

Supporting information Schäfer et al. 2005

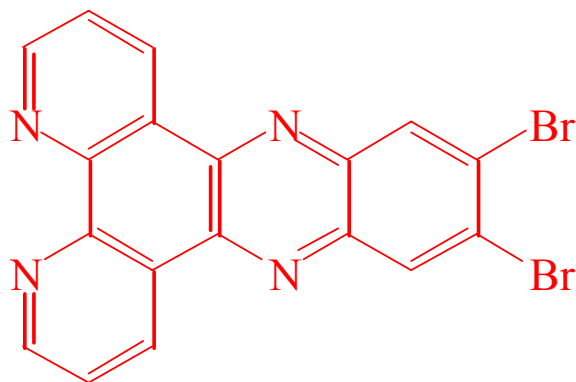
Experimental Section

General.

Unless otherwise noted, all Pd catalyzed crosscoupling reactions were conducted under an atmosphere of dry, deoxygenated argon using standard Schlenk techniques. Acetonitrile was distilled from CaH₂. Toluene was distilled from sodium benzophenone ketyl under an argon atmosphere prior to use. All other solvents were used as received.

Infrared spectra were recorded using a Perkin-Elmer 2000 FT-IR; ¹H-NMR spectra were recorded on a Bruker 400 MHz/200 Mhz spectrophotometer, UV/Visible spectra were obtained using a AnalytikJena specord S600 UV-vis. Emission spectra were recorded using a Perkin-Elmer LS50B spectrometer equipped with a Hamamatsu R928 red-sensitive detector. The mass spectra were recorded using a SSQ 170, Finigan Mat at the Friedrich Schiller University Jena. Electrospray-Mass spectra were recorded on a Finnigan MAT, MAT 95 XL. The positive ES mass spectra were obtained with voltages of 3-4kV applied to the electrospray needle. The microwave assisted reactions were carried out using a Microwave Laboratory Systems MLS EM-2 microwave system.

dppzBr₂ L1



¹H-NMR (ppm; CDCl₃)

7,730 phen(2H, dd);

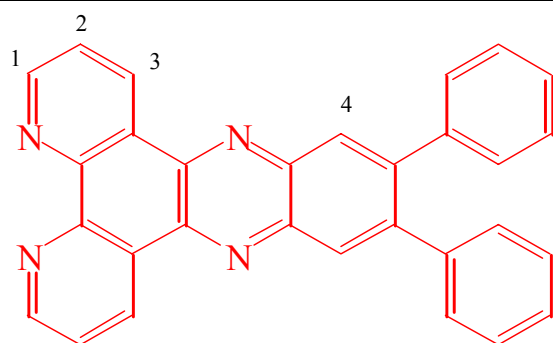
8,559 H4(2H, s);

9,233 phen(2H, d(lc));

9,529 phen(2H, d(lc));

EI-MS m/z = 440 (100%) corresponding pattern

dppz(Ph)₂ L2



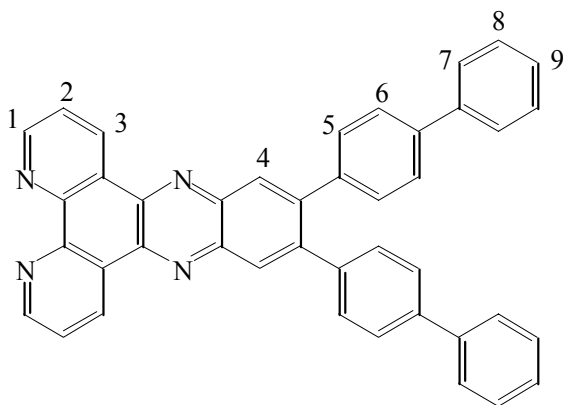
¹H-NMR

7,305 phenyl (10H, s)
7,808 H2-phen (2H, dd)
8,363 H4 (2H, s)
9,300 H3-phen (2H, d)
9,626 H1-phen (2H, d)

MS(DEI, EI +Q1MS)

m/z = 434 (100%)

dppz(BPh)₂ L3



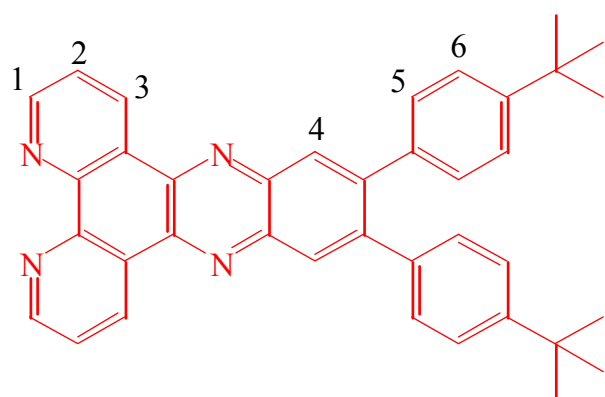
¹H-NMR (d₆-DMSO, δ = 2,485 ppm, T = 300K)

7,43 H7, H8, H9 (10H, m)
7,70 H6, H5 (8H, m)
7,91 H2(2H, dd);
8,31 H4(2H, s);
9,19 H3(2H, d(lc));
9,44 H1(2H, d(lc));

MS(DEI, EI +Q1MS)

m/z = 586 (100%)

dppz(TBPh)₂ L4



C₃₈H₃₄N₄
546,704
C 83,48; H 6,27; N 10,25

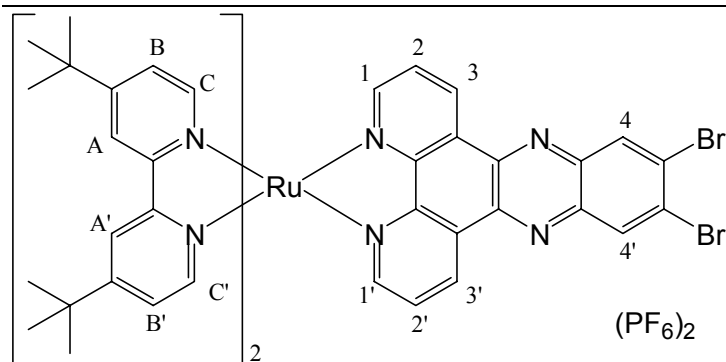
¹H-NMR (CD₂Cl₂, δ = 5,336 ppm, T = 300°C)

1,321 CH₃ (tert.-butyl, 18H, s)
7,325 H₆, H₅(8H, m);
7,794 H₃ (2H, dd);
8,361 H₄ (2H, s);
9,215 H₃ (2H, d(lc));
9,622 H₁ (2H, d(lc));

MS(DEI, EI +Q1MS LMR UP LR)

m/z = 546 (30%), m/z = 531 (35%), m/z = 475 (35%)

(tbbpy)₂Ru(dppz(Br)₂) RuL1

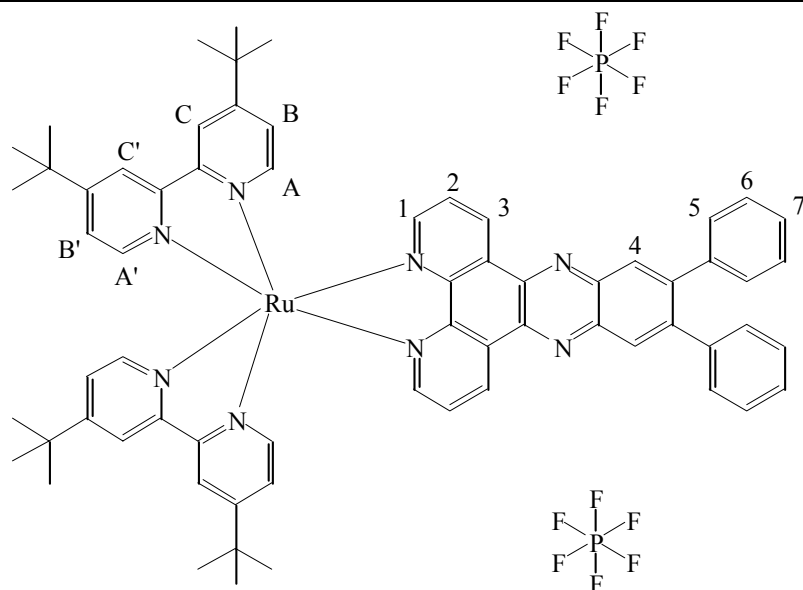


CD₃CN 400MHz]

1,347 CH₃bpy (tert.-butyl, 18H, s)
1,441 CH₃bpy (tert.-butyl, 18H, s)
7,233 HBbpy (2H, d);
7,466 HB'bpy (2H, d);
7,565 HA bpy (2H, d);
7,659 HA'bpy (2H, d);

7,888 H2phen (2H, dd);
8,143 H3phen (2H,d);
8,476 HC bpy (2H, s);
8,515 HC' bpy (2H, s);
8,844 H4 (2H, s);
9,556 H1phen (2H, d);

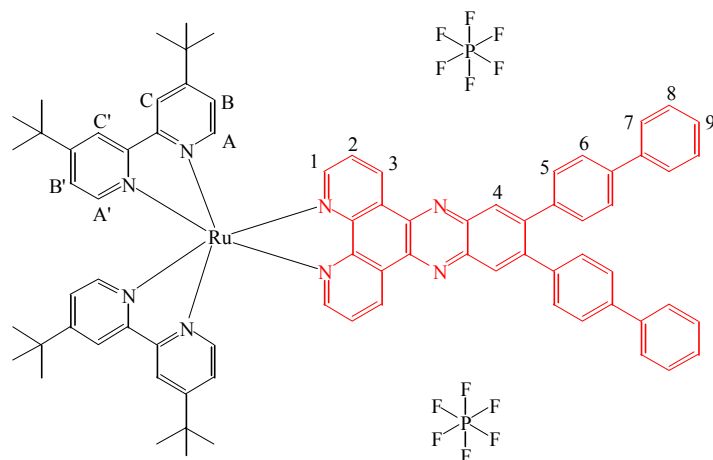
(tbbpy)₂Ru(dppz(Ph)₂) RuL2



¹H-NMR (d₃-CD₃CN, δ = 1,943 ppm, T = 300K)

1,327 CH₃(tert.-butyl, 18H, s)
1,434 CH₃(tert.-butyl, 18H, s)
7,256 HB' (2H, d(lc))
7,353 H5, H6, H7 (10H, m);
7,475 HB (2H, d(lc))
7,620 HA' (2H, d);
7,694 HA (2H, d);
7,896 H2 (2H, dd);
8,146 H3 (2H, d(lc));
8,422 H4 (2H, s);
8,512 HC' (2H, s);
8,551 HC (2H, s);
9,589 H1 (2H, d);

(tbbpy)₂Ru(dppz(BPh)₂) RuL3



¹H-NMR (d₃-CD₃CN, δ = 1,930 ppm, T = 300 K)

[Dez07-2004, EXPNO 30, 400MHz]

1,277 CH₃(tert.-butyl, 18H, s)

1,471 CH₃(tert.-butyl, 18H, s)

7,412 H₇, H₈, H₉ (10H, m)

7,211 H₆ (4H, d);

7,272 H₅ (4H, d)

7,348 H_{B'} (2H, d);

7,522 H_B (2H, d);

7,772 H_A, H_{A'} (4H, d);

7,799 H₂ (2H, dd);

7,968 H₄ (2H, s);

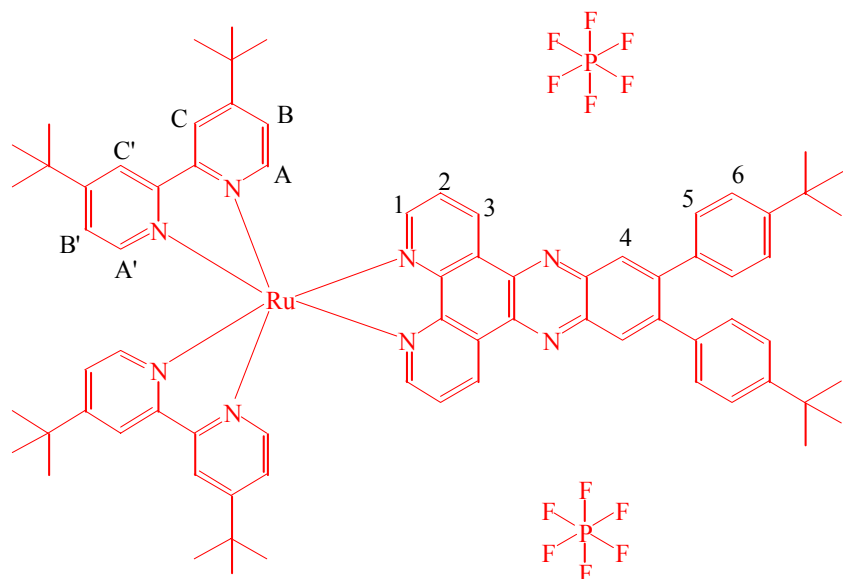
8,241 H₃ (2H, d);

8,571 H_C (2H, s);

8,639 H_{C'} (2H, s);

9,175 H₁ (2H, d);

(tbbpy)₂Ru(dppz(TBPh)₂) RuL₄



¹H-NMR (CD₃CN, δ = 1,949 ppm, T = 300K)

1,312 CH₃(tert-butyl, 18H, s)
1,329 CH₃(tert-butyl, 18H, s)
1,468 CH₃(tert-butyl, 18H, s)

7,228 H₆, H₅(8H, m);
7,328 H_{B'} (2H, d(lc));
7,505 H_B (2H, d(lc));
7,703 H_{A'} (2H, d);
7,736 H_A (2H, d);
7,774 H₂ (2H, dd);
8,031 H₄ (2H, s);
8,161 H₃ (2H, (lc));
8,517 H_{C'} (2H, s);
8,566 H_C (2H, s);
9,268 H₁ (2H, d(lc));