Supporting Information

Terpyridine-fused Polyaromatic Hydrocarbons generated via Cyclodehydrogenation and used as Ligands in Ru(II) Complexes

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Table S1. Crystal Data and Structure Refinement Details for 1-(2,2':6',2"-terpyrid-4'-yl)-2,3,4,5,6-pentaphenylbenzene (**1**).

	1.3$CHCl_3$	
Empirical formula	C54 H38 Cl9 N3	
Formula weight	1047.92	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 11.5279(5) Å	α = 90
	b = 17.3151(8) Å	β = 95.0820
	c = 25.3288(12) Å	γ = 90
Volume	5035.9(4) $Å^3$	
Z	4	
Density (calculated)	1.382 g/cm^3	
Absorption coefficient	0.541 mm^{-1}	
F(000)	2144	
Crystal size	0.39 x 0.38 x 0.27 mm^3	
Theta range for data collection	1.61 to 26.50°.	
Index ranges	-14<=h<=14, -21<=k<=21, -31<=l<=29	
Reflections collected	44768	
Independent reflections	10440 [R(int) = 0.0285]	
Completeness to theta = 26.50°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8678 and 0.8169	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10440 / 0 / 595	
Goodness-of-fit on F^2	1.035	
R_1 [I>sigma(I)]	0.0595	
wR_2 (all data)	0.1707	

[a] $R_1 = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma wF_o^2]^{1/2}$; goodness of fit = $\{\Sigma[w(F_o^2 - F_c^2)^2/(N_{obs} - N_{param}\}^{1/2}$; $w = [\sigma^2(F_o^2) + (g_1P)^2 + g_2P]^{-1;}$ $P = [\max(F_o^2;0) + 2F_c^2]/3$.

Table S2. Crystal Data and Structure Refinement Details for 1-(2,2':6',2"-terpyrid-4'-yl)-2,3,4,5,6-penta-(4-*tert*-butylphenyl)benzene (**2**).

	2.2CH_2Cl_2	
Empirical formula	C73 H79 Cl4 N3	
Formula weight	1140.19	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.2579(7) Å	α = 66.3110
	b = 16.5216(9) Å	β = 70.3760
	c = 18.2312(10) Å	γ = 76.7660
Volume	3165.7(3) $Å^3$	
Z	2	
Density (calculated)	1.196 g/cm^3	
Absorption coefficient	0.231 mm^{-1}	
F(000)	1212	
Crystal size	0.45 x 0.37 x 0.20 mm^3	
Theta range for data collection	1.77 to 26.00°.	
Index ranges	-15<=h<=15, -20<=k<=20, -22<=l<=22	
Reflections collected	31713	
Independent reflections	12437 [R(int) = 0.0297]	
Completeness to theta = 26.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.7814	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12437 / 0 / 721	
Goodness of fit on F2	1.076	
R_1 [I>sigma(I)]	0.0801	
wR_2 (all data)	0.2070	

[a] $R_1 = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma wF_o^2]^{1/2}$; goodness of fit = $\{\Sigma[w(F_o^2 - F_c^2)^2/(N_{obs} - N_{param}\}^{1/2}$; $w = [\sigma^2(F_o^2) + (g_1P)^2 + g_2P]^{-1;}$ $P = [\max(F_o^2;0) + 2F_c^2]/3$.

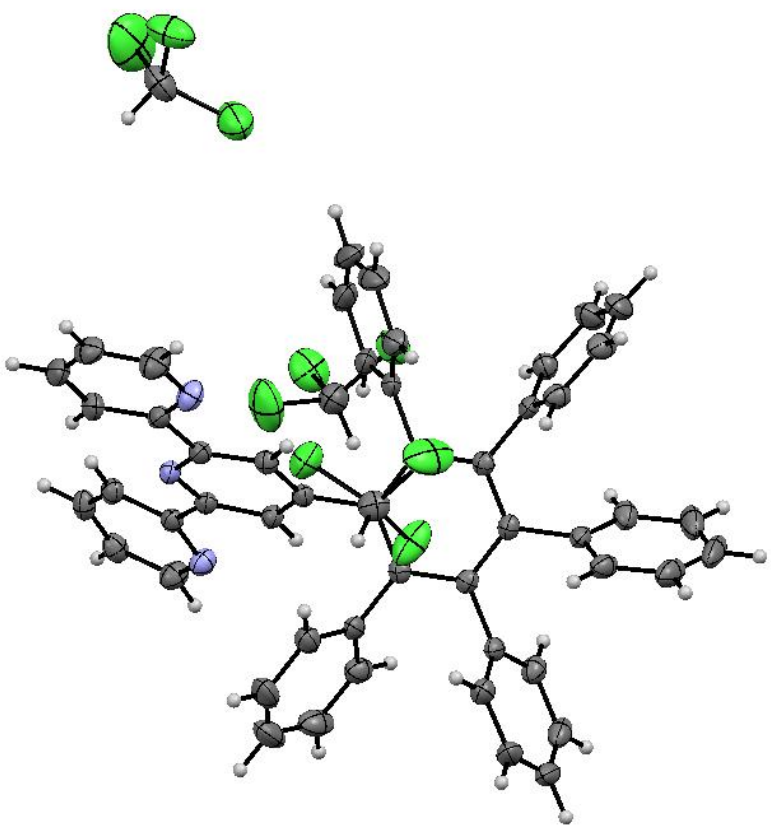

Figure S1. ORTEP diagram showing molecular structure of 1-(2,2':6',2"-Terpyrid-4'-yl)-2,3,4,5,6-pentaphenylbenzene (**1**). Ellipsoids are drawn at 50% probability level.

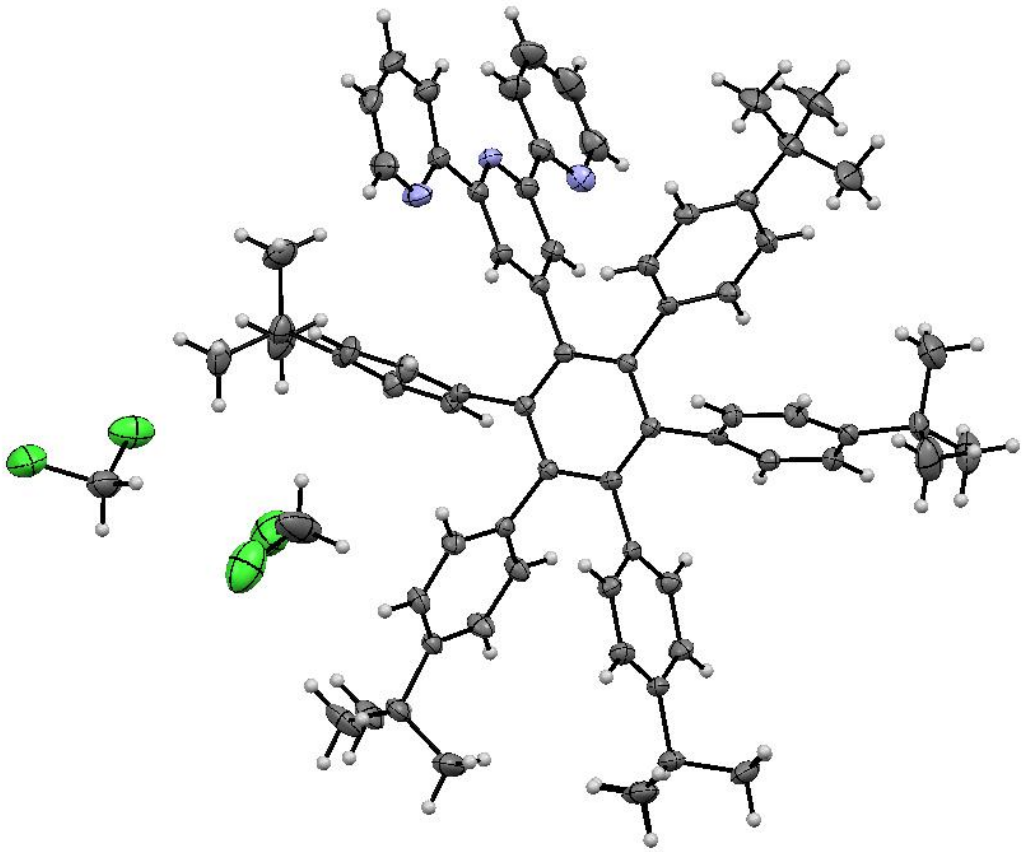

Figure S2. ORTEP diagram showing molecular structure of 1-(2,2':6',2"-Terpyrid-4'-yl)-2,3,4,5,6-penta-(4-*tert*-butylphenyl)benzene (**2**). Ellipsoids are drawn at 50% probability level.

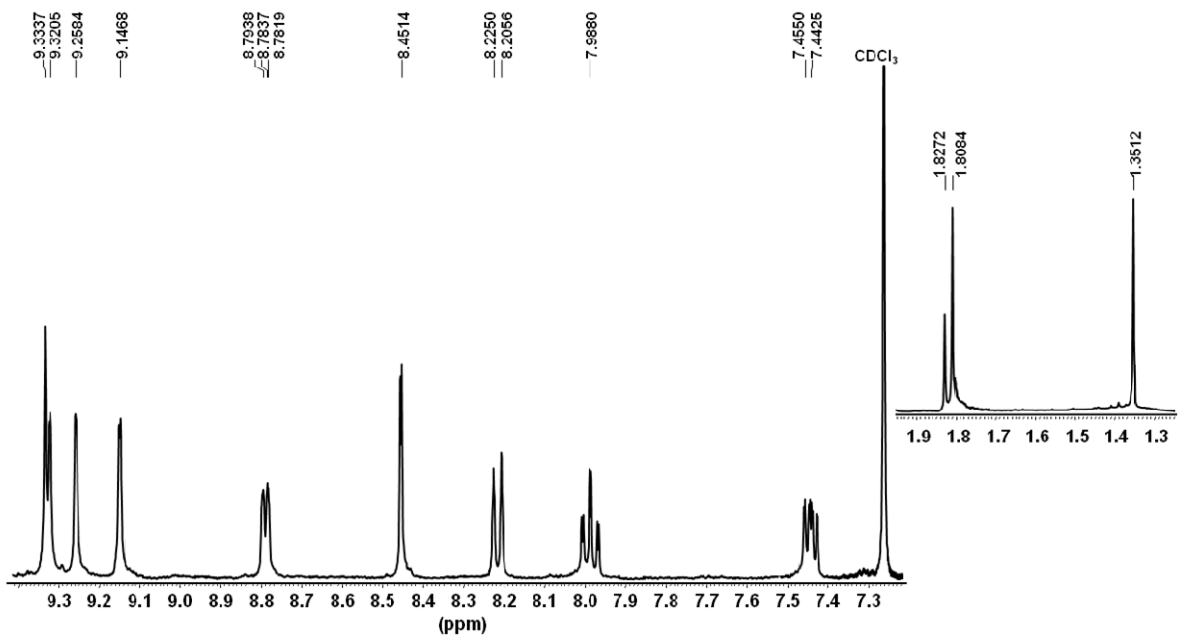

Figure S3. ^{1}H NMR Spectrum of **4** ($CDCl_3$) showing the aromatic region with inset portion of aliphatic region.

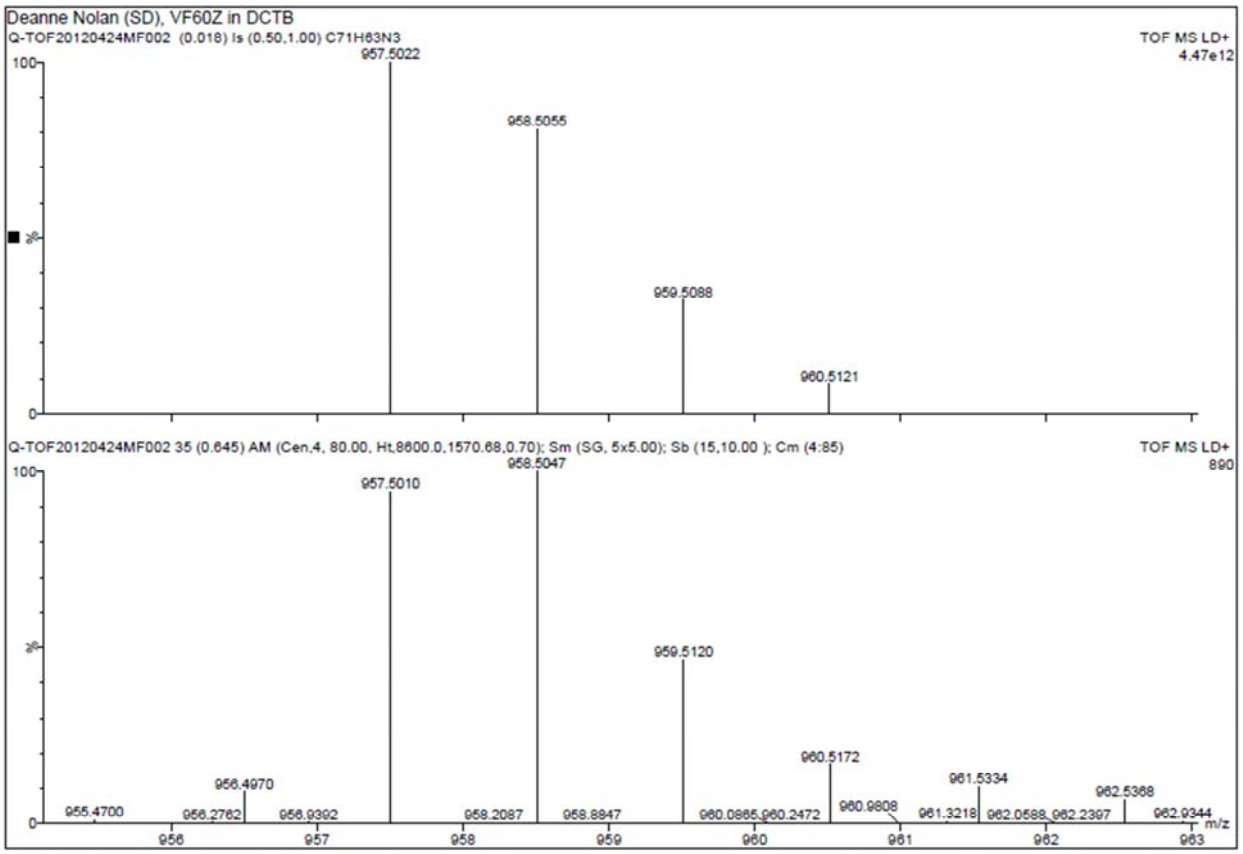

Figure S4. The experimental (+)-MALDI-TOF spectra of **4** (lower spectrum) and the simulated isotopic distribution pattern for ($M^{+\bullet}$) (DCTB matrix, upper spectrum).

Additional ^{1}H NMR Spectra:

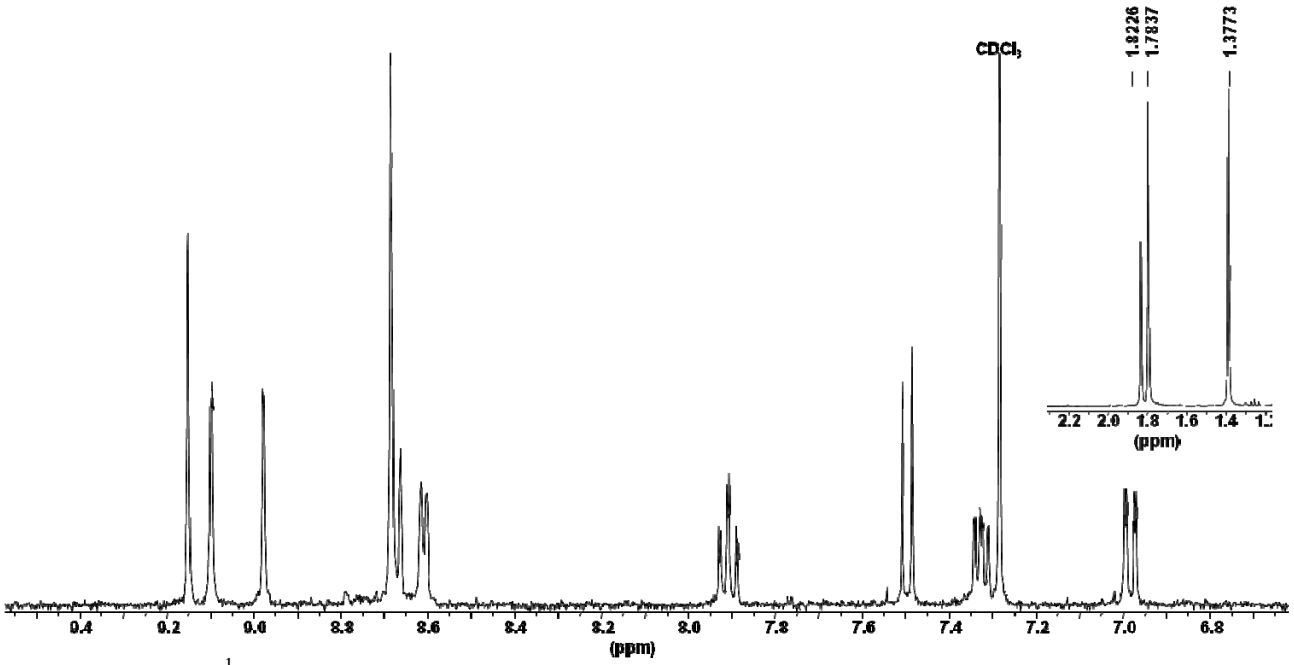

Figure S5. ^{1}H NMR Spectrum of **3** ($CDCl_3$) showing the aromatic region with inset portion of aliphatic region.

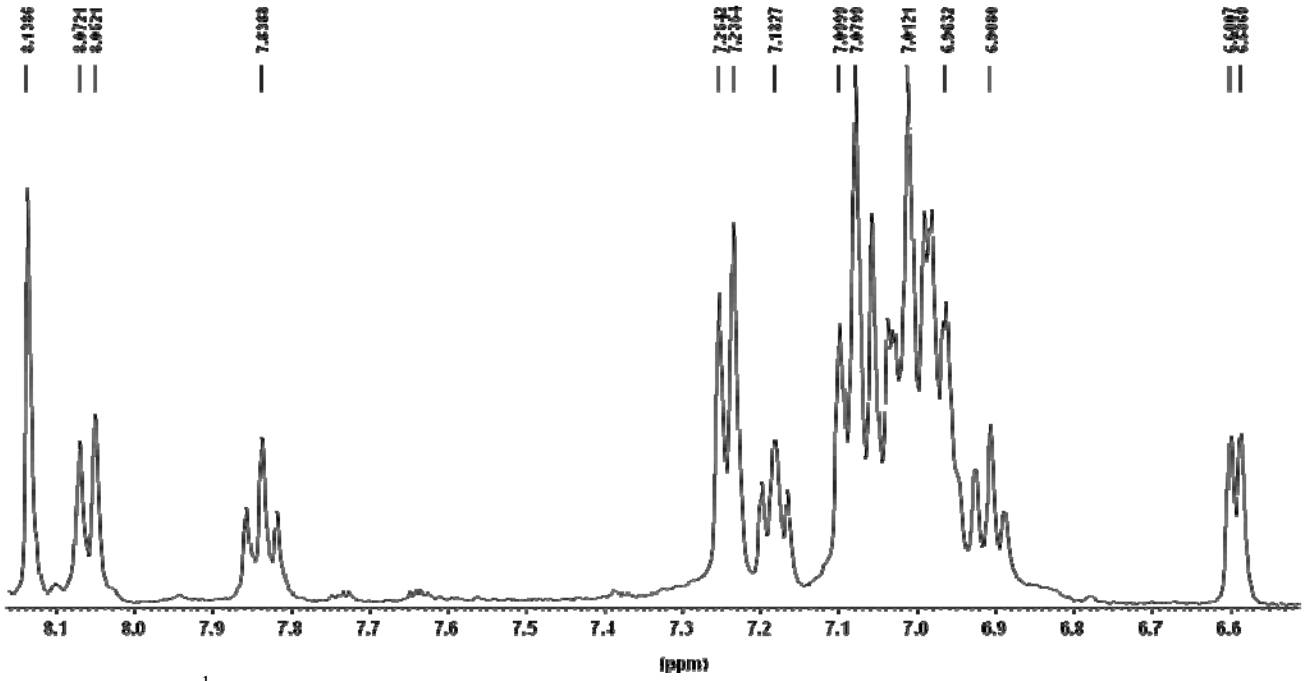

Figure S6. ^{1}H NMR Spectrum of **6** (CD_3CN) showing the aromatic region.

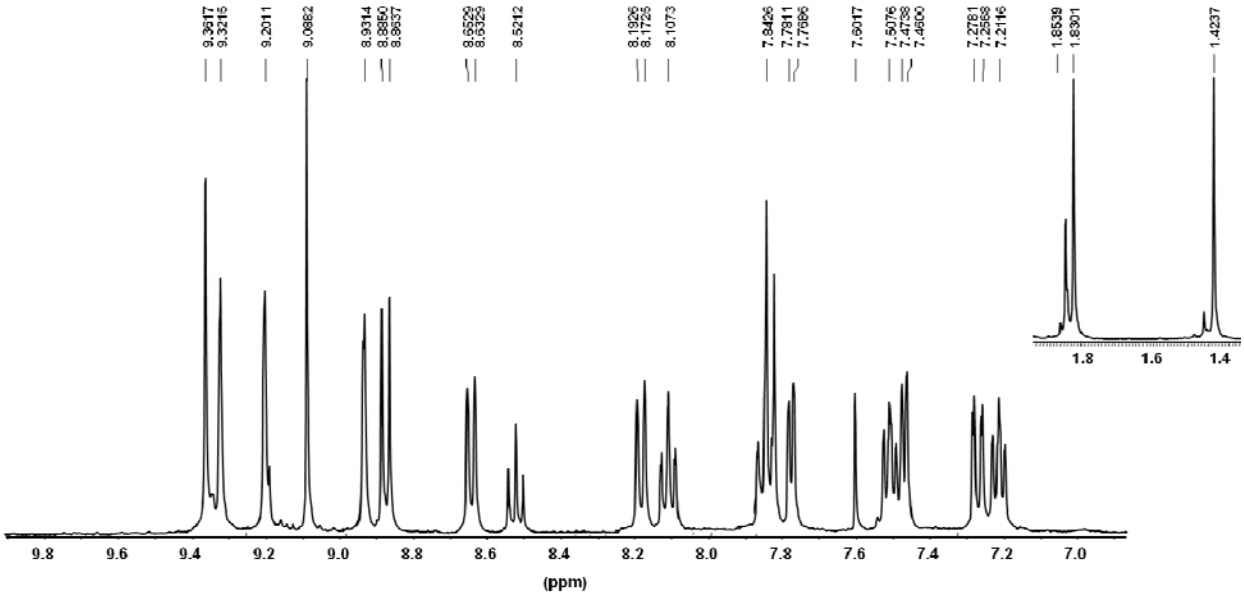

Figure S7. ^{1}H NMR Spectrum of **8** (CD_3CN) showing the aromatic region with inset portion of aliphatic region.