

Supplementary Information

Table S1. Selected bond lengths, bond angles and torsion angles of compounds **1**, **2** and **3** in the crystalline state.

		1	2	3	
<i>d</i> / Å	N1–N2	1.356(2)	1.359(2)	1.374(2)	
	N1–C2	1.345(2)	1.343(3)	1.343(2)	
	N2–C1	1.314(2)	1.317(3)	1.327(2)	
	N3–C1	1.350(2)	1.347(3)	1.343(2)	
	N3–C2	1.327(2)	1.326(3)	1.338(2)	
	N4–C1	1.452(2)	1.449(4)	1.441(2)	
	O1–N4	1.227(2)	1.228(3)	1.239(2)	
	O2–N4	1.228(2)	1.218(3)	1.233(2)	
	N5–C2	1.383(2)	1.383(3)	1.410(2)	
	N5–N6	1.256(2)	1.252(3)	1.250(2)	
	N6–N7	1.124(2)	1.112(3)	1.123(2)	
	N1–C3	-	1.463(4)	-	
	< / °	N1–N2–C1	100.0(1)	100.9(2)	103.6(1)
		N1–C2–N3	110.7(1)	112.0(2)	116.1(1)
N2–N1–C2		110.5(1)	109.1(2)	104.6(1)	
N2–C1–N3		118.5(1)	118.0(2)	117.5(1)	
C1–N3–C2		100.3(1)	100.0(2)	98.2(1)	
N2–C1–N4		119.9(1)	120.2(2)	120.7(1)	
O1–N4–O2		124.9(2)	124.8(2)	123.6(1)	
N1–C2–N5		118.7(2)	118.8(2)	116.9(1)	
N6–N5–C2		115.3(1)	113.5(2)	115.3(1)	
N5–N6–N7		170.4(2)	171.8(2)	172.2(2)	
N2–N1–C3		-	121.9(2)	-	
< / °		N2–C1–N4–O1	180.0(2)	–180.0(2)	179.0(1)
		N1–C2–N5–N6	180.0(2)	180.0(2)	–174.9(1)
	C1–N2–N1–C3	-	180.0(2)	-	

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