Table S1 Selected bond distances (Å) and angles (°) for [pypz$^{R(1)py}$]·H$_2$O

N1–N2	1.356(5)	**N1–N2–C3**	103.9(4)
N1–C5	1.383(5)	**N2–N1–C5**	112.4(4)
N1–C6	1.431(6)	**N2–C3–C4**	112.0(4)
N2–C3	1.342(5)	**N1–C5–C4**	105.5(4)
C3–C4	1.390(6)	**C3–C4–C5**	106.2(4)
C4–C5	1.370(6)	**N2–C3–C11**	120.1(4)
C5–C16	1.477(6)	**N1–C5–C6**	129.3(4)
C3–C11	1.486(6)		

Table S2 Dihedral angles between planes for [pz$^{R(1)py}$py]·H$_2$O

Plane 1: N1N2C3C4C5	
Plane 2: N1'C6C7C8C9C10	
Plane 3: N1''C11C12C13C14C15	
Plane 4: C16C17C18C19C20C21	
1-2	57.9(2)
1-3	20.8(2)
1-4	28.7(2)
2-3	46.5(2)
2-4	59.3(2)
3-4	15.7(2)