Supplementary Material (ESI) for New Journal of Chemistry

Hydroxybenziphthalocyanines: Non-aromatic phthalocyanine analogs that exhibit strong UV-visible absorptions

Roshinee Costa[a], Andrew J. Schick[b], Nathan B. Paul[b], William S. Durfee[b] and Christopher J. Ziegler[a]

[a] *Department of Chemistry, University of Akron, Akron, OH 44325-3601 USA. Fax: (330) 972-7370; Tel: (330) 972-2531 ; E-mail: ziegler@uakron.edu*

[b] *Department of Chemistry, Buffalo State College, 1300 Elmwood Avenue, Buffalo, NY 14222-1095*

Supporting Information

X-ray crystallographic details

Structure of compound **4**: The asymmetric unit of **4** is shown in Figure S3. The compound crystallizes in the P-1 space group. There are three pyridine molecules associated with compound 4 in the asymmetric unit. Two of these pyridine solvates are engaged in hydrogen bonding to the resorcinol hydroxides with O-N distances of 2.622(3) and 2.740(3) Å. These hydrogen bonding interactions are shown in Figure S4. As in previously published structures of benziphthalocyanine, the ionizable hydrogen atoms on the nitrogen atom positions were located on the difference map; two are on the peripheral nitrogen atoms adjacent to the benzene ring, and one is on the internal isoindoline nitrogen across from the benzene ring.

Structure of compound **5**. The asymmetric unit is shown in Figure S5. This compound crystallizes in the P-1 space group. In addition to compound **5**, there are two methanol solvent molecules that engage in hydrogen bonding to the compound and two disordered solvent water molecules with partial occupancy. The occupancy for these two water molecules are approximately 65 and 20% respectively.

Compound **5** engages in hydrogen bonding with the two methanol solvate molecules via both NH-O and OH-N interactions. Figure S6 shows these two hydrogen bonding interactions. One methanol solvent is encapsulated in compound **5**, with hydrogen bond distances of 2.739(3) and 2.722(3) Å for the NH-O and OH-N interactions respectively. The second methanol is engaged in hydrogen bonding with the terminal Schiff base nitrogens, with distances of 2.781(3) and 2.986(3) Å for the NH-O and OH-N interactions respectively.

Structure of compound **7**: The asymmetric unit of compound **7** is shown in Figure S7. This compound crystallizes in the $Pna2_1$ space group, and the asymmetric unit contains the Schiff base molecule plus two equivalents of pyridine. Hydrogen atoms were observed on the resorcinolic hydroxide groups, and on the terminal isoindoline nitrogen positions.

There are three types of hydrogen bonding interactions observed in this structure. First, intramolecular hydrogen bonds are observed between the resorcinolic hydroxide groups and the central isoindoline nitrogens that have OH-N distances of 2.509(4) and 2.487(4) Å. In addition, there are long hydrogen bonding interactions between the solvent pyridine molecules and the terminal isoindoline Schiff base nitrogens that measure 2.938(4) and 2.874(4) Å. Both of these hydrogen bonding interactions are shown in Figure S8. Lastly, we also observe some weak hydrogen bonding interactions between equivalents of compound **7**. These interactions take place between the terminal Schiff base nitrogens and the resorcinolic hydroxide groups, and the NH-O interactions measure 2.908(4) and 2.822(4) Å in distance.

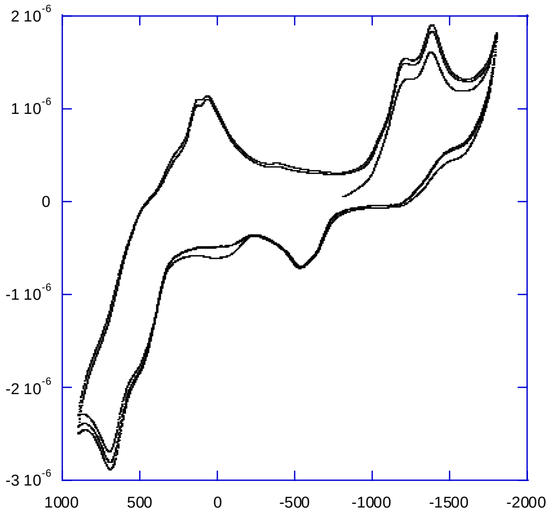

Figure S1. Cyclic voltammetry of **3** (left) and **4** (right) in DMSO/0.2 M [*n*-Bu_4N][PF_6] recorded using gold working electrode. Potentials are referenced to a Ag/AgCl (THF/0.2 M [*n*-Bu_4N][PF_6])nonaqueous reference electrode.

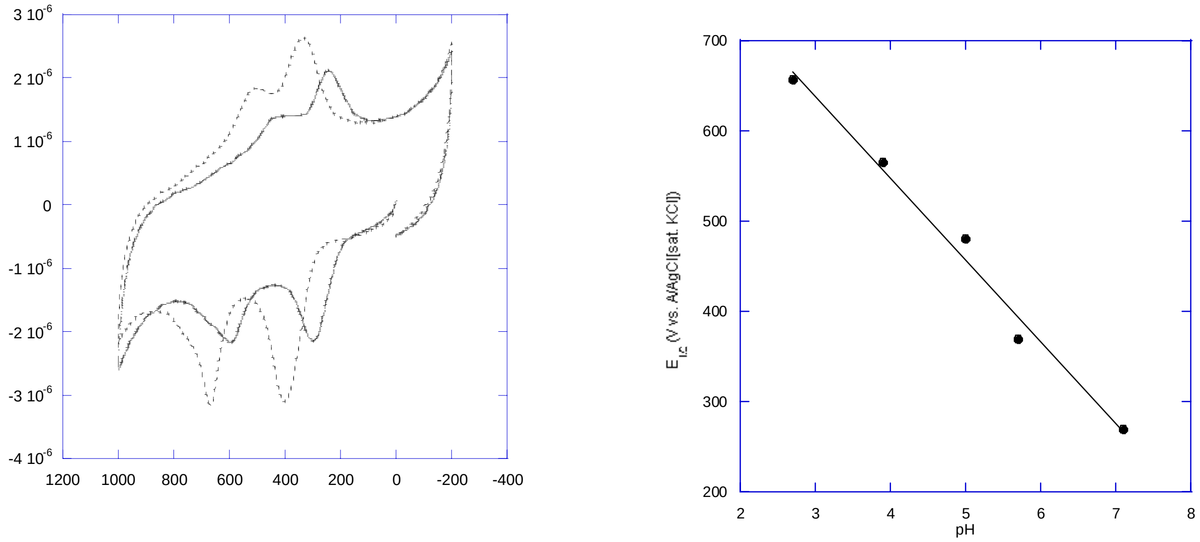

Figure S2. Left: The cyclic voltammetry of **3** adsorbed on a glassy carbon working electrode recorded in aqueous buffer. Voltammograms for pH 6 (dashed line) and pH 7 (solid line) are shown. Potentials are reported versus an aqueous Ag/AgCl (sat. KCl) reference electrode. Right: $E_{1/2}$ as a function of pH. The slope of the least-squares line is -90 mV/pH.

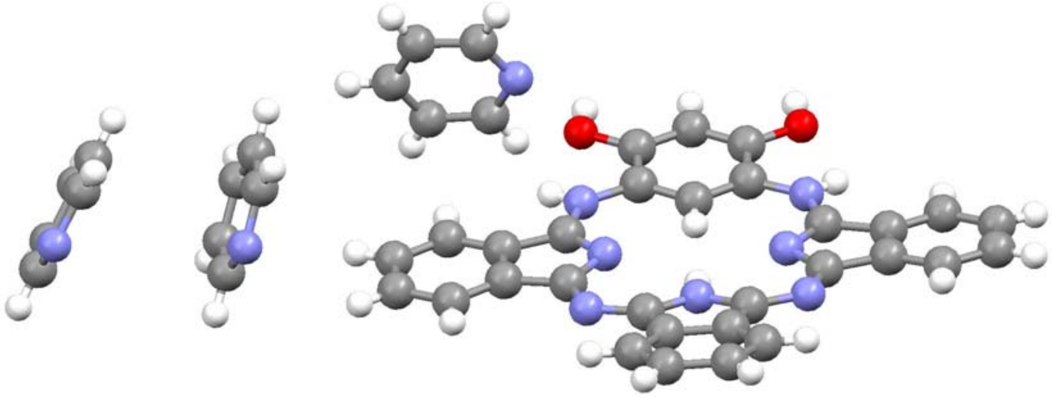

Figure S3. The asymmetric unit of compound **4**.

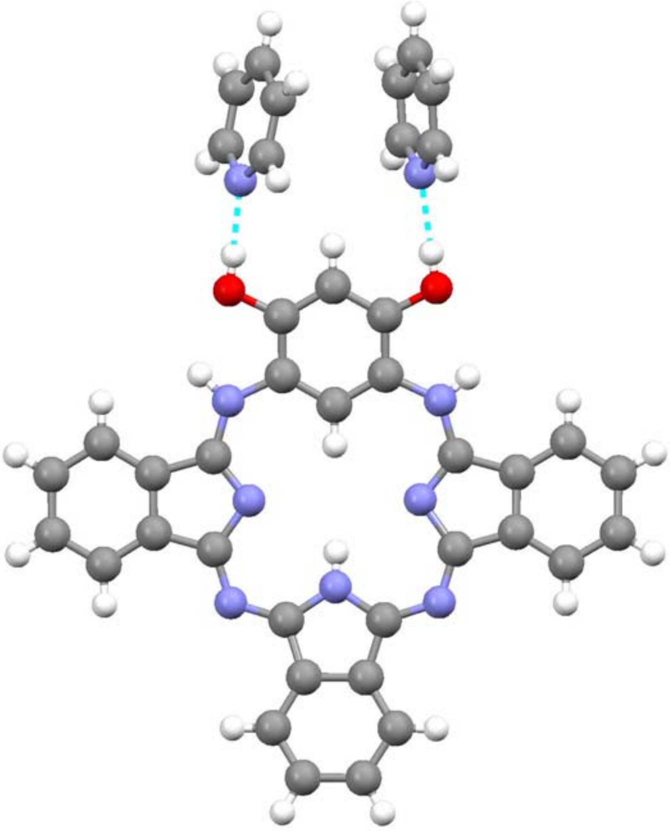

Figure S4. Hydrogen bonding interactions observed in the structure of **4**.

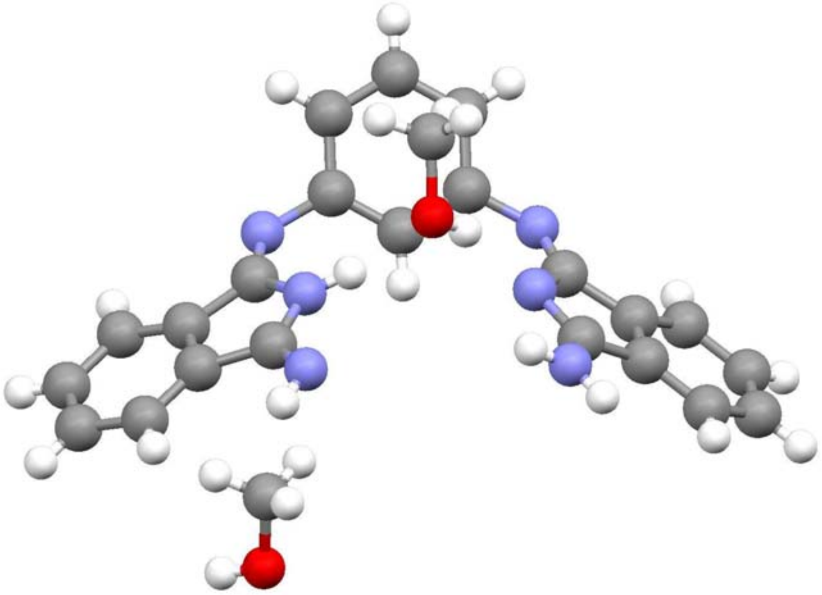

Figure S5. The asymmetric unit of compound **5**.

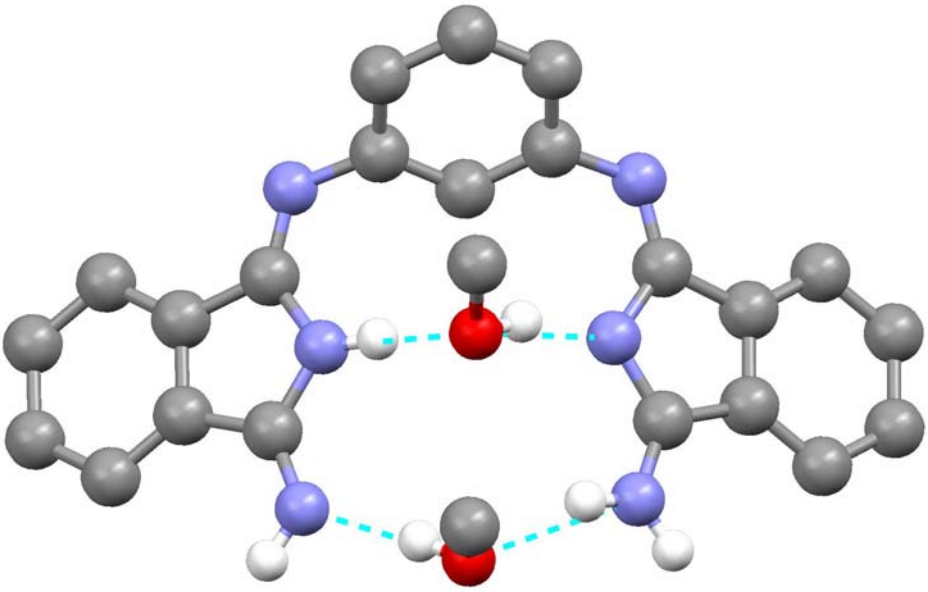

Figure S6. Hydrogen bonding interactions observed in the structure of **5**.

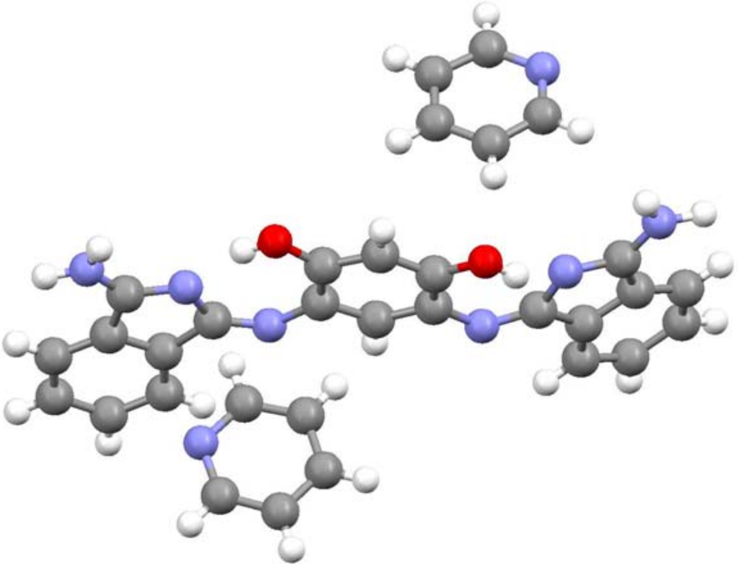

Figure S7. The asymmetric unit of compound **7**.

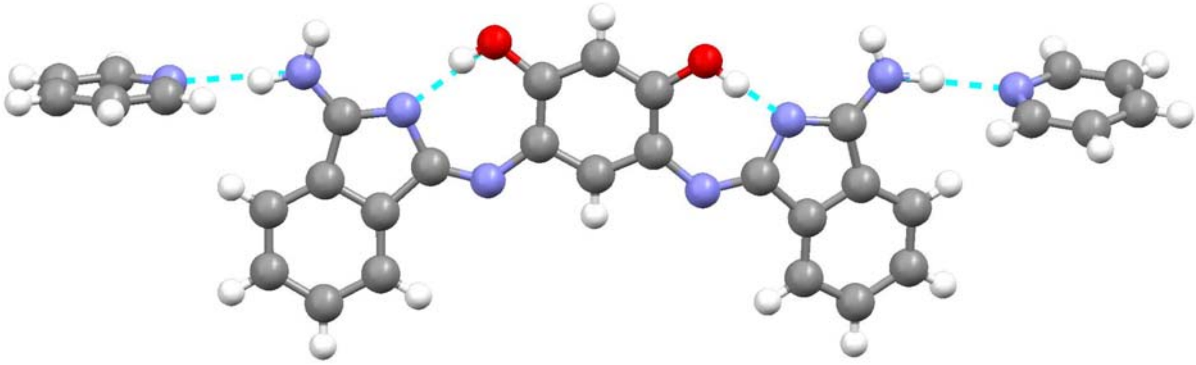

Figure S8. Interamolecular and solvent hydrogen bonding interactions observed in the structure of **7**.

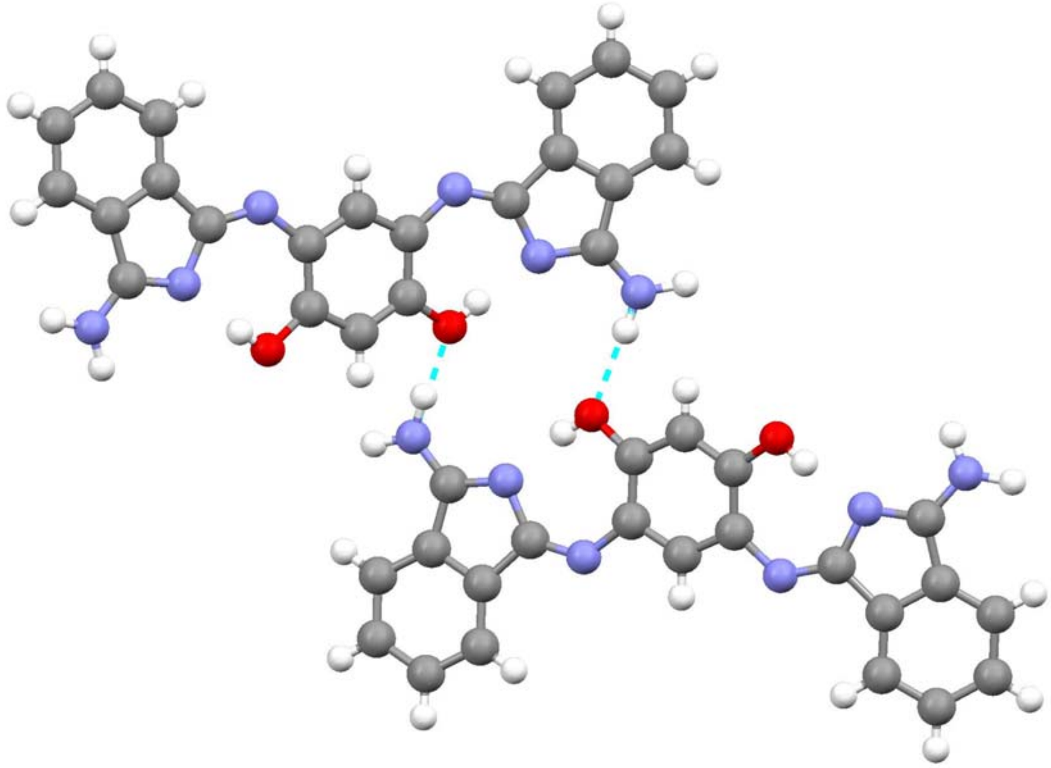

Figure S9. Hydrogen bonding interactions observed between equivalents of **7**.

References

1) J.A. Elvidge, J. H. Golden, *J. Chem. Soc.*, **1957**, 700.

2) G. M. Sheldrick, SHELXTL, Crystallographic Software Package,Version 6.10, Bruker-AXS: Madison, WI, 2000.