5)	119.1(4)

C(1)-C(6)-N(6)	120.5(4)
C(5)-C(6)-N(6)	120.3(4)
N(6)-C(7)-N(8)	109.5(5)
N(6)-C(7)-H(7)	125.3
N(8)-C(7)-H(7)	125.3
N(7)-C(8)-N(8)	114.9(5)
N(7)-C(8)-H(8)	122.6
N(8)-C(8)-H(8)	122.6
N(5)-C(9)-N(3)	109.7(6)
N(5)-C(9)-H(9)	125.1
N(3)-C(9)-H(9)	125.1
N(4)-C(10)-N(5)	116.0(6)
N(4)-C(10)-H(10)	122.0
N(5)-C(10)-H(10)	122.0
C(12)-C(11)-C(16)	119.8(4)
C(12)-C(11)-Cl(3)	119.8(4)
C(16)-C(11)-Cl(3)	120.4(4)
C(11)-C(12)-C(13)	121.6(5)
C(11)-C(12)-N(9)	120.3(5)
C(13)-C(12)-N(9)	118.1(5)
C(12)-C(13)-C(14)	118.1(4)
C(12)-C(13)-Cl(4)	120.4(4)
C(14)-C(13)-Cl(4)	121.5(4)
C(15)-C(14)-C(13)	121.6(4)
C(15)-C(14)-N(10)	119.8(4)
C(13)-C(14)-N(10)	118.7(4)
C(14)-C(15)-C(16)	119.8(4)
C(14)-C(15)-N(11)	120.2(4)
C(16)-C(15)-N(11)	120.0(4)
C(15)-C(16)-C(11)	119.1(4)
C(15)-C(16)-N(14)	119.4(4)
C(11)-C(16)-N(14)	121.3(4)
N(16)-C(17)-N(14)	110.2(6)
N(16)-C(17)-H(17)	124.9
N(14)-C(17)-H(17)	124.9
N(15)-C(18)-N(16)	116.2(6)
N(15)-C(18)-H(18)	121.9
N(16)-C(18)-H(18)	121.9

N(13)-C(19)-N(11)	110.0(6)
N(13)-C(19)-C(20)	38.9(4)
N(11)-C(19)-C(20)	71.2(4)
N(13)-C(19)-H(19)	125.0
N(11)-C(19)-H(19)	125.0
C(20)-C(19)-H(19)	163.7
N(12)-C(20)-N(13)	116.0(6)
N(12)-C(20)-C(19)	77.6(4)
N(13)-C(20)-C(19)	38.5(4)
N(12)-C(20)-H(20)	122.0
N(13)-C(20)-H(20)	122.0
C(19)-C(20)-H(20)	160.4

Symmetry transformations used to generate equivalent atoms:

Table S10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **5**. 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}	U^{12}
Cl(1)	73(1)	78(1)	46(1)	-15(1)	23(1)	5(1)
Cl(2)	46(1)	78(1)	61(1)	21(1)	12(1)	32(1)
Cl(3)	65(1)	85(1)	50(1)	23(1)	-12(1)	2(1)
Cl(4)	43(1)	62(1)	70(1)	-10(1)	3(1)	17(1)
N(1)	53(3)	71(4)	38(3)	9(3)	-1(2)	6(3)
N(2)	43(2)	52(3)	39(2)	-3(2)	6(2)	6(2)
N(3)	32(2)	48(3)	44(3)	17(2)	-1(2)	-5(2)
N(4)	44(3)	72(3)	46(3)	22(2)	0(2)	-10(2)
N(5)	50(3)	179(8)	70(4)	58(5)	-21(3)	-29(4)
N(6)	31(2)	29(2)	63(3)	4(2)	12(2)	-1(2)
N(7)	35(2)	39(3)	117(5)	11(3)	23(3)	0(2)
N(8)	48(3)	44(3)	145(6)	23(3)	34(3)	17(2)
N(9)	46(3)	76(4)	40(3)	-8(3)	7(2)	-12(3)
N(10)	45(3)	61(3)	42(3)	8(2)	0(2)	1(2)
N(11)	38(2)	50(3)	47(3)	-8(2)	11(2)	-4(2)
N(12)	91(4)	80(4)	80(4)	-38(3)	43(3)	-39(3)
N(13)	69(4)	128(6)	62(4)	-25(4)	30(3)	-25(4)
N(14)	35(2)	27(2)	65(3)	1(2)	2(2)	2(2)
N(15)	37(3)	37(3)	118(5)	6(3)	8(3)	1(2)
N(16)	54(3)	37(3)	175(7)	15(4)	13(4)	17(3)
O(1)	84(4)	161(6)	55(3)	20(3)	-28(3)	-35(4)

O(2)	119(4)	81(4)	58(3)	31(3)	1(3)	11(3)
O(3)	89(3)	72(3)	56(3)	-24(2)	15(2)	-9(3)
O(4)	52(2)	98(4)	54(3)	2(2)	23(2)	-2(2)
O(5)	104(4)	121(5)	67(3)	-44(3)	25(3)	-24(4)
O(6)	120(5)	163(6)	60(3)	-11(3)	43(3)	-62(5)
O(7)	72(3)	139(5)	63(3)	27(3)	-24(3)	-41(3)
O(8)	140(5)	76(4)	91(4)	41(3)	-37(4)	-24(4)
C(1)	41(3)	34(3)	35(3)	-3(2)	9(2)	-7(2)
C(2)	38(3)	38(3)	37(3)	6(2)	-1(2)	-1(2)
C(3)	26(2)	42(3)	40(3)	6(2)	4(2)	6(2)
C(4)	31(2)	35(3)	30(2)	3(2)	9(2)	0(2)
C(5)	28(2)	27(2)	39(3)	7(2)	-1(2)	-6(2)
C(6)	33(2)	22(2)	48(3)	1(2)	11(2)	-3(2)
C(7)	48(3)	32(3)	106(5)	11(3)	29(3)	4(2)
C(8)	38(3)	49(4)	116(6)	17(4)	30(3)	9(3)
C(9)	41(3)	142(7)	62(4)	41(5)	-12(3)	-21(4)
C(10)	56(4)	109(6)	49(4)	32(4)	-8(3)	-14(4)
C(11)	37(3)	37(3)	36(3)	7(2)	-4(2)	-6(2)
C(12)	35(3)	44(3)	35(3)	-2(2)	8(2)	-9(2)
C(13)	34(3)	33(3)	46(3)	-3(2)	3(2)	-2(2)
C(14)	34(2)	36(3)	39(3)	3(2)	-2(2)	-2(2)
C(15)	30(2)	31(2)	41(3)	-5(2)	6(2)	-3(2)
C(16)	33(2)	24(2)	49(3)	0(2)	-1(2)	0(2)
C(17)	51(4)	30(3)	117(6)	11(3)	2(4)	5(3)
C(18)	45(4)	42(4)	157(8)	4(4)	17(4)	6(3)
C(19)	78(4)	78(4)	72(4)	-8(4)	25(4)	-26(4)
C(20)	84(5)	101(5)	65(4)	-33(4)	34(4)	-24(4)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **5**.

	x	y	z	U(eq)
H(7)	812711701	112773		
H(8)	61069867	134980		
H(9)	73568529	-9899		
H(10)	84069958	-182186		
H(17)	7063-1645	629979		
H(18)	8956165	565797		
H(19)	69822701	426390		

H(20)	6879-663	334699

Table S12. Torsion angles [°] for **5**.

C(9)-N(3)-N(4)-C(10)	0.1(8)
C(5)-N(3)-N(4)-C(10)	176.6(6)
C(7)-N(6)-N(7)-C(8)	1.7(7)
C(6)-N(6)-N(7)-C(8)	-179.6(5)
C(19)-N(11)-N(12)-C(20)	1.7(8)
C(15)-N(11)-N(12)-C(20)	-173.5(6)
C(17)-N(14)-N(15)-C(18)	-1.2(8)
C(16)-N(14)-N(15)-C(18)	178.1(6)
C(6)-C(1)-C(2)-C(3)	-0.3(7)
Cl(1)-C(1)-C(2)-C(3)	178.8(4)
C(6)-C(1)-C(2)-N(1)	-179.2(5)
Cl(1)-C(1)-C(2)-N(1)	-0.1(7)
O(2)-N(1)-C(2)-C(1)	87.6(7)
O(1)-N(1)-C(2)-C(1)	-95.4(7)
O(2)-N(1)-C(2)-C(3)	-91.4(6)
O(1)-N(1)-C(2)-C(3)	85.6(7)
C(1)-C(2)-C(3)-C(4)	-1.1(8)
N(1)-C(2)-C(3)-C(4)	177.9(5)
C(1)-C(2)-C(3)-Cl(2)	179.7(4)
N(1)-C(2)-C(3)-Cl(2)	-1.4(7)
C(2)-C(3)-C(4)-C(5)	0.9(7)
Cl(2)-C(3)-C(4)-C(5)	-179.9(4)
C(2)-C(3)-C(4)-N(2)	-174.8(4)
Cl(2)-C(3)-C(4)-N(2)	4.4(7)
O(3)-N(2)-C(4)-C(3)	104.7(6)
O(4)-N(2)-C(4)-C(3)	-72.4(6)
O(3)-N(2)-C(4)-C(5)	-71.1(6)
O(4)-N(2)-C(4)-C(5)	111.8(5)
C(3)-C(4)-C(5)-C(6)	0.6(7)
N(2)-C(4)-C(5)-C(6)	176.2(4)
C(3)-C(4)-C(5)-N(3)	-177.7(4)
N(2)-C(4)-C(5)-N(3)	-2.1(7)
C(9)-N(3)-C(5)-C(4)	129.1(7)
N(4)-N(3)-C(5)-C(4)	-46.6(7)
C(9)-N(3)-C(5)-C(6)	-49.1(9)
N(4)-N(3)-C(5)-C(6)	135.2(5)

C(2)-C(1)-C(6)-C(5)	1.8(7)
Cl(1)-C(1)-C(6)-C(5)	-177.3(3)
C(2)-C(1)-C(6)-N(6)	178.3(4)
Cl(1)-C(1)-C(6)-N(6)	-0.8(6)
C(4)-C(5)-C(6)-C(1)	-2.0(7)
N(3)-C(5)-C(6)-C(1)	176.3(4)
C(4)-C(5)-C(6)-N(6)	-178.4(4)
N(3)-C(5)-C(6)-N(6)	-0.2(7)
C(7)-N(6)-C(6)-C(1)	97.1(7)
N(7)-N(6)-C(6)-C(1)	-81.3(6)
C(7)-N(6)-C(6)-C(5)	-86.4(8)
N(7)-N(6)-C(6)-C(5)	95.2(6)
N(7)-N(6)-C(7)-N(8)	-1.7(8)
C(6)-N(6)-C(7)-N(8)	179.8(6)
C(8)-N(8)-C(7)-N(6)	0.8(9)
N(6)-N(7)-C(8)-N(8)	-1.3(9)
C(7)-N(8)-C(8)-N(7)	0.3(10)
C(10)-N(5)-C(9)-N(3)	1.4(11)
N(4)-N(3)-C(9)-N(5)	-1.0(10)
C(5)-N(3)-C(9)-N(5)	-177.1(7)
N(3)-N(4)-C(10)-N(5)	0.8(9)
C(9)-N(5)-C(10)-N(4)	-1.4(11)
C(16)-C(11)-C(12)-C(13)	1.5(7)
Cl(3)-C(11)-C(12)-C(13)	178.2(4)
C(16)-C(11)-C(12)-N(9)	-177.3(4)
Cl(3)-C(11)-C(12)-N(9)	-0.7(7)
O(6)-N(9)-C(12)-C(11)	-92.1(7)
O(5)-N(9)-C(12)-C(11)	90.5(7)
O(6)-N(9)-C(12)-C(13)	89.0(8)
O(5)-N(9)-C(12)-C(13)	-88.4(7)
C(11)-C(12)-C(13)-C(14)	0.6(7)
N(9)-C(12)-C(13)-C(14)	179.5(4)
C(11)-C(12)-C(13)-Cl(4)	-178.9(4)
N(9)-C(12)-C(13)-Cl(4)	0.0(6)
C(12)-C(13)-C(14)-C(15)	-1.8(7)
Cl(4)-C(13)-C(14)-C(15)	177.7(4)
C(12)-C(13)-C(14)-N(10)	179.6(4)
Cl(4)-C(13)-C(14)-N(10)	-0.9(7)

O(7)-N(10)-C(14)-C(15)	93.5(7)
O(8)-N(10)-C(14)-C(15)	-85.0(7)
O(7)-N(10)-C(14)-C(13)	-87.8(7)
O(8)-N(10)-C(14)-C(13)	93.7(7)
C(13)-C(14)-C(15)-C(16)	0.8(7)
N(10)-C(14)-C(15)-C(16)	179.4(4)
C(13)-C(14)-C(15)-N(11)	-178.8(4)
N(10)-C(14)-C(15)-N(11)	-0.2(7)
N(12)-N(11)-C(15)-C(14)	-106.3(7)
C(19)-N(11)-C(15)-C(14)	79.6(8)
N(12)-N(11)-C(15)-C(16)	74.1(7)
C(19)-N(11)-C(15)-C(16)	-100.0(7)
C(14)-C(15)-C(16)-C(11)	1.4(7)
N(11)-C(15)-C(16)-C(11)	-179.0(4)
C(14)-C(15)-C(16)-N(14)	-174.3(4)
N(11)-C(15)-C(16)-N(14)	5.3(7)
C(12)-C(11)-C(16)-C(15)	-2.5(7)
Cl(3)-C(11)-C(16)-C(15)	-179.1(4)
C(12)-C(11)-C(16)-N(14)	173.1(4)
Cl(3)-C(11)-C(16)-N(14)	-3.6(6)
C(17)-N(14)-C(16)-C(15)	-118.5(7)
N(15)-N(14)-C(16)-C(15)	62.4(7)
C(17)-N(14)-C(16)-C(11)	65.9(8)
N(15)-N(14)-C(16)-C(11)	-113.2(6)
C(18)-N(16)-C(17)-N(14)	-0.5(9)
N(15)-N(14)-C(17)-N(16)	1.1(8)
C(16)-N(14)-C(17)-N(16)	-178.1(6)
N(14)-N(15)-C(18)-N(16)	0.9(10)
C(17)-N(16)-C(18)-N(15)	-0.3(11)
C(20)-N(13)-C(19)-N(11)	3.7(9)
N(12)-N(11)-C(19)-N(13)	-3.6(9)
C(15)-N(11)-C(19)-N(13)	171.1(6)
N(12)-N(11)-C(19)-C(20)	-1.1(6)
C(15)-N(11)-C(19)-C(20)	173.6(6)
N(11)-N(12)-C(20)-N(13)	0.7(10)
N(11)-N(12)-C(20)-C(19)	-1.1(5)
C(19)-N(13)-C(20)-N(12)	-2.8(11)

Symmetry transformations used to generate equivalent atoms:

Table S13. Hydrogen bonds for **5** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)<(DHA) C(17)-	
H(17)...N(7)#1	0.93	2.55	3.225(7)	129.9
C(9)-H(9)...N(7)	0.93	2.57	3.202(10)	125.6
C(8)-H(8)...O(6)#2	0.93	2.56	3.211(8)	127.4
C(7)-H(7)...O(4)#3	0.93	2.44	3.158(7)	134.1
C(7)-H(7)...N(15)#4	0.93	2.65	3.296(7)127.2 C(17)-	
H(17)...N(7)#1	0.93	2.55	3.225(7)	129.9
C(9)-H(9)...N(7)	0.93	2.57	3.202(10)	125.6
C(8)-H(8)...O(6)#2	0.93	2.56	3.211(8)	127.4
C(7)-H(7)...O(4)#3	0.93	2.44	3.158(7)	134.1
C(7)-H(7)...N(15)#4	0.93	2.65	3.296(7)	127.2
C(7)-H(7)...N(15)#4	0.93	2.65	3.296(7)	127.2
C(7)-H(7)...O(4)#3	0.93	2.44	3.158(7)	134.1
C(8)-H(8)...O(6)#2	0.93	2.56	3.211(8)	127.4
C(9)-H(9)...N(7)	0.93	2.57	3.202(10)	125.6
C(17)-H(17)...N(7)#1	0.93	2.55	3.225(7)	129.9
C(7)-H(7)...N(15)#4	0.93	2.65	3.296(7)	127.2
C(7)-H(7)...O(4)#3	0.93	2.44	3.158(7)	134.1
C(8)-H(8)...O(6)#2	0.93	2.56	3.211(8)	127.4
C(9)-H(9)...N(7)	0.93	2.57	3.202(10)	125.6
C(17)-H(17)...N(7)#1	0.93	2.55	3.225(7)	129.9

Symmetry transformations used to generate equivalent atoms:

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

Table S14. 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	U(eq)
N(1)	-3441(3)	6019(2)	4186(1)	48(1)
N(2)	-1015(3)	4617(2)	3979(1)	46(1)
N(3)	-953(2)	5810(2)	3452(1)	30(1)
N(4)	-1034(3)	4585(2)	1973(1)	50(1)
N(5)	1859(3)	4794(2)	772(1)	44(1)
N(6)	4618(3)	6733(3)	1094(1)	64(1)
N(7)	4533(2)	8320(2)	2542(1)	36(1)
N(8)	1763(3)	7640(2)	3746(1)	44(1)

N(9)	-1904(2)	-330(2)	456(1)	40(1)
N(10)	-39(3)	-1298(2)	1389(1)	41(1)
N(11)	-212(2)	162(2)	1470(1)	30(1)
N(12)	-1793(2)	426(2)	2993(1)	43(1)
N(13)	14(3)	1612(2)	4320(1)	37(1)
N(14)	3329(3)	2950(3)	3906(1)	60(1)
N(15)	4871(2)	2926(2)	2296(1)	41(1)
N(16)	3177(2)	1159(2)	1160(1)	43(1)
O(1)	648(2)	3933(2)	650(1)	56(1)
O(2)	3055(3)	4978(3)	222(1)	79(1)
O(3)	5816(2)	8554(2)	2031(1)	57(1)
O(4)	4472(2)	9038(2)	3172(1)	48(1)
O(5)	-1556(2)	1239(2)	4463(1)	55(1)
O(6)	903(2)	2007(2)	4905(1)	51(1)
O(7)	5554(2)	3753(2)	2782(1)	72(1)
O(8)	5650(2)	2786(2)	1614(1)	64(1)
C(1)	-2535(3)	4814(3)	4394(2)	46(1)
C(2)	-2400(3)	6611(3)	3595(1)	42(1)
C(3)	486(3)	6049(2)	2851(1)	31(1)
C(4)	397(3)	5369(2)	2102(1)	32(1)
C(5)	1861(3)	5554(2)	1505(1)	34(1)
C(6)	3289(3)	6527(2)	1647(1)	37(1)
C(7)	3241(3)	7282(2)	2407(1)	31(1)
C(8)	1832(3)	7009(2)	3026(1)	31(1)
C(9)	-1077(3)	-1517(3)	779(1)	42(1)
C(10)	-1325(3)	691(2)	910(1)	35(1)
C(11)	703(3)	882(2)	2094(1)	29(1)
C(12)	-158(3)	965(2)	2872(1)	30(1)
C(13)	796(3)	1607(2)	3513(1)	31(1)
C(14)	2493(3)	2287(2)	3332(1)	33(1)
C(15)	3265(3)	2219(2)	2508(1)	31(1)
C(16)	2411(3)	1404(2)	1894(1)	30(1)

Table S15. Bond lengths [Å] and angles [°] for **6**.

N(1)-C(2)	1.308(3)
N(1)-C(1)	1.340(3)
N(2)-C(1)	1.313(3)
N(2)-N(3)	1.361(3)

N(3)-C(2)	1.329(3)
N(3)-C(3)	1.431(2)
N(4)-C(4)	1.323(3)
N(4)-H(4A)	0.8600
N(4)-H(4B)	0.8600
N(5)-O(1)	1.236(2)
N(5)-O(2)	1.242(2)
N(5)-C(5)	1.404(3)
N(6)-C(6)	1.318(3)
N(6)-H(6A)	0.8600
N(6)-H(6B)	0.8600
N(7)-O(4)	1.240(2)
N(7)-O(3)	1.253(2)
N(7)-C(7)	1.394(3)
N(8)-C(8)	1.325(3)
N(8)-H(8A)	0.8600
N(8)-H(8B)	0.8600
N(9)-C(10)	1.307(3)
N(9)-C(9)	1.352(3)
N(10)-C(9)	1.303(3)
N(10)-N(11)	1.368(2)
N(11)-C(10)	1.329(3)
N(11)-C(11)	1.430(2)
N(12)-C(12)	1.325(3)
N(12)-H(12A)	0.8600
N(12)-H(12B)	0.8600
N(13)-O(5)	1.234(2)
N(13)-O(6)	1.246(2)
N(13)-C(13)	1.408(3)
N(14)-C(14)	1.314(3)
N(14)-H(14A)	0.8600
N(14)-H(14B)	0.8600
N(15)-O(8)	1.238(2)
N(15)-O(7)	1.245(2)
N(15)-C(15)	1.392(3)
N(16)-C(16)	1.325(3)
N(16)-H(16A)	0.8600
N(16)-H(16B)	0.8600

C(1)-H(1A)	0.9300
C(2)-H(2A)	0.9300
C(3)-C(8)	1.390(3)
C(3)-C(4)	1.393(3)
C(4)-C(5)	1.436(3)
C(5)-C(6)	1.431(3)
C(6)-C(7)	1.440(3)
C(7)-C(8)	1.438(3)
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
C(11)-C(16)	1.388(3)
C(11)-C(12)	1.394(3)
C(12)-C(13)	1.433(3)
C(13)-C(14)	1.432(3)
C(14)-C(15)	1.433(3)
C(15)-C(16)	1.443(3)

C(2)-N(1)-C(1)	101.80(19)
C(1)-N(2)-N(3)	101.54(19)
C(2)-N(3)-N(2)	108.93(18)
C(2)-N(3)-C(3)	129.31(19)
N(2)-N(3)-C(3)	121.75(17)
C(4)-N(4)-H(4A)	120.0
C(4)-N(4)-H(4B)	120.0
H(4A)-N(4)-H(4B)	120.0
O(1)-N(5)-O(2)	117.77(18)
O(1)-N(5)-C(5)	120.82(18)
O(2)-N(5)-C(5)	121.40(19)
C(6)-N(6)-H(6A)	120.0
C(6)-N(6)-H(6B)	120.0
H(6A)-N(6)-H(6B)	120.0
O(4)-N(7)-O(3)	117.33(17)
O(4)-N(7)-C(7)	121.66(17)
O(3)-N(7)-C(7)	121.01(17)
C(8)-N(8)-H(8A)	120.0
C(8)-N(8)-H(8B)	120.0
H(8A)-N(8)-H(8B)	120.0
C(10)-N(9)-C(9)	102.19(18)

C(9)-N(10)-N(11)	101.89(19)
C(10)-N(11)-N(10)	109.01(17)
C(10)-N(11)-C(11)	129.89(18)
N(10)-N(11)-C(11)	121.09(17)
C(12)-N(12)-H(12A)	120.0
C(12)-N(12)-H(12B)	120.0
H(12A)-N(12)-H(12B)	120.0
O(5)-N(13)-O(6)	118.72(17)
O(5)-N(13)-C(13)	121.19(17)
O(6)-N(13)-C(13)	120.08(18)
C(14)-N(14)-H(14A)	120.0
C(14)-N(14)-H(14B)	120.0
H(14A)-N(14)-H(14B)	120.0
O(8)-N(15)-O(7)	117.57(18)
O(8)-N(15)-C(15)	121.55(17)
O(7)-N(15)-C(15)	120.85(17)
C(16)-N(16)-H(16A)	120.0
C(16)-N(16)-H(16B)	120.0
H(16A)-N(16)-H(16B)	120.0
N(2)-C(1)-N(1)	116.2(2)
N(2)-C(1)-H(1A)	121.9
N(1)-C(1)-H(1A)	121.9
N(1)-C(2)-N(3)	111.5(2)
N(1)-C(2)-H(2A)	124.2
N(3)-C(2)-H(2A)	124.2
C(8)-C(3)-C(4)	123.80(18)
C(8)-C(3)-N(3)	118.31(17)
C(4)-C(3)-N(3)	117.78(18)
N(4)-C(4)-C(3)	118.53(19)
N(4)-C(4)-C(5)	123.00(18)
C(3)-C(4)-C(5)	118.47(18)
N(5)-C(5)-C(6)	120.29(19)
N(5)-C(5)-C(4)	119.42(18)
C(6)-C(5)-C(4)	120.27(18)
N(6)-C(6)-C(5)	120.9(2)
N(6)-C(6)-C(7)	120.6(2)
C(5)-C(6)-C(7)	118.52(18)
N(7)-C(7)-C(8)	119.06(17)

N(7)-C(7)-C(6)	120.33(18)
C(8)-C(7)-C(6)	120.58(18)
N(8)-C(8)-C(3)	119.20(19)
N(8)-C(8)-C(7)	122.79(18)
C(3)-C(8)-C(7)	118.01(17)
N(10)-C(9)-N(9)	115.7(2)
N(10)-C(9)-H(9)	122.1
N(9)-C(9)-H(9)	122.1
N(9)-C(10)-N(11)	111.2(2)
N(9)-C(10)-H(10)	124.4
N(11)-C(10)-H(10)	124.4
C(16)-C(11)-C(12)	124.35(18)
C(16)-C(11)-N(11)	117.92(17)
C(12)-C(11)-N(11)	117.69(18)
N(12)-C(12)-C(11)	119.15(18)
N(12)-C(12)-C(13)	122.93(19)
C(11)-C(12)-C(13)	117.90(18)
N(13)-C(13)-C(14)	120.09(17)
N(13)-C(13)-C(12)	119.20(18)
C(14)-C(13)-C(12)	120.67(18)
N(14)-C(14)-C(13)	121.04(19)
N(14)-C(14)-C(15)	120.75(19)
C(13)-C(14)-C(15)	118.21(17)
N(15)-C(15)-C(14)	120.02(17)
N(15)-C(15)-C(16)	119.18(17)
C(14)-C(15)-C(16)	120.80(18)
N(16)-C(16)-C(11)	119.80(18)
N(16)-C(16)-C(15)	122.97(18)
C(11)-C(16)-C(15)	117.23(17)

Symmetry transformations used to generate equivalent atoms:

Table S16. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **6**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	36(1)	63(1)	45(1)	-10(1)	8(1)	-9(1)
N(2)	51(1)	44(1)	43(1)	4(1)	10(1)	-4(1)
N(3)	30(1)	32(1)	29(1)	-3(1)	4(1)	-6(1)
N(4)	45(1)	58(1)	50(1)	-26(1)	14(1)	-26(1)

N(5)	42(1)	50(1)	39(1)	-18(1)	7(1)	-8(1)
N(6)	47(1)	96(2)	52(1)	-36(1)	24(1)	-35(1)
N(7)	29(1)	45(1)	36(1)	-4(1)	-2(1)	-10(1)
N(8)	40(1)	61(1)	34(1)	-17(1)	7(1)	-20(1)
N(9)	35(1)	57(1)	31(1)	-13(1)	-1(1)	-13(1)
N(10)	48(1)	35(1)	41(1)	-12(1)	-2(1)	-5(1)
N(11)	32(1)	31(1)	27(1)	-9(1)	-1(1)	-7(1)
N(12)	38(1)	57(1)	34(1)	-14(1)	5(1)	-22(1)
N(13)	42(1)	39(1)	30(1)	-7(1)	6(1)	-11(1)
N(14)	48(1)	98(2)	35(1)	-33(1)	9(1)	-37(1)
N(15)	33(1)	55(1)	35(1)	-17(1)	5(1)	-16(1)
N(16)	33(1)	67(1)	30(1)	-21(1)	4(1)	-13(1)
O(1)	64(1)	56(1)	49(1)	-27(1)	7(1)	-24(1)
O(2)	58(1)	123(2)	59(1)	-54(1)	29(1)	-34(1)
O(3)	42(1)	84(1)	46(1)	-12(1)	10(1)	-36(1)
O(4)	43(1)	53(1)	49(1)	-21(1)	3(1)	-17(1)
O(5)	49(1)	74(1)	42(1)	-18(1)	17(1)	-30(1)
O(6)	53(1)	76(1)	26(1)	-14(1)	1(1)	-16(1)
O(7)	58(1)	106(2)	53(1)	-44(1)	17(1)	-52(1)
O(8)	48(1)	100(2)	45(1)	-35(1)	20(1)	-35(1)
C(1)	49(2)	51(2)	38(1)	-2(1)	10(1)	-13(1)
C(2)	33(1)	46(1)	44(1)	1(1)	0(1)	-1(1)
C(3)	27(1)	36(1)	29(1)	-3(1)	5(1)	-7(1)
C(4)	32(1)	30(1)	33(1)	-5(1)	2(1)	-6(1)
C(5)	31(1)	38(1)	32(1)	-11(1)	3(1)	-5(1)
C(6)	30(1)	46(1)	35(1)	-8(1)	6(1)	-4(1)
C(7)	26(1)	37(1)	29(1)	-5(1)	0(1)	-8(1)
C(8)	29(1)	37(1)	28(1)	-6(1)	-1(1)	-2(1)
C(9)	44(1)	48(2)	36(1)	-18(1)	5(1)	-18(1)
C(10)	33(1)	43(1)	30(1)	-6(1)	-1(1)	-4(1)
C(11)	31(1)	32(1)	24(1)	-9(1)	-3(1)	-5(1)
C(12)	30(1)	27(1)	33(1)	-4(1)	-1(1)	-6(1)
C(13)	36(1)	34(1)	23(1)	-9(1)	4(1)	-7(1)
C(14)	32(1)	40(1)	28(1)	-11(1)	0(1)	-7(1)
C(15)	27(1)	38(1)	29(1)	-11(1)	2(1)	-8(1)
C(16)	32(1)	33(1)	25(1)	-6(1)	-2(1)	-3(1)

Table S17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **6**.

	x	y	z	U(eq)
H(4A)	-18824503	234861		
H(4B)	-11164156	151561		
H(6A)	46346280	64077		
H(6B)	54707321	118677		
H(8A)	8937453	409953		
H(8B)	25898236	386153		
H(12A)	-231032	259451		
H(12B)	-2337471	347051		
H(14A)	28572980	439971		
H(14B)	43483354	378871		
H(16A)	2615678	80951		
H(16B)	42361481	103551		
H(1A)	-29574154	480856		
H(2A)	-26417483	331150		
H(9)	-1239-2432	57851		
H(10)	-16491660	84942		

Table S18. Torsion angles [°] for **6**.

C(1)-N(2)-N(3)-C(2)	0.5(2)
C(1)-N(2)-N(3)-C(3)	-178.47(18)
C(9)-N(10)-N(11)-C(10)	0.0(2)
C(9)-N(10)-N(11)-C(11)	179.02(18)
N(3)-N(2)-C(1)-N(1)	-0.4(3)
C(2)-N(1)-C(1)-N(2)	0.1(3)
C(1)-N(1)-C(2)-N(3)	0.2(2)
N(2)-N(3)-C(2)-N(1)	-0.4(3)
C(3)-N(3)-C(2)-N(1)	178.40(19)
C(2)-N(3)-C(3)-C(8)	80.7(3)
N(2)-N(3)-C(3)-C(8)	-100.6(2)
C(2)-N(3)-C(3)-C(4)	-95.5(3)
N(2)-N(3)-C(3)-C(4)	83.1(3)
C(8)-C(3)-C(4)-N(4)	-173.6(2)
N(3)-C(3)-C(4)-N(4)	2.4(3)
C(8)-C(3)-C(4)-C(5)	6.3(3)
N(3)-C(3)-C(4)-C(5)	-177.70(19)
O(1)-N(5)-C(5)-C(6)	178.7(2)

O(2)-N(5)-C(5)-C(6)	-2.2(4)
O(1)-N(5)-C(5)-C(4)	-2.6(3)
O(2)-N(5)-C(5)-C(4)	176.4(2)
N(4)-C(4)-C(5)-N(5)	-4.7(3)
C(3)-C(4)-C(5)-N(5)	175.4(2)
N(4)-C(4)-C(5)-C(6)	174.0(2)
C(3)-C(4)-C(5)-C(6)	-6.0(3)
N(5)-C(5)-C(6)-N(6)	0.3(4)
C(4)-C(5)-C(6)-N(6)	-178.3(2)
N(5)-C(5)-C(6)-C(7)	-179.9(2)
C(4)-C(5)-C(6)-C(7)	1.5(3)
O(4)-N(7)-C(7)-C(8)	-1.9(3)
O(3)-N(7)-C(7)-C(8)	177.6(2)
O(4)-N(7)-C(7)-C(6)	176.3(2)
O(3)-N(7)-C(7)-C(6)	-4.3(3)
N(6)-C(6)-C(7)-N(7)	4.6(4)
C(5)-C(6)-C(7)-N(7)	-175.2(2)
N(6)-C(6)-C(7)-C(8)	-177.3(2)
C(5)-C(6)-C(7)-C(8)	3.0(3)
C(4)-C(3)-C(8)-N(8)	177.6(2)
N(3)-C(3)-C(8)-N(8)	1.6(3)
C(4)-C(3)-C(8)-C(7)	-1.9(3)
N(3)-C(3)-C(8)-C(7)	-177.89(18)
N(7)-C(7)-C(8)-N(8)	-4.2(3)
C(6)-C(7)-C(8)-N(8)	177.6(2)
N(7)-C(7)-C(8)-C(3)	175.33(19)
C(6)-C(7)-C(8)-C(3)	-2.9(3)
N(11)-N(10)-C(9)-N(9)	0.1(2)
C(10)-N(9)-C(9)-N(10)	-0.2(3)
C(9)-N(9)-C(10)-N(11)	0.2(2)
N(10)-N(11)-C(10)-N(9)	-0.2(2)
C(11)-N(11)-C(10)-N(9)	-179.06(19)
C(10)-N(11)-C(11)-C(16)	-92.1(3)
N(10)-N(11)-C(11)-C(16)	89.1(2)
C(10)-N(11)-C(11)-C(12)	90.2(3)
N(10)-N(11)-C(11)-C(12)	-88.5(2)
C(16)-C(11)-C(12)-N(12)	-179.9(2)
N(11)-C(11)-C(12)-N(12)	-2.4(3)

C(16)-C(11)-C(12)-C(13)	-1.2(3)
N(11)-C(11)-C(12)-C(13)	176.33(18)
O(5)-N(13)-C(13)-C(14)	168.6(2)
O(6)-N(13)-C(13)-C(14)	-10.9(3)
O(5)-N(13)-C(13)-C(12)	-9.1(3)
O(6)-N(13)-C(13)-C(12)	171.5(2)
N(12)-C(12)-C(13)-N(13)	3.2(3)
C(11)-C(12)-C(13)-N(13)	-175.42(18)
N(12)-C(12)-C(13)-C(14)	-174.4(2)
C(11)-C(12)-C(13)-C(14)	6.9(3)
N(13)-C(13)-C(14)-N(14)	-1.5(3)
C(12)-C(13)-C(14)-N(14)	176.1(2)
N(13)-C(13)-C(14)-C(15)	178.09(19)
C(12)-C(13)-C(14)-C(15)	-4.3(3)
O(8)-N(15)-C(15)-C(14)	173.7(2)
O(7)-N(15)-C(15)-C(14)	-8.0(3)
O(8)-N(15)-C(15)-C(16)	-5.4(3)
O(7)-N(15)-C(15)-C(16)	172.9(2)
N(14)-C(14)-C(15)-N(15)	-3.5(3)
C(13)-C(14)-C(15)-N(15)	176.9(2)
N(14)-C(14)-C(15)-C(16)	175.5(2)
C(13)-C(14)-C(15)-C(16)	-4.0(3)
C(12)-C(11)-C(16)-N(16)	173.9(2)
N(11)-C(11)-C(16)-N(16)	-3.5(3)
C(12)-C(11)-C(16)-C(15)	-6.9(3)
N(11)-C(11)-C(16)-C(15)	175.63(18)
N(15)-C(15)-C(16)-N(16)	7.7(3)
C(14)-C(15)-C(16)-N(16)	-171.4(2)
N(15)-C(15)-C(16)-C(11)	-171.5(2)
C(14)-C(15)-C(16)-C(11)	9.4(3)

Symmetry transformations used to generate equivalent atoms:

Table S19. Hydrogen bonds for **6** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(10)-H(10)...O(8)#1	0.93	2.57	3.187(3)	124.1
C(9)-H(9)...O(1)#2	0.93	2.50	3.293(3)	143.5
C(2)-H(2A)...O(4)#1	0.93	2.60	3.308(3)	133.0
C(2)-H(2A)...O(3)#1	0.93	2.56	3.350(3)	142.4

C(2)-H(2A)...N(7)#1	0.93	2.59	3.270(3)	130.2
N(16)-H(16B)...O(8)	0.86	1.91	2.539(2)	129.0
N(16)-H(16A)...N(9)#2	0.86	2.17	2.949(2)	150.5
N(14)-H(14B)...O(7)	0.86	1.85	2.501(3)	131.2
N(14)-H(14A)...O(6)	0.86	1.86	2.510(3)	131.2
N(14)-H(14A)...N(1)#3	0.86	2.56	3.273(3)	141.0
N(12)-H(12B)...O(5)	0.86	1.90	2.538(2)	130.0
N(12)-H(12A)...O(3)#4	0.86	2.21	3.016(2)	155.9
N(8)-H(8B)...O(4)	0.86	1.89	2.527(2)	129.5
N(8)-H(8A)...O(6)#3	0.86	2.13	2.924(2)	153.0
N(6)-H(6B)...O(3)	0.86	1.85	2.507(2)	132.3
N(6)-H(6A)...O(2)#5	0.86	2.50	3.172(3)	135.9
N(6)-H(6A)...O(2)	0.86	1.86	2.518(3)	132.3
N(4)-H(4B)...O(1)	0.86	1.90	2.534(2)	129.1
N(4)-H(4A)...O(7)#1	0.86	2.12	2.909(3)	151.8

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z #2 -x,-y,-z #3 -x,-y+1,-z+1 #4 x-1,y-1,z

#5 -x+1,-y+1,-z

Table S20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **7**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	5350(2)	10302(2)	1634(2)	63(1)
O(2)	6340(2)	11033(2)	3585(2)	55(1)
O(3)	6822(2)	6506(2)	5847(2)	68(1)
O(4)	6251(2)	7473(2)	7136(2)	65(1)
N(1)	3040(2)	9992(2)	1687(2)	42(1)
N(2)	1980(2)	10312(2)	1583(2)	46(1)
N(3)	1018(2)	10695(3)	1350(3)	77(1)
N(4)	5626(2)	10327(2)	2815(2)	36(1)
N(5)	7260(2)	8895(2)	5212(2)	43(1)
N(6)	7910(2)	9235(2)	4647(2)	43(1)
N(7)	8623(2)	9512(2)	4290(2)	66(1)
N(8)	6209(2)	7246(2)	6054(2)	40(1)
N(9)	3646(2)	6828(2)	4879(2)	37(1)
N(10)	2661(2)	6294(2)	4148(2)	37(1)
N(11)	1811(2)	5717(2)	3650(2)	58(1)
N(12)	1913(2)	8181(2)	2589(2)	32(1)

N(13)	1166(2)	8464(2)	3216(2)	43(1)
N(14)	-22(2)	7655(2)	1201(2)	55(1)
C(1)	3773(2)	9258(2)	2753(2)	30(1)
C(2)	5109(2)	9429(2)	3356(2)	30(1)
C(3)	5924(2)	8786(2)	4456(2)	32(1)
C(4)	5359(2)	7953(2)	4913(2)	31(1)
C(5)	4050(2)	7716(2)	4303(2)	30(1)
C(6)	3260(2)	8391(2)	3214(2)	29(1)
C(7)	31(2)	8129(2)	2331(3)	53(1)
C(8)	1170(2)	7699(2)	1398(2)	43(1)

Table S21. Bond lengths [Å] and angles [°] for **7**.

O(1)-N(4)	1.207(2)
O(2)-N(4)	1.210(2)
O(3)-N(8)	1.200(3)
O(4)-N(8)	1.211(2)
N(1)-N(2)	1.237(3)
N(1)-C(1)	1.402(3)
N(2)-N(3)	1.117(3)
N(4)-C(2)	1.459(3)
N(5)-N(6)	1.238(3)
N(5)-C(3)	1.399(3)
N(6)-N(7)	1.109(3)
N(8)-C(4)	1.466(3)
N(9)-N(10)	1.235(3)
N(9)-C(5)	1.400(3)
N(10)-N(11)	1.114(3)
N(12)-C(8)	1.341(3)
N(12)-N(13)	1.368(2)
N(12)-C(6)	1.418(3)
N(13)-C(7)	1.304(3)
N(14)-C(8)	1.297(3)
N(14)-C(7)	1.348(3)
C(1)-C(6)	1.379(3)
C(1)-C(2)	1.399(3)
C(2)-C(3)	1.387(3)
C(3)-C(4)	1.385(3)

C(4)-C(5)	1.385(3)
C(5)-C(6)	1.392(3)
C(7)-H(7)	0.9300
C(8)-H(8)	0.9300

N(2)-N(1)-C(1)	117.77(18)
N(3)-N(2)-N(1)	170.4(3)
O(1)-N(4)-O(2)	123.7(2)
O(1)-N(4)-C(2)	118.12(18)
O(2)-N(4)-C(2)	118.09(18)
N(6)-N(5)-C(3)	118.71(18)
N(7)-N(6)-N(5)	171.2(2)
O(3)-N(8)-O(4)	125.3(2)
O(3)-N(8)-C(4)	117.7(2)
O(4)-N(8)-C(4)	117.0(2)
N(10)-N(9)-C(5)	117.87(18)
N(11)-N(10)-N(9)	169.8(2)
C(8)-N(12)-N(13)	109.34(17)
C(8)-N(12)-C(6)	129.82(18)
N(13)-N(12)-C(6)	120.83(16)
C(7)-N(13)-N(12)	101.20(19)
C(8)-N(14)-C(7)	102.7(2)
C(6)-C(1)-C(2)	119.38(19)
C(6)-C(1)-N(1)	124.21(19)
C(2)-C(1)-N(1)	116.41(19)
C(3)-C(2)-C(1)	121.42(19)
C(3)-C(2)-N(4)	120.53(18)
C(1)-C(2)-N(4)	118.04(18)
C(4)-C(3)-C(2)	117.01(18)
C(4)-C(3)-N(5)	114.68(19)
C(2)-C(3)-N(5)	128.3(2)
C(5)-C(4)-C(3)	123.40(19)
C(5)-C(4)-N(8)	118.76(18)
C(3)-C(4)-N(8)	117.75(18)
C(4)-C(5)-C(6)	117.89(19)
C(4)-C(5)-N(9)	115.85(18)
C(6)-C(5)-N(9)	126.24(18)
C(1)-C(6)-C(5)	120.77(18)

C(1)-C(6)-N(12)	120.20(18)
C(5)-C(6)-N(12)	119.02(18)
N(13)-C(7)-N(14)	116.2(2)
N(13)-C(7)-H(7)	121.9
N(14)-C(7)-H(7)	121.9
N(14)-C(8)-N(12)	110.6(2)
N(14)-C(8)-H(8)	124.7
N(12)-C(8)-H(8)	124.7

Symmetry transformations used to generate equivalent atoms:

Table S22. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **7**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	77(1)	72(1)	47(1)	2(1)	36(1)	-20(1)
O(2)	56(1)	43(1)	68(1)	-7(1)	27(1)	-15(1)
O(3)	51(1)	63(1)	78(1)	11(1)	19(1)	25(1)
O(4)	72(1)	81(2)	33(1)	9(1)	14(1)	4(1)
N(1)	34(1)	46(1)	44(1)	12(1)	16(1)	5(1)
N(2)	44(1)	47(1)	41(1)	10(1)	14(1)	7(1)
N(3)	54(2)	92(2)	82(2)	31(2)	27(1)	34(2)
N(4)	34(1)	37(1)	40(1)	-2(1)	20(1)	-2(1)
N(5)	25(1)	60(1)	41(1)	6(1)	11(1)	-6(1)
N(6)	26(1)	53(1)	46(1)	4(1)	12(1)	-3(1)
N(7)	37(1)	91(2)	74(2)	12(1)	29(1)	-4(1)
N(8)	28(1)	45(1)	41(1)	5(1)	9(1)	-2(1)
N(9)	32(1)	40(1)	35(1)	3(1)	11(1)	-5(1)
N(10)	36(1)	35(1)	43(1)	5(1)	20(1)	-1(1)
N(11)	47(1)	48(1)	67(2)	6(1)	14(1)	-14(1)
N(12)	24(1)	38(1)	34(1)	0(1)	11(1)	0(1)
N(13)	28(1)	55(1)	48(1)	-2(1)	19(1)	3(1)
N(14)	30(1)	67(2)	54(1)	-1(1)	6(1)	-10(1)
C(1)	31(1)	32(1)	27(1)	-2(1)	12(1)	3(1)
C(2)	31(1)	32(1)	32(1)	-3(1)	17(1)	-3(1)
C(3)	28(1)	38(1)	31(1)	-4(1)	14(1)	-2(1)
C(4)	27(1)	36(1)	29(1)	1(1)	11(1)	3(1)
C(5)	29(1)	33(1)	30(1)	-2(1)	16(1)	0(1)
C(6)	24(1)	32(1)	30(1)	-1(1)	11(1)	0(1)

C(7)	28(1)	66(2)	65(2)	2(1)	20(1)	1(1)
C(8)	33(1)	51(2)	37(1)	-3(1)	9(1)	-7(1)

Table S23. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **7**.

	x	y	z	U(eq)
H(7)	-7018213	247164		
H(8)	14697434	79751		

Table S24. Torsion angles [°] for **7**.

C(5)-N(9)-N(10)-N(11)	176.4(13)
C(8)-N(12)-N(13)-C(7)	-0.4(3)
C(6)-N(12)-N(13)-C(7)	-179.4(2)
N(2)-N(1)-C(1)-C(6)	37.8(3)
N(2)-N(1)-C(1)-C(2)	-143.0(2)
C(6)-C(1)-C(2)-C(3)	-3.5(3)
N(1)-C(1)-C(2)-C(3)	177.3(2)
C(6)-C(1)-C(2)-N(4)	177.90(18)
N(1)-C(1)-C(2)-N(4)	-1.3(3)
O(1)-N(4)-C(2)-C(3)	126.8(2)
O(2)-N(4)-C(2)-C(3)	-50.7(3)
O(1)-N(4)-C(2)-C(1)	-54.6(3)
O(2)-N(4)-C(2)-C(1)	127.8(2)
C(1)-C(2)-C(3)-C(4)	1.2(3)
N(4)-C(2)-C(3)-C(4)	179.70(18)
C(1)-C(2)-C(3)-N(5)	-176.1(2)
N(4)-C(2)-C(3)-N(5)	2.5(3)
N(6)-N(5)-C(3)-C(4)	151.4(2)
N(6)-N(5)-C(3)-C(2)	-31.4(3)
C(2)-C(3)-C(4)-C(5)	2.2(3)
N(5)-C(3)-C(4)-C(5)	179.83(19)
C(2)-C(3)-C(4)-N(8)	178.55(19)
N(5)-C(3)-C(4)-N(8)	-3.8(3)
O(3)-N(8)-C(4)-C(5)	101.1(2)
O(4)-N(8)-C(4)-C(5)	-80.2(3)
O(3)-N(8)-C(4)-C(3)	-75.4(3)
O(4)-N(8)-C(4)-C(3)	103.3(2)

C(3)-C(4)-C(5)-C(6)	-3.1(3)
N(8)-C(4)-C(5)-C(6)	-179.42(19)
C(3)-C(4)-C(5)-N(9)	178.50(19)
N(8)-C(4)-C(5)-N(9)	2.2(3)
N(10)-N(9)-C(5)-C(4)	-152.95(19)
N(10)-N(9)-C(5)-C(6)	28.9(3)
C(2)-C(1)-C(6)-C(5)	2.6(3)
N(1)-C(1)-C(6)-C(5)	-178.27(19)
C(2)-C(1)-C(6)-N(12)	-178.06(18)
N(1)-C(1)-C(6)-N(12)	1.1(3)
C(4)-C(5)-C(6)-C(1)	0.6(3)
N(9)-C(5)-C(6)-C(1)	178.80(19)
C(4)-C(5)-C(6)-N(12)	-178.73(18)
N(9)-C(5)-C(6)-N(12)	-0.6(3)
C(8)-N(12)-C(6)-C(1)	73.4(3)
N(13)-N(12)-C(6)-C(1)	-107.8(2)
C(8)-N(12)-C(6)-C(5)	-107.3(3)
N(13)-N(12)-C(6)-C(5)	71.5(3)
N(12)-N(13)-C(7)-N(14)	0.3(3)
C(8)-N(14)-C(7)-N(13)	-0.1(3)
C(7)-N(14)-C(8)-N(12)	-0.2(3)
N(13)-N(12)-C(8)-N(14)	0.4(3)
C(6)-N(12)-C(8)-N(14)	179.3(2)

Symmetry transformations used to generate equivalent atoms:

Table S25. Hydrogen bonds for **7** [Å and °].

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

Table S26. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **8**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	6391(3)	1625(3)	1331(1)	30(1)
N(2)	5398(3)	266(4)	1373(1)	44(1)
N(3)	6335(3)	1640(4)	2372(1)	45(1)
N(4)	4033(3)	2320(4)	204(2)	42(1)
N(5)	4586(3)	3580(3)	-1008(1)	36(1)
N(6)	7745(3)	3631(4)	-1032(1)	54(1)

N(7)	10180(3)	2393(4)	66(1)	36(1)
N(8)	9422(3)	1677(3)	1281(1)	34(1)
N(9)	10470(3)	2973(4)	1576(1)	49(1)
N(10)	10973(4)	343(5)	2133(2)	69(1)
O(1)	3245(3)	3633(4)	-966(1)	61(1)
O(2)	4836(2)	3994(3)	-1534(1)	58(1)
O(3)	10609(3)	3248(4)	-338(1)	62(1)
O(4)	11022(2)	1296(3)	446(1)	54(1)
C(1)	6717(3)	2005(4)	714(1)	28(1)
C(2)	5463(3)	2446(4)	143(1)	28(1)
C(3)	5830(3)	3051(4)	-440(1)	29(1)
C(4)	7404(3)	3127(4)	-482(1)	32(1)
C(5)	8583(3)	2580(4)	96(1)	32(1)
C(6)	8221(3)	2063(4)	684(1)	28(1)
C(7)	6926(3)	2417(4)	1933(1)	38(1)
C(8)	5415(4)	351(5)	2004(2)	48(1)
C(9)	9759(4)	148(5)	1620(2)	51(1)
C(10)	11351(4)	2078(6)	2082(2)	64(1)

Table S27. Bond lengths [Å] and angles [°] for **8**.

N(1)-C(7)	1.342(3)
N(1)-N(2)	1.365(3)
N(1)-C(1)	1.419(3)
N(2)-C(8)	1.306(4)
N(3)-C(7)	1.311(4)
N(3)-C(8)	1.353(4)
N(4)-C(2)	1.324(4)
N(4)-H(4B)	0.84(3)
N(4)-H(4A)	0.91(3)
N(5)-O(2)	1.214(3)
N(5)-O(1)	1.227(3)
N(5)-C(3)	1.430(3)
N(6)-C(4)	1.316(3)
N(6)-H(6A)	0.8600
N(6)-H(6B)	0.8600
N(7)-O(3)	1.197(3)
N(7)-O(4)	1.234(3)

N(7)-C(5)	1.454(4)
N(8)-C(9)	1.328(4)
N(8)-N(9)	1.365(3)
N(8)-C(6)	1.422(3)
N(9)-C(10)	1.305(4)
N(10)-C(9)	1.298(4)
N(10)-C(10)	1.347(5)
C(1)-C(6)	1.365(4)
C(1)-C(2)	1.423(4)
C(2)-C(3)	1.413(4)
C(3)-C(4)	1.435(4)
C(4)-C(5)	1.416(4)
C(5)-C(6)	1.402(4)
C(7)-H(7)	0.9300
C(8)-H(8)	0.9300
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300

C(7)-N(1)-N(2)	109.5(2)
C(7)-N(1)-C(1)	130.0(2)
N(2)-N(1)-C(1)	120.5(2)
C(8)-N(2)-N(1)	101.8(2)
C(7)-N(3)-C(8)	102.7(2)
C(2)-N(4)-H(4B)	115(2)
C(2)-N(4)-H(4A)	115(2)
H(4B)-N(4)-H(4A)	128(3)
O(2)-N(5)-O(1)	119.0(2)
O(2)-N(5)-C(3)	121.0(2)
O(1)-N(5)-C(3)	120.0(2)
C(4)-N(6)-H(6A)	120.0
C(4)-N(6)-H(6B)	120.0
H(6A)-N(6)-H(6B)	120.0
O(3)-N(7)-O(4)	122.8(3)
O(3)-N(7)-C(5)	119.4(3)
O(4)-N(7)-C(5)	117.7(3)
C(9)-N(8)-N(9)	110.1(2)
C(9)-N(8)-C(6)	129.7(3)
N(9)-N(8)-C(6)	120.2(2)

C(10)-N(9)-N(8)	100.6(3)
C(9)-N(10)-C(10)	102.3(3)
C(6)-C(1)-N(1)	120.2(2)
C(6)-C(1)-C(2)	120.7(2)
N(1)-C(1)-C(2)	119.0(2)
N(4)-C(2)-C(3)	124.7(3)
N(4)-C(2)-C(1)	117.3(3)
C(3)-C(2)-C(1)	118.0(2)
C(2)-C(3)-N(5)	118.6(2)
C(2)-C(3)-C(4)	122.2(2)
N(5)-C(3)-C(4)	119.2(2)
N(6)-C(4)-C(5)	121.2(3)
N(6)-C(4)-C(3)	122.3(3)
C(5)-C(4)-C(3)	116.5(2)
C(6)-C(5)-C(4)	121.2(2)
C(6)-C(5)-N(7)	118.8(2)
C(4)-C(5)-N(7)	119.8(2)
C(1)-C(6)-C(5)	121.3(2)
C(1)-C(6)-N(8)	117.8(2)
C(5)-C(6)-N(8)	120.8(2)
N(3)-C(7)-N(1)	110.3(3)
N(3)-C(7)-H(7)	124.9
N(1)-C(7)-H(7)	124.9
N(2)-C(8)-N(3)	115.8(3)
N(2)-C(8)-H(8)	122.1
N(3)-C(8)-H(8)	122.1
N(10)-C(9)-N(8)	110.6(3)
N(10)-C(9)-H(9)	124.7
N(8)-C(9)-H(9)	124.7
N(9)-C(10)-N(10)	116.4(3)
N(9)-C(10)-H(10)	121.8
N(10)-C(10)-H(10)	121.8

Symmetry transformations used to generate equivalent atoms:

Table S28. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **8**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	31(1)	36(2)	26(1)	-1(1)	12(1)	-7(1)

N(2)	54(2)	45(2)	38(2)	0(1)	19(1)	-18(1)
N(3)	52(2)	57(2)	29(1)	-1(1)	17(1)	-3(2)
N(4)	26(2)	67(2)	34(2)	5(2)	10(1)	-1(1)
N(5)	33(2)	47(2)	28(1)	2(1)	7(1)	8(1)
N(6)	36(2)	96(2)	34(2)	17(2)	16(1)	3(2)
N(7)	26(1)	55(2)	29(1)	2(1)	10(1)	6(1)
N(8)	26(1)	45(2)	31(1)	2(1)	6(1)	0(1)
N(9)	38(2)	63(2)	39(2)	-6(2)	-2(1)	-6(1)
N(10)	56(2)	86(3)	53(2)	17(2)	-5(2)	12(2)
O(1)	27(1)	108(2)	47(1)	18(1)	11(1)	18(1)
O(2)	49(2)	95(2)	31(1)	21(1)	13(1)	16(1)
O(3)	39(1)	95(2)	58(2)	15(1)	22(1)	0(1)
O(4)	36(1)	69(2)	61(2)	7(1)	18(1)	10(1)
C(1)	31(2)	31(2)	23(1)	-1(1)	10(1)	-3(1)
C(2)	28(2)	28(2)	29(2)	-4(1)	10(1)	-2(1)
C(3)	29(2)	33(2)	25(1)	-1(1)	7(1)	2(1)
C(4)	33(2)	38(2)	28(2)	-3(1)	11(1)	-1(1)
C(5)	25(2)	39(2)	32(2)	-1(1)	11(1)	-4(1)
C(6)	26(2)	30(2)	28(2)	-3(1)	7(1)	2(1)
C(7)	38(2)	50(2)	24(2)	-5(1)	8(1)	-6(2)
C(8)	59(2)	57(2)	36(2)	4(2)	25(2)	-11(2)
C(9)	47(2)	50(2)	53(2)	15(2)	8(2)	6(2)
C(10)	47(2)	87(3)	46(2)	1(2)	-8(2)	-1(2)

Table S29. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **8**.

	x	y	z	U(eq)
H(6A)	86983632	-104565		
H(6B)	70153960	-137965		
H(7)	76173380	202545		
H(8)	4831-426	218858		
H(9)	9202-916	150661		
H(10)	121952609	239177		
H(4B)	3320(40)	2520(40)	-149(15)	32(9)
H(4A)	3960(40)	1750(40)	584(17)	53(10)

Table S30. Torsion angles [°] for **8**.

C(7)-N(1)-N(2)-C(8)	0.0(3)
C(1)-N(1)-N(2)-C(8)	179.9(3)
C(9)-N(8)-N(9)-C(10)	-0.6(3)
C(6)-N(8)-N(9)-C(10)	-178.9(3)
C(7)-N(1)-C(1)-C(6)	53.7(4)
N(2)-N(1)-C(1)-C(6)	-126.1(3)
C(7)-N(1)-C(1)-C(2)	-121.9(3)
N(2)-N(1)-C(1)-C(2)	58.3(4)
C(6)-C(1)-C(2)-N(4)	178.5(3)
N(1)-C(1)-C(2)-N(4)	-5.9(4)
C(6)-C(1)-C(2)-C(3)	-3.9(4)
N(1)-C(1)-C(2)-C(3)	171.7(2)
N(4)-C(2)-C(3)-N(5)	0.4(4)
C(1)-C(2)-C(3)-N(5)	-177.1(3)
N(4)-C(2)-C(3)-C(4)	-178.8(3)
C(1)-C(2)-C(3)-C(4)	3.8(4)
O(2)-N(5)-C(3)-C(2)	-175.0(3)
O(1)-N(5)-C(3)-C(2)	5.4(4)
O(2)-N(5)-C(3)-C(4)	4.2(4)
O(1)-N(5)-C(3)-C(4)	-175.3(3)
C(2)-C(3)-C(4)-N(6)	177.6(3)
N(5)-C(3)-C(4)-N(6)	-1.6(4)
C(2)-C(3)-C(4)-C(5)	-0.6(4)
N(5)-C(3)-C(4)-C(5)	-179.8(3)
N(6)-C(4)-C(5)-C(6)	179.2(3)
C(3)-C(4)-C(5)-C(6)	-2.5(4)
N(6)-C(4)-C(5)-N(7)	-6.3(4)
C(3)-C(4)-C(5)-N(7)	172.0(3)
O(3)-N(7)-C(5)-C(6)	-159.7(3)
O(4)-N(7)-C(5)-C(6)	22.9(4)
O(3)-N(7)-C(5)-C(4)	25.7(4)
O(4)-N(7)-C(5)-C(4)	-151.7(3)
N(1)-C(1)-C(6)-C(5)	-174.7(2)
C(2)-C(1)-C(6)-C(5)	0.9(4)
N(1)-C(1)-C(6)-N(8)	2.0(4)
C(2)-C(1)-C(6)-N(8)	177.5(2)
C(4)-C(5)-C(6)-C(1)	2.5(4)
N(7)-C(5)-C(6)-C(1)	-172.1(3)

C(4)-C(5)-C(6)-N(8)	-174.1(3)
N(7)-C(5)-C(6)-N(8)	11.4(4)
C(9)-N(8)-C(6)-C(1)	66.7(4)
N(9)-N(8)-C(6)-C(1)	-115.5(3)
C(9)-N(8)-C(6)-C(5)	-116.7(4)
N(9)-N(8)-C(6)-C(5)	61.2(4)
C(8)-N(3)-C(7)-N(1)	-0.3(3)
N(2)-N(1)-C(7)-N(3)	0.2(3)
C(1)-N(1)-C(7)-N(3)	-179.6(3)
N(1)-N(2)-C(8)-N(3)	-0.2(4)
C(7)-N(3)-C(8)-N(2)	0.3(4)
C(10)-N(10)-C(9)-N(8)	-0.2(4)
N(9)-N(8)-C(9)-N(10)	0.5(4)
C(6)-N(8)-C(9)-N(10)	178.6(3)
N(8)-N(9)-C(10)-N(10)	0.5(4)
C(9)-N(10)-C(10)-N(9)	-0.2(5)

Symmetry transformations used to generate equivalent atoms:

Table S31. Hydrogen bonds for **8** [Å and °].

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

DSC plots for the title compounds

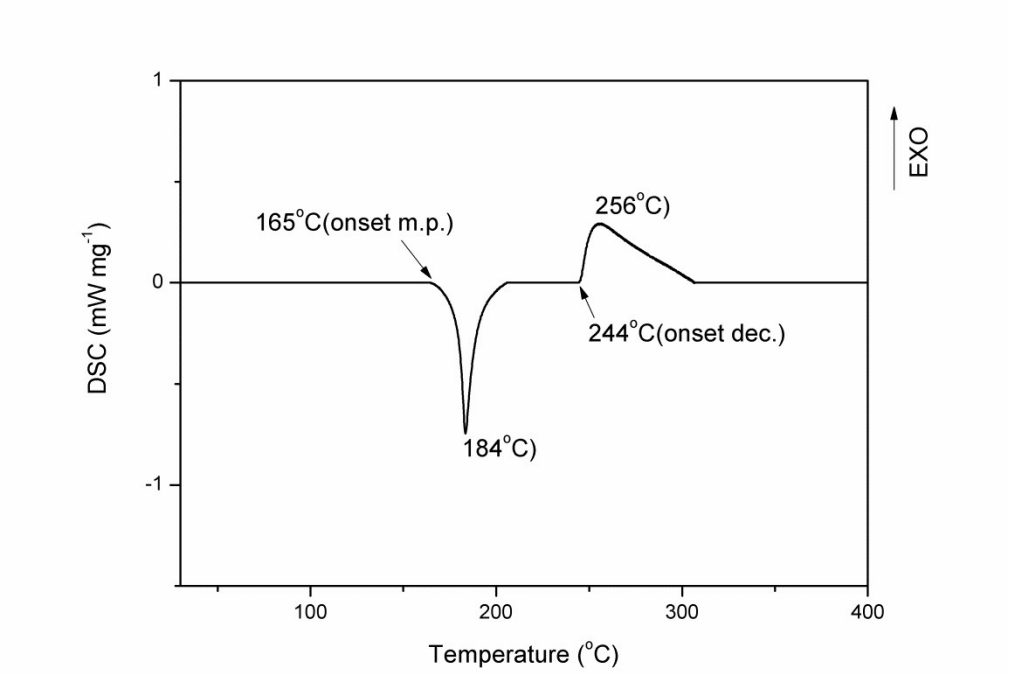


Fig. S5 DSC plot for compound **4**

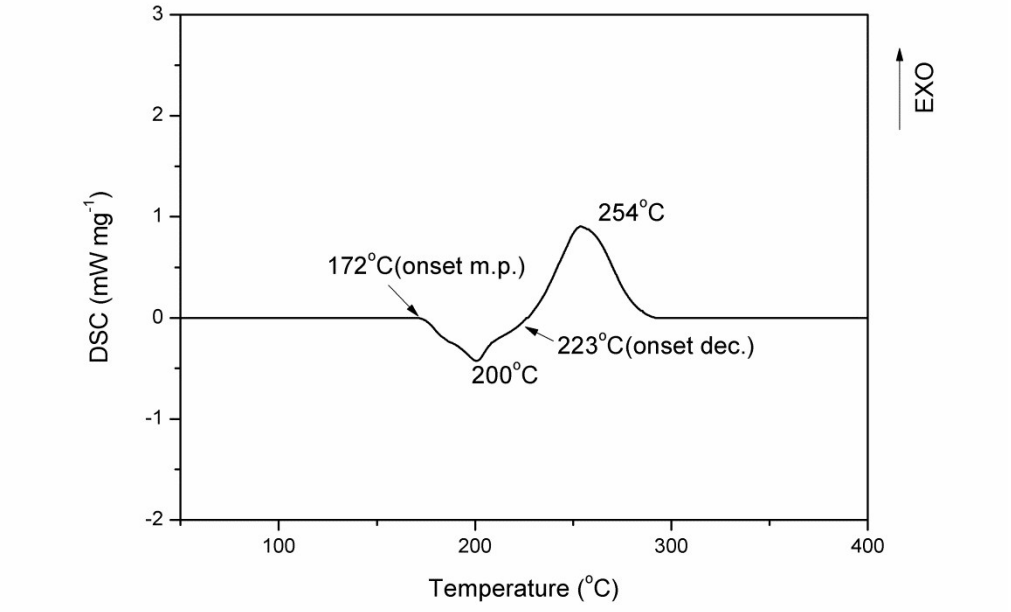


Fig. S6 DSC plot for compound **5**

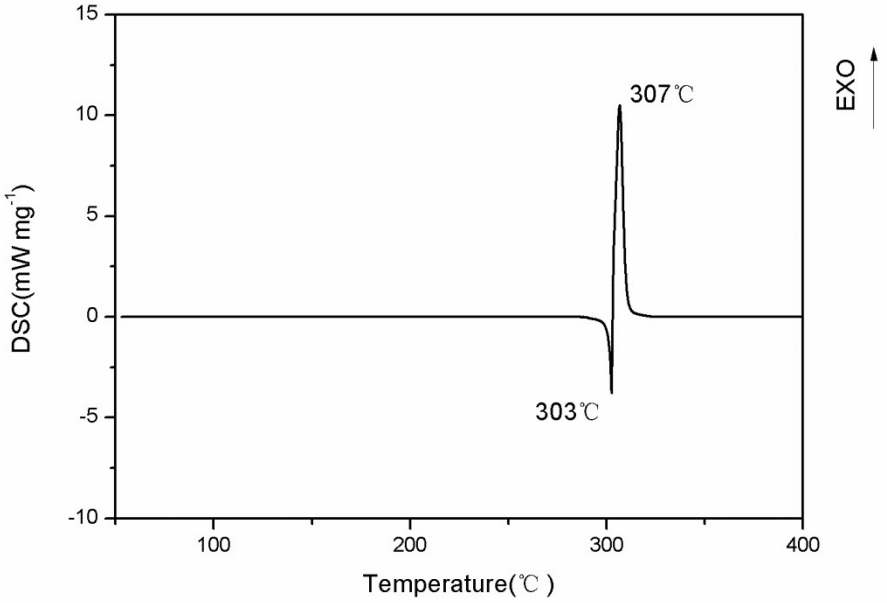


Fig. S7 DSC plot for compound **6**

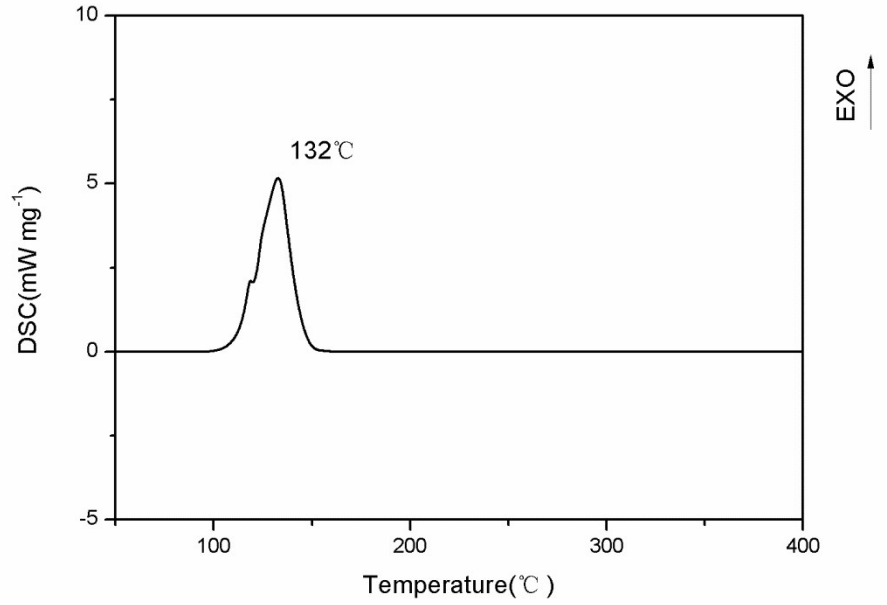


Fig. S8 DSC plot for compound **7**

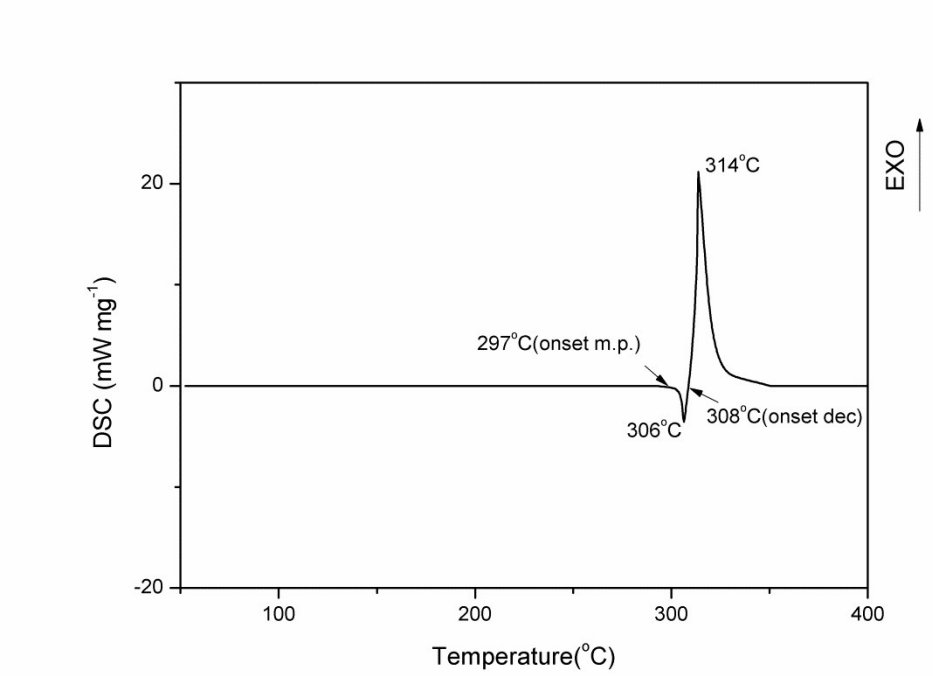


Fig. S9 DSC plot for compound **8**

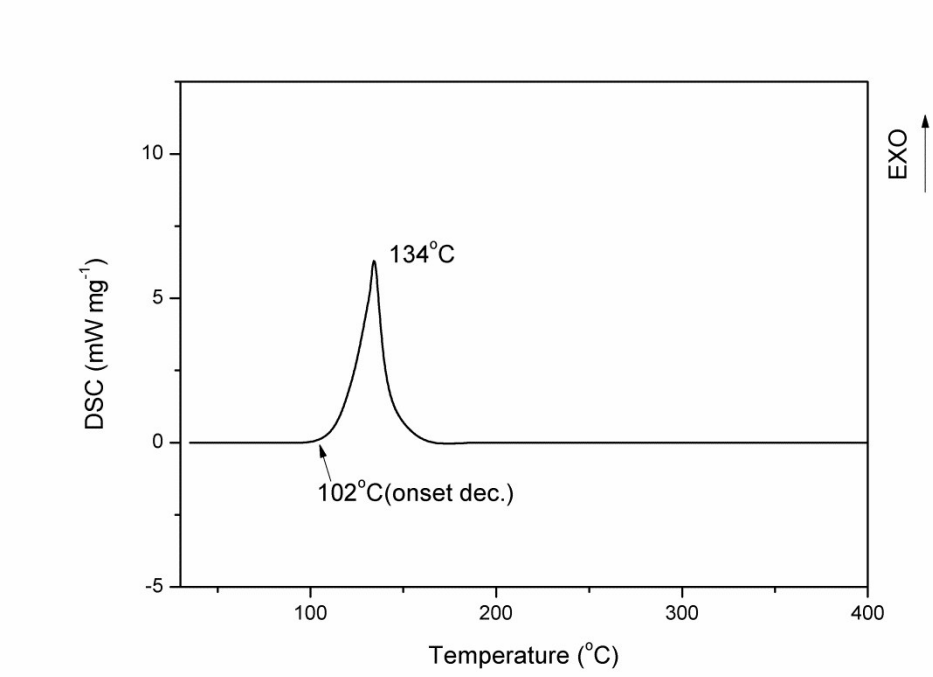


Fig. S10 DSC plot for compound **9**

Theoretical study

All calculations were carried out at Gaussian 09 package.[2] All molecules were optimized at DFT/B3LYP[3] functional 6-31G** basis set,[4] and the structures were conformed to be true local-energy minima on the potenital-energy surface with frequency analysis. The change of enthalpy for the reactions at 298 K can be expressed as

$$\Delta H_{298} = \sum \Delta_f H_P - \sum \Delta_f H_R \quad (1)$$

where $\Delta_f H_R$ and $\Delta_f H_P$ are the HOF of reactants and products at 298 K, respectively, and ΔH_{298} can be calculated using the following expression:

$$\Delta H_{298} = \Delta E_{298} + \Delta(PV) = \Delta E_0 + \Delta ZPE + \Delta H_T + \Delta nRT \quad (2)$$

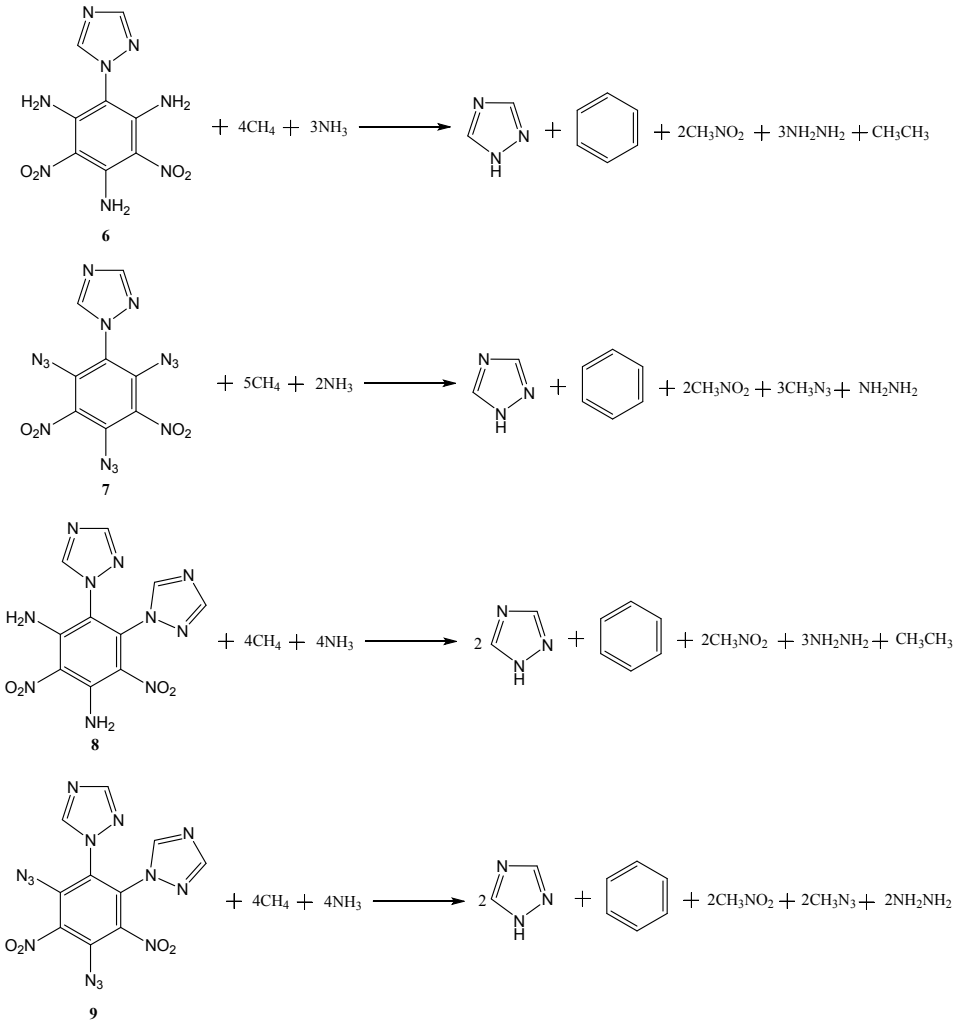
where ΔE_0 is the change in total energy between the products and the reactants at 0 K; ΔZPE is the difference between the zero-point energies (*ZPE*) of the products and the reactants at 0 K; ΔH_T is thermal correction from 0 to 298 K. The $\Delta(PV)$ value in eq (2) is the *PV* work term. It equals $\Delta(nRT)$ for the reactions of ideal gas. For the isodesmic reactions, $\Delta n = 0$, so $\Delta(PV) = 0$. On the left side of Eq. (1), apart from target compound, all the others are called reference compounds. The HOF of reference compounds are available either from the experiments[5] or from the high level computing like G2 method.[6] Molar enthalpy of formation in solid state calculated by $\Delta_f H_s = \Delta_f H_g - \Delta_f H_{sub}$, enthalpy of formation in gas state ($\Delta_f H_g$) was calculated by DFT method in combination with the isodesmic reactions, the sublimation enthalpy ($\Delta_f H_{sub}$) was evaluated by the electrostatic potential method.

The detonation velocity and detonation pressure were calculated by the Kamlet-Jacobs formulas (3) and (4)[7] as follows:

$$D = 1.01(NM^{1/2}Q^{1/2})^{1/2}(1+1.30\rho) \quad (3)$$

$$P = 1.558\rho^2 NM^{1/2}Q^{1/2} \quad (4)$$

where D is the detonation velocity (km s^{-1}), P is the detonation pressure (GPa), N is the moles of detonation gases per gram of explosive, M is the average molecular weight (g mol^{-1}) of these gases. Q is the heat of detonation (cal g^{-1}), and is the loaded density (g cm^{-3}) of explosives.



Scheme 1 Isodesmic reaction

Table S32 Calculated total energy (E_0), zero point energy (ZPE), and thermal correction (H_T) and experimental gaseous heat of formation ($\Delta_f H_{gas}$) for the reference compounds. E_0 and ZPE are in (a.u.), H_{sub} and HOF are in (kJ mol^{-1}).

Compd.	ZPE	H_T	E_0	$E_{cor.}$	ΔH_T	$\Delta_f H_{gas}$	ΔH_{sub}	$\Delta H_{f,solid}$
CH_4	0.04416	0.04692	-40.478950	-40.432030	10.01	-74.6[a]		
NH_3	0.03377	0.03674	-56.523305	-56.486565	10.00	-45.9[a]		
CH_3CH_3	0.07303	0.07537	-79.759748	-79.684378	10.47	-84.0[a]		
CH_3NO_2	0.04894	0.05219	-244.963435	-244.911245	11.62	-74.7[a]		
CH_3N_3	0.04945	0.05364	-204.046787	-203.993147	14.22	238.4[a]		
NH_2NH_2	0.05224	0.05522	-111.815351	-111.760131	11.06	93.4[a]		
benzene	0.09861	0.10171	-232.157596	-232.055886	14.00	82.9[a]		
1,2,4-triazole	0.05877	0.06189	-242.195875	-242.133985	11.83	192.7[a]		
6	0.19248	0.20531	-1048.21335	-1048.00804	45.84	207.40	175.63	31.77
7	0.14956	0.16824	-1372.852635	-1372.684395	59.44	1253.65	239.01	1014.68
8	0.21441	0.22927	-1233.851790	-1233.622520	52.61	537.43	221.19	316.24
9	0.18548	0.20439	-1450.281089	-1450.076699	62.08	1239.2	264.66	974.62

					8

[a] The experimental data are taken from Ref.4.

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Table S33 Predicted heats of formation ($\Delta H_{f,solid}$), densities (ρ), detonation velocities (*D*), detonation pressures (*P*), and oxygen balance (OB) for the title compounds together with TNT, RDX and HMX

Comp.	$\Delta H_{f,solid}$(kJ mol^{-1})	ρ(g cm^{-3})	D(km s^{-1})	P(GPa)	OB(%)
6	31.77	1.73	6.55	18.53	-91.36
7	1014.68	1.77	7.50	24.67	-58.07
8	316.24	1.73	6.56	18.67	-96.32
9	974.62	1.75	7.13	22.19	-74.95
TNT	-67.36	1.65	6.94	22.00	-73.97

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