Supporting Information

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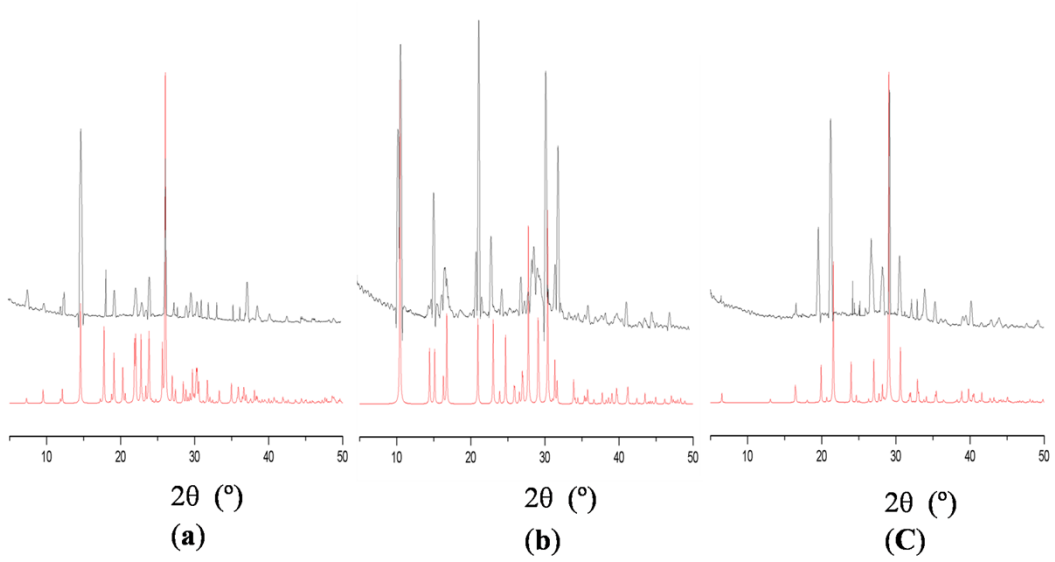

Table S1.

Selected bond lengths (Å) and angles (°) for **1–3**.

1	N(1)-C(3)	1.333(4)	C(3)-N(1)-C(2)	122.1(3)
	N(1)-N(3)	1.319(5)	N(3)-N(1)-C(2)	129.5(3)
	N(1)-C(2)	1.455(4)	N(3)-N(4)-N(2)	105.2(3)
	N(4)-N(3)	1.316(5)	C(3)-N(2)-N(4)	110.6(3)
	N(4)-N(2)	1.356(5)	N(4)-N(3)-N(1)	108.8(3)
	N(2)-C(3)	1.274(5)	C(5)-N(7)-C(6)	116.3(3)
	N(7)-C(5)	1.332(4)	C(4)-N(9)-C(6)	115.5(3)
	N(7)-C(6)	1.338(4)	C(4)-N(6)-C(5)	119.9(3)
	N(9)-C(4)	1.330(4)	C(4)-N(6)-H(5)	120.1
	N(9)-C(6)	1.351(4)	C(5)-N(6)-H(5)	120.1
	N(6)-C(4)	1.353(4)	N(5)-C(4)-N(9)	120.6(3)
	N(6)-C(5)	1.362(4)	N(5)-C(4)-N(6)	117.8(3)
	N(6)-H(5)	0.8600	N(9)-C(4)-N(6)	121.5(3)
	C(4)-N(5)	1.315(4)	N(8)-C(6)-N(7)	117.7(3)
	C(6)-N(8)	1.328(4)	N(8)-C(6)-N(9)	116.2(3)
	C(5)-N(10)	1.300(4)	N(7)-C(6)-N(9)	126.1(3)
	C(3)-H(8)	0.9300	N(10)-C(5)-N(7)	121.2(3)
	C(2)-C(1)	1.516(5)	N(10)-C(5)-N(6)	118.2(3)
	C(2)-H(12)	0.91(4)	N(7)-C(5)-N(6)	120.6(3)
	C(2)-H(9)	0.914(19)	N(2)-C(3)-N(1)	107.1(3)
	C(1)-O(2)	1.228(4)	N(2)-C(3)-H(8)	126.5
	C(1)-O(3)	1.256(4)	N(1)-C(3)-H(8)	126.5
	O(1)-H(10)	0.95(4)	N(1)-C(2)-C(1)	113.0(3)
	O(1)-H(11)	0.90(5)	N(1)-C(2)-H(12)	106(3)
	N(8)-H(2)	0.8600	C(1)-C(2)-H(12)	107(3)
	N(5)-H(4)	0.8600	N(1)-C(2)-H(9)	108(3)
	N(5)-H(3)	0.8600	C(1)-C(2)-H(9)	104(3)
	N(10)-H(7)	0.8600	H(12)-C(2)-H(9)	118(4)
	N(10)-H(6)	0.8600	O(2)-C(1)-O(3)	126.6(3)
	H(7)-N(10)-H(6)	0.8600	O(2)-C(1)-C(2)	119.2(3)
	C(5)-N(10)-H(6)	120.0	O(3)-C(1)-C(2)	114.2(3)
	H(4)-N(5)-H(3)	120.0	H(10)-O(1)-H(11)	93(4)
	H(4)-N(5)-H(3)	120.0	C(6)-N(8)-H(1)	120.0
	C(4)-N(5)-H(3)	120.0	C(6)-N(8)-H(2)	120.0
	C(4)-N(5)-H(4)	120.0	H(1)-N(8)-H(2)	120.0
2	N(2)-C(2)	1.335(4)	C(2)-N(2)-H(4)	122(3)
	N(2)-N(5)	1.366(4)	N(5)-N(2)-H(4)	126(3)
	N(2)-H(4)	1.06(6)	N(5)-N(4)-N(3)	108.7(3)
	N(4)-N(5)	1.269(4)	C(2)-N(3)-N(4)	109.1(3)
	N(4)-N(3)	1.360(4)	C(2)-N(3)-H(1)	125.4
	N(3)-C(2)	1.329(4)	N(4)-N(3)-H(1)	125.4
	N(3)-H(1)	0.8600	N(4)-N(5)-N(2)	107.6(3)

	N(1)-C(2)	1.322(5)	C(2)-N(1)-H(2)	120.0
	N(1)-H(2)	0.8600	C(2)-N(1)-H(3)	120.0
	N(1)-H(3)	0.8600	H(2)-N(1)-H(3)	120.0
	O(2)-C(1)	1.280(4)	N(1)-C(2)-N(3)	127.8(3)
	O(1)-C(1)	1.217(4)	N(1)-C(2)-N(2)	126.8(3)
	C(1)-C(1)#1	1.548(6)	N(3)-C(2)-N(2)	105.4(3)
	C(2)-N(2)-N(5)	109.2(3)	O(1)-C(1)-O(2)	126.2(3)
	O(2)-C(1)-C(1)#1	113.8(3)	O(1)-C(1)-C(1)#1	120.0(3)
3	O(1)-N(1)	1.234(2)	C(2)-N(4)-H(4)	132.3(15)
	O(2)-N(1)	1.248(2)	N(3)-N(4)-H(4)	119.6(15)
	O(3)-N(1)	1.239(2)	C(1)-N(5)-C(2)	108.62(17)
	O(4)-N(2)	1.237(2)	C(1)-N(5)-H(5)	128.5(19)
	O(5)-N(2)	1.209(2)	C(2)-N(5)-H(5)	122.8(19)
	O(6)-N(2)	1.256(2)	C(1)-N(6)-H(6A)	119.3(17)
	N(3)-C(1)	1.320(3)	C(1)-N(6)-H(6B)	121.8(17)
	N(3)-N(4)	1.388(3)	H(6A)-N(6)-H(6B)	119(2)
	N(3)-H(3)	0.84(2)	C(2)-N(7)-H(7A)	120.1(14)
	N(4)-C(2)	1.314(3)	H(7A)-N(7)-H(7B)	118.5(18)
	N(4)-H(4)	0.92(2)	N(6)-C(1)-N(3)	121(2)
	N(5)-C(1)	1.355(3)	N(6)-C(1)-N(5)	126.7(2)
	N(5)-C(2)	1.358(3)	N(3)-C(1)-N(5)	125.66(19)
	N(5)-H(5)	0.83(3)	N(7)-C(2)-N(4)	107.61(17)
	N(6)-C(1)	1.312(3)	N(7)-C(2)-N(5)	126.8(2)
	N(6)-H(6A)	0.82(3)	N(7)-C(2)-N(5)	125.4(2)
	N(6)-H(6B)	0.93(3)	N(4)-C(2)-N(5)	107.70(18)
	N(7)-C(2)	1.312(3)	O(1)-N(1)-O(3)	119.77(18)
	N(7)-H(7A)	0.99(2)	O(1)-N(1)-O(2)	119.60(18)
	N(7)-H(7B)	0.84(3)	O(3)-N(1)-O(2)	120.60(18)
	O(4)-N(2)-O(6)	118.58(17)	O(5)-N(2)-O(4)	120.83(17)
	C(1)-N(3)-N(4)	107.95(17)	O(5)-N(2)-O(6)	120.57(17)
	C(1)-N(3)-H(3)	130.9(15)	N(4)-N(3)-H(3)	120.3(15)
	C(2)-N(4)-N(3)	108.06(17)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+1.

Table S2.

Hydrogen bond lengths (Å) and angles (°) for **1–3**.

	d(D-H···A) [Å]	d(D−H) [Å]	d(H···A)[Å]	d(D···A) [Å]	<(DHA) [°]
1	O(1)-H(11) ···O(3)#1	0.90(5)	1.91(5)	2.773(4)	162(4)
	N(10)-H(6) ···N(4)#2	0.86	2.11	2.939(4)	161.8
	N(10)-H(7) ···N(7)#3	0.86	2.19	3.047(4)	175.8
	N(5)-H(3) ···O(3)#4	0.86	2.32	2.849(4)	120.4
	N(5)-H(4) ···N(9)#5	0.86	2.16	3.016(4)	178.0
	N(8)-H(2) ···•O(3)#6	0.86	2.04	2.830(4)	152.6
	N(8)-H(1) ···N(2)#7	0.86	2.22	3.022(4)	154.8
	O(1)-H(10) ···O(2)	0.95(4)	1.81(5)	2.754(4)	173(4)
	N(5)-H(3) ···O(1)	0.86	2.39	3.095(4)	139.2
	N(6)-H(5) ···O(1)	0.86	1.88	2.707(4)	160.6
2	N(2)-H(4) ···O(1)#2	1.06(6)	2.12(6)	2.872(4)	126(4)
	N(2)-H(4) ···O(2)#3	1.06(6)	1.82(6)	2.710(4)	138(5)
	N(1)-H(3) ···O(1)#2	0.86	2.31	2.994(4)	137.2
	N(1)-H(2) ···N(5)#4	0.86	2.33	3.184(5)	175.8
	N(3)-H(1) ···O(2)#5	0.86	1.70	2.561(3)	173.9
3	N3-H3···O6	0.84(2)	1.82(2)	2.655(2)	176(2)
	N3-H3···O5	0.84(2)	2.51(2)	3.072(2)	125.7(19)
	N4-H4···O4#1	0.92(2)	1.82(2)	2.737(2)	172(2)
	N4-H4···O5	0.92(2)	2.55(2)	3.126(2)	120.6(18)
	N5-H5···O3	0.83(3)	1.93(3)	2.752(2)	171(3)
	N6-H6A···O1#2	0.82(3)	2.46(3)	3.122(3)	139(2)
	N6-H6A···O2#2	0.82(3)	2.53(3)	3.327(3)	167(2)
	N6-H6B···O1#3	0.93(3)	2.01(3)	2.920(3)	166(2)
	N6-H6B···O3#3	0.93(3)	2.34(3)	3.069(2)	136(2)
	N7-H7A···O4#4	0.99(2)	2.18(2)	2.970(2)	135.9(19)
	N7-H7A···O5#5	0.99(2)	2.18(2)	3.101(3)	154.4(19)
	N7-H7B···O2	0.84(3)	2.10(3)	2.940(3)	172(3)
	N7-H7B···O6#4	0.84(3)	2.54(3)	3.016(3)	117(2)

Symmetry transformations used to generate equivalent atoms for **1**: #1 -x,-y,-z+1; #2 x-1,y,z; #3 -x,-y+1,-z; #4 -x+1,-y,-z+1; #5 -x+2,-y,-z; #6 x+1,y,z-1; #7 -x+1,-y+1,-z.

Symmetry transformations used to generate equivalent atoms for **2**: #1 -x+1,-y+1,-z+1;#2 x,-y+3/2,z-1/2; #3 -x+1,y+1/2,-z+1/2; #4 -x,y-1/2,-z+1/2; #5 x-1,y,z.

Symmetry transformations used to generate equivalent atoms for **3**: #1 -x, y+1/2, -z+1/2; #2 x, y-1, z; #3 -x+1, y-1/2, -z+3/2; #4 x, y+1, z; #5 -x, y+1/2, -z+1/2.