Supporting Information for the Manuscript

"Effects Induced by Axial Ligands Binding to Tetrapyrrole-Based Aromatic Metallomacrocycles"

Yang Yang

Department of Chemistry, Case Western Reserve University, Cleveland, Ohio 44106

yxy130@case.edu

Table S1. Selected Bond Lengths of MgPc, $[MgPc]^+$, and $[MgPc]^-$

bond[a]	MgPc	$[MgPc]^+$	$[MgPc]^-$	
$Mg\text{-}N_p$	2.008	2.002	2.008	2.019
$N_p\text{-}C_\alpha$	1.372	1.373	1.381	1.374
$C_\alpha\text{-}N_m$	1.334	1.334	1.319	1.357
$C_\alpha\text{-}C_\beta$	1.462	1.466	1.470	1.443
$C_\beta\text{-}C_\gamma$	1.395	1.390	1.394	1.403
$C_\beta\text{-}C_\beta$	1.413	1.411	1.411	1.426
$C_\gamma\text{-}C_\delta$	1.394	1.401	1.396	1.389
$C_\delta\text{-}C_\delta$	1.408	1.402	1.406	1.416

[a]The lettering scheme is given below.

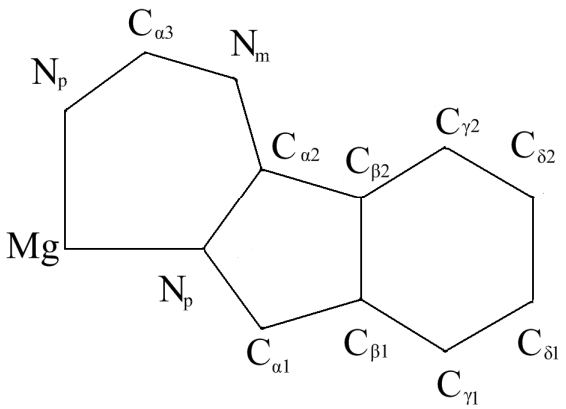

Table S2. Charges from Electrostatic Potentials using a Grid based method (CHELPG charges)

MMc	ligand		M	Mc	L	N_{Mc}	N_L	X[a]
MgPc		**1**	0.995	-0.995		-0.603		
MgPc	py[b]	**1a**	0.765	-0.911	0.146	-0.510	-0.305	
MgP		**2**	0.947	-0.947		-0.570		
MgP	py	**2a**	0.592	-0.732	0.140	-0.403	-0.267	
MgTAP		**3**	1.085	-1.085		-0.748		
MgTAP	py	**3a**	0.921	-1.048	0.127	-0.687	-0.352	
MgTBP		**4**	0.774	-0.774		-0.331		
MgTBP	py	**4a**	0.639	-0.773	0.134	-0.330	-0.232	
MgNc		**5**	1.031	-1.031		-0.624		
MgNc	py	**5a**	0.893	-1.017	0.124	-0.583	-0.343	
BePc		**6**	0.803	-0.803		-0.573		
BePc	py	**6a**	0.721	-0.899	0.178	-0.542	-0.197	
AlPcCl		**10**	1.081	-0.602		-0.547		-0.479
AlPcCl	py	**10a**	1.610	-1.119	0.092	-0.724	-0.262	-0.583
AlPcF		**11**	1.457	-0.889		-0.684		-0.568
AlPcF	py	**11a**	1.765	-1.146	0.040	-0.718	-0.337	-0.659

[a]X; halogen. [b]Pyridine.

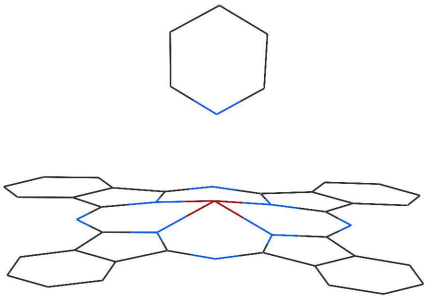

Figure S1. a) The structure of magnesium phthalocyanine bound by pyridine, **1a**.

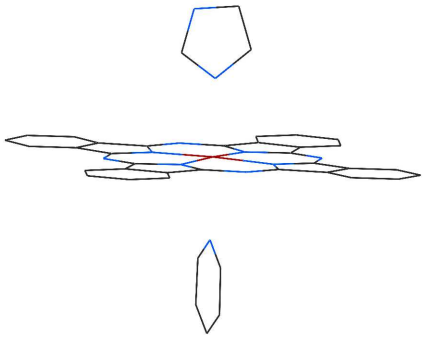

Figure S1. b) The structure of magnesium phthalocyanine bound by a pyridine and an imidazole, **1f**.

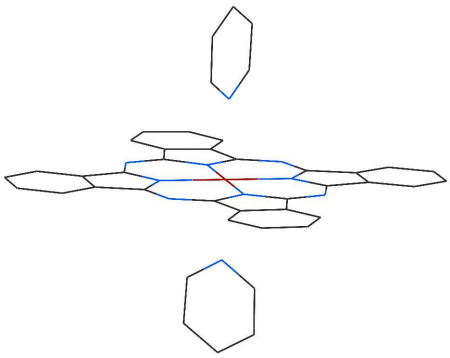

Figure S1. c) The structure of magnesium phthalocyanine bound by two pyridines, **1g**.

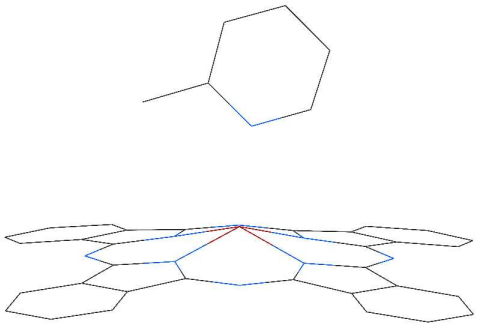

Figure S2. a) The structure of magnesium phthalocyanine bound by 2-picoline, **1b**.

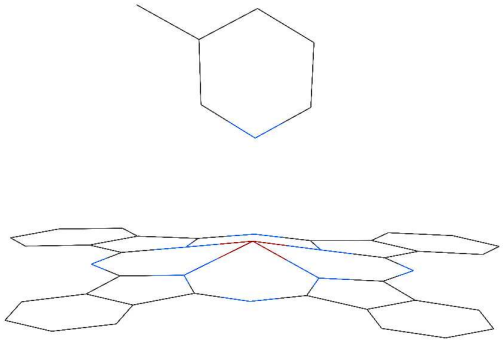

Figure S2. b) The structure of magnesium phthalocyanine bound by 3-picoline.

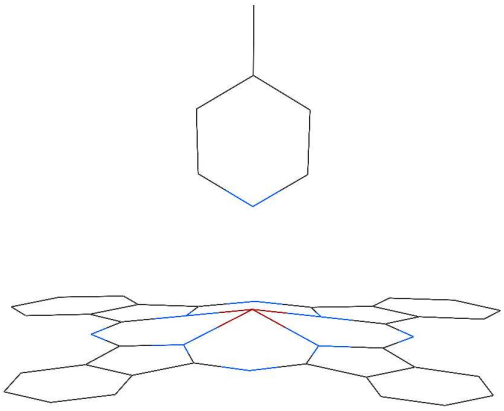

Figure S2. c) The structure of magnesium phthalocyanine bound by 4-picoline.

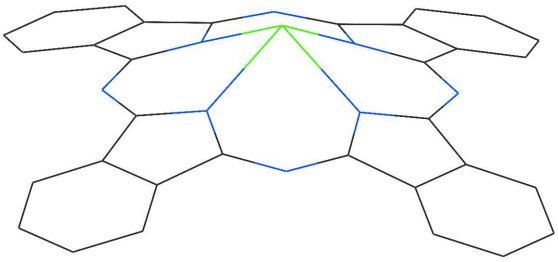

Figure S3. a) The structure of bare calcium phthalocyanine, **9**.

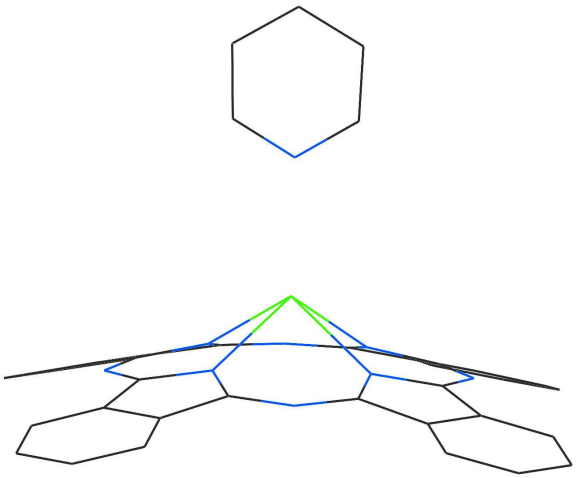

Figure S3. b) The structure of calcium phthalocyanine bound by one pyridine ligand, **9a**.

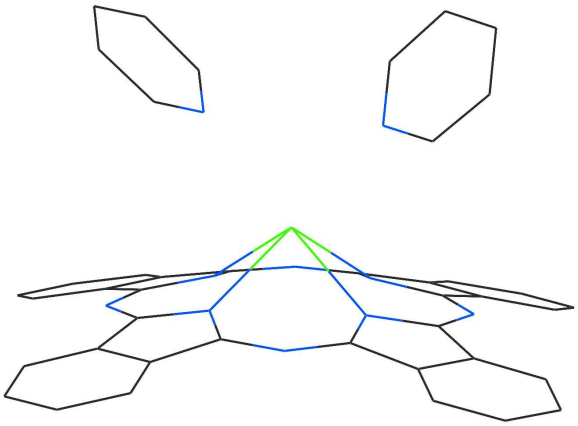

Figure S3. b) The structure of calcium phthalocyanine bound by two pyridine ligands, **9b**.

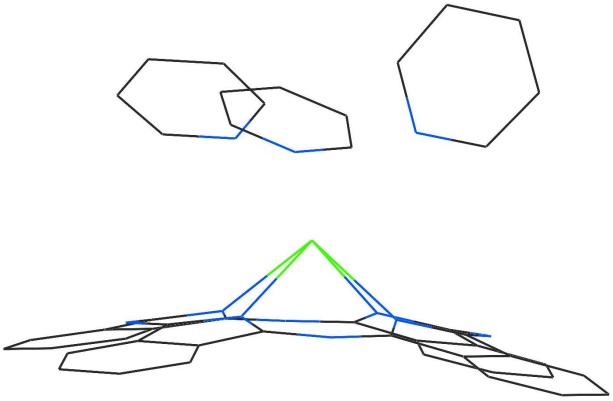

Figure S3. b) The structure of calcium phthalocyanine bound by three pyridine ligands, **9c**.

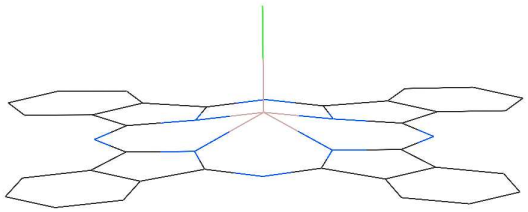

Figure S4. a) The structure of aluminum phthalocyanine chloride, **10**.

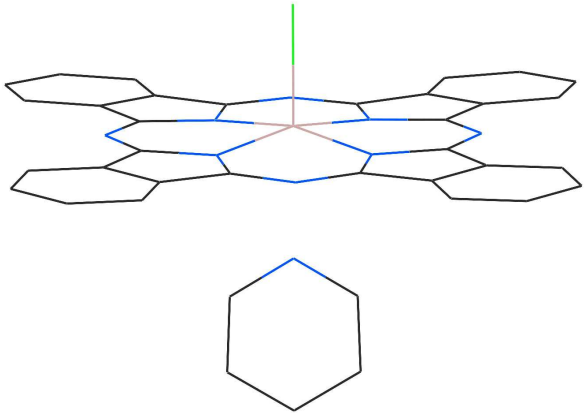

Figure S4. b) The structure of aluminum phthalocyanine chloride bound by a pyridine ligand, **10a**.

Complete Reference for Gaussian 09:

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision A.2, Gaussian, Inc., Wallingford CT, 2009.