Supporting Information For: A DFT Based Assay for Tailor-made Terpyridine Ligand-Metal Complexation Properties.

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Supp-Tab. 1: M-N Bond Lengths (Å), Dihedral angle and N-M-N bond angles (in degrees) in Functionalized TPy-M Complexes. The Corresponding Geometrical Parameters in Unfunctionalized TPy-M Complexes are also Given for Comparison.

Metal		EDGs					EWGs			
Geometric Parameters		TPy-M	CH ₃	C ₆ H ₅	OCH ₃	NH ₂	CF ₃	CN	COOH	NO ₂
Co	M-N	1.94	1.935	1.934	1.930	1.943	1.931	1.928	1.935	1.927
	M-N'	1.85	1.851	1.851	1.853	1.858	1.851	1.851	1.852	1.850
	M-N''	1.94	1.935	1.933	1.939	1.949	1.931	1.928	1.934	1.927
	Dihedral Angle	-30.31	-8.48	-0.32	-0.42	-31.40	-3.78	-0.58	2.06	23.54
Ru	M-N	2.040	2.044	2.053	2.040	2.070	2.048	2.045	2.048	2.047
	M-N'	1.979	1.980	1.979	1.953	1.939	1.981	1.981	1.981	1.982
	M-N''	2.070	2.064	2.051	2.096	2.070	2.047	2.046	2.046	2.046
	Dihedral Angle	0.90	3.25	4.72	6.37	1.13	0.96	-1.07	3.89	-0.80
Fe	M-N	2.00	1.951	1.956	1.952	1.949	1.952	1.954	1.956	1.953
	M-N'	1.88	1.901	1.903	1.894	1.889	1.903	1.902	1.903	1.903
	M-N''	1.94	1.976	1.963	1.985	1.990	1.960	1.954	1.955	1.953
	Dihedral Angle	2.65	-1.91	0.68	1.41	-5.98	1.20	-2.18	-1.25	-0.78
Mo	M-N	2.096	2.100	2.130	2.139	2.133	2.093	2.151	2.177	2.143
	M-N'	2.087	2.081	2.055	2.045	2.044	2.08	2.078	2.133	2.060
	M-N''	2.094	2.094	2.159	2.154	2.152	2.10	2.150	2.177	2.187
	Dihedral Angle	1.07	-8.10	16.70	21.77	19.14	9.01	0.66	-0.41	14.32
Au	M-N	2.625	2.801	2.80	2.597	2.771	2.784	2.807	2.765	2.791
	M-N'	2.235	2.240	2.158	2.240	2.162	2.156	2.154	2.148	2.155
	M-N''	2.595	2.784	2.782	2.603	2.793	2.784	2.802	2.993	2.823
	Dihedral Angle	-80.84	-133.74	-134.60	2.46	-137.03	-137.98	137.00	-140.67	-140.24

Supp-Tab. 2: BSSE Corrected Binding Energies (kcal/mol) of Unfunctionalized and Functionalized Terpyridine-Metal Complexes.

Metals		EDGs				EWGs			
	M-tpy	CH ₃	C ₆ H ₅	OCH ₃	NH ₂	CF ₃	CN	COOH	NO ₂
Co	-86.03	-87.97	-78.56	-61.49	-96.13	-82.95	-82.39	-84.96	-85.96
Ru	-94.69	-93.62	-94.65	-34.32	-97.26	-87.85	-90.23	-94.62	-94.18
Fe	-68.52	-69.96	-78.62	-57.54	-72.91	-65.76	-67.64	-65.69	-66.01
Mo	-87.85	-93.56	-95.70	-79.57	-96.26	-84.46	-85.46	-92.05	-91.68
Au	-37.71	-41.28	-41.48	-24.03	-42.86	-38.03	-37.46	-30.05	-37.33

Supp-Tab. 3: Comparison of Hirshfeld (black) and NPA(red) charges for NO₂ Functionalized TPy-M Complexes (M=Co, Fe, Ru, Mo, Au)

Metals/Atom center		Co		Ru		Fe		Mo		Au	
		Co	NO ₂	Ru	NO ₂	Fe	NO ₂	Mo	NO ₂	Au	NO ₂
M	Hirshfeld	-0.008	-0.020	0.101	-0.277	-0.071	0.076	0.443	0.445	0.796	0.789
	NPA	-0.050	-0.088	0.226	0.225	0.330	0.367	0.488	0.501	0.398	0.406
N	Hirshfeld	-0.007	-0.001	-0.035	0.021	-0.004	-0.004	-0.055	-0.063	-0.139	-0.143
	NPA	-0.230	-0.218	-0.125	-0.124	-0.126	-0.127	-0.164	-0.166	-0.336	-0.334
N'	Hirshfeld	-0.018	-0.019	-0.037	0.008	-0.007	-0.010	-0.080	-0.069	-0.091	-0.092
	NPA	-0.211	-0.209	-0.127	-0.127	-0.117	-0.119	-0.179	-0.171	-0.322	-0.336
N''	Hirshfeld	-0.008	0.001	-0.035	0.021	-0.006	-0.004	-0.053	-0.069	-0.138	-0.143
	NPA	0.232	-0.218	-0.130	-0.124	-0.134	-0.127	-0.171	-0.173	-0.338	-0.334
Cl(Metal)	Hirshfeld	-0.868	-0.814	-0.813	-0.606	-0.775	-0.865	-0.886	-0.681	-1.112	-1.028
	NPA	-0.945	-0.874	-0.151	-0.091	-0.269	-0.208	-0.173	-0.088	-0.834	-0.793
Cl(TPy)	Hirshfeld	-0.024	-0.006	-0.026	-0.020	-0.023	-0.019	-0.048	-0.019	-0.021	0.003
	NPA	0.050	0.071	0.028	0.040	0.027	0.038	0.014	0.030	0.054	0.080
Net Charge gained by NO ₂	Hirshfeld	-	-0.201	-	-0.230	-	-0.210	-	-0.279	-	-0.219
	NPA	-	-0.330	-	-0.201	-	-0.195	-	-0.216	-	-0.340
Net Charge lost by pyridine C-atoms	Hirshfeld	-	0.063	-	0.225	-	0.140	-	0.055	-	0.115
	NPA	-	0.540	-	0.271	-	0.231	-	0.257	-	0.562

Supp-Fig. 1: Molecular orbitals of unfunctionalized TPy-M complexes.

EDGs-TPy-Ru

CH₃-TPy-Ru CF₃-TPy-Ru C₆H₅-TPy-Ru

CN-TPy-Ru

OCH₃-TPy-Ru

COOH-TPy-Ru

NH₂-TPy-Ru NO₂-TPy-Ru

Supp-Fig. 2: Optimized EDG and EWG functionalized TPy-Ru complexes.

Supp-Fig. 3: Super imposed images of unfunctionalized TPy-Co and NO₂ functionalized TPy-Co complexes

Supp-Fig. 4: Molecular Orbitals of EDG Functionalized TPy-Co Complexes.

Supp-Fig. 5: Electrostatic Potentials of EDG Functionalized TPY-Co Complexes.