Electronic Supplementary Information (ESI) for

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Synthetic Procedures

1,3-Bis(3-pyridyl)-l,3-propanedione

To a suspension of NaH (2.0 g, 60% in oil, 0.05mol) in 50 mL anhydrous THF was added 3.425g (0.025mol) methyl nicotinate. The mixture was stirred at room temperature for 10 min and then 3.0 mL (3.0g, 0.025mol) 3-acepyridine was slowly added to the mixture. After completing the addition of 3-acepyridine, the mixture was kept with stirring for about 5 hours. The mixture was filtered. A yellow solid was obtained, then was dissolved in 50 mL diluted acetic acid solution (3 $mol \cdot L^{-1}$). The mixture was stirred for 30 min then filtered and washed by water. A yellowy solid was obtained and dried in vacuum to give 3.1 g of primary products 1,3-bis(3-pyridyl)-l,3-propanedione; yielding : 55%, m.p.: 208-210°C. IR (ν/cm^{-1}): 3400 s, 3101 w, 2925 w, 2847 w, 1589 vs, 1544 s, 1446 s, 1409 m, 1250 m, 1119 m, 1017 m, 796 s, 698 s.

3,5-bis(3-pyridyl)-1-H-pyrazole (Hbppz)

2.3g (0.01mol) 1,3-bis(3-pyridyl)-l,3-propanedione was added in ethanol (30 mL) and the mixture was treated with an excess of hydrazine (80%, 5mL), then refluxed for 10 hours. The solution was kept standing in air to evaporate the ethanol solvent. Several days later colorless block crystals were obtained. The block crystals were recrystallized in ethanol to give 1.69g Hbppz; yielding 76%, mp: 243-244°C. IR(ν/cm^{-1}): 3402 s, 3141 m, 3015 m, 1606 vs, 1577 s, 1438 s, 1193 m, 1050 m, 996 m, 964 m, 837 s, 706 s. ^{1}HNMR (400MHz, CD_3OD, 298K): δ 9.01 (m s, 2H, CH_{py}), 8.52 (m d, 4H, J_{HH} = 4.40, CH_{py}), 8.24 (m d, 2H, J_{HH} = 4.45, CH_{py}), 7.52 (m q, 2H, J_{HH} = 5.2, 7.6, 12.4, CH_{py}), 7.26 (s, H, CH_{pz}).

X-ray structure of 3,5-bis(3-pyridyl)-1-H-pyrazole

Crystal data for the ligand:$C_{13}H_{10}N_4$, Monoclinic, space group Cc, *M*r = 222.25 Å, *a* = 18.395(3) Å, *b* = 5.3096(9) Å, *c* = 11.993(2) Å, *β* = 109.004(3) º, *V* = 1107.5(3) $Å^3$, *Z* = 4, ρ_{cald} = 1.333 $g \cdot cm^{-3}$, *F*(000) = 464, *T* = 293(2) K, 2744 reflections collected, 979 uniq with (R_{int} = 0.0274), *R*1[I>2σ(I)] = 0.0458, *wR*2 = 0.1076 final (for all data) *R*1 = 0.0520, *wR*2 = 0.1110, GOF = 1.077. Data collection was performed on a Bruker Smart Apex CCD diffractometer (Mo-Kα, λ = 0.71073 Å).

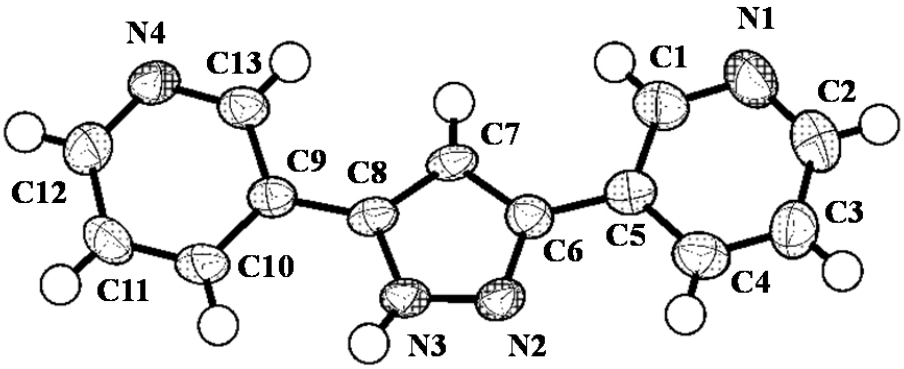

Fig. S1 XP drawing of Hbppz with the thermal ellipsoids drawn of the 30% probability level.

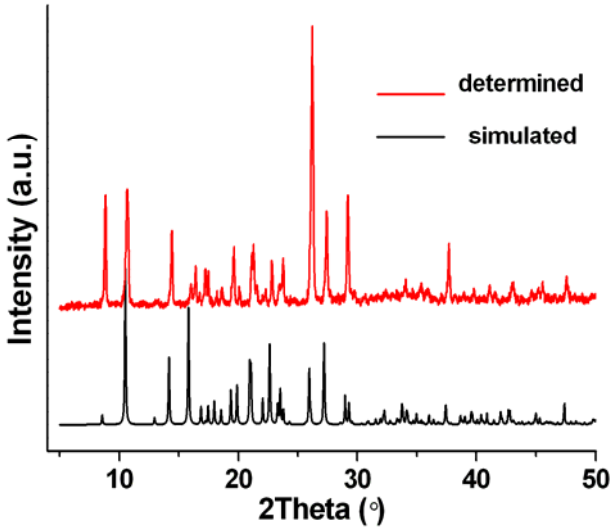

Fig. S2 Comparison of experimental XRPD (X-ray Powder Diffraction) for bulk sample to simulated pattern from single-crystal X-ray data.

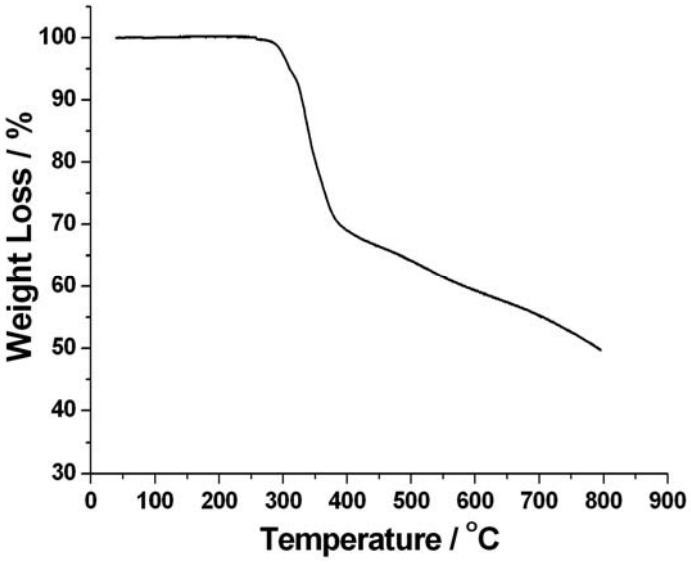

Fig. S3 TGA plot of the complex.