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Supporting Information

Lipophilic M(α,α'-OC_5H_{11})$_8$Phthalocyanines (M = H_2 and Ni(II)): Synthesis, Electronic Structure, and its Utility for Applications on Highly Efficient Carbonyl Reduction

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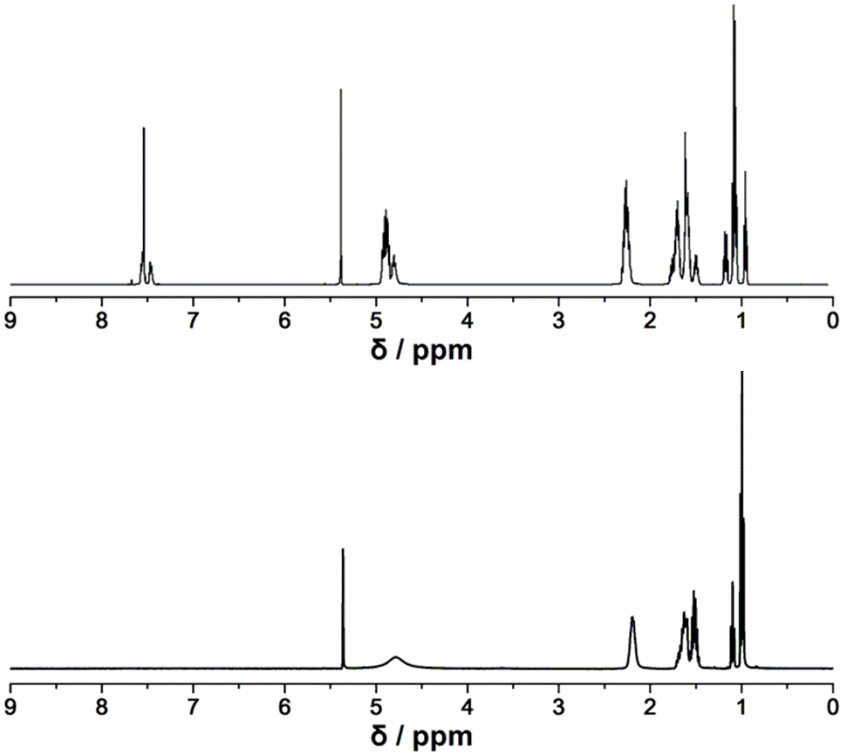

Figure S1. ^{1}HNMR spectra of H_2-Pc **2** (up) and Ni(II)Pc **3a** (bottom) in CD_2Cl_2.

Table S1. TD-DFT spectra of the B3LYP optimized geometries of **2** and **3a** calculated with the CAM-B3LYP functional and 6-31G(d) basis sets.

2							
Band[a]	#[b]	Calc[c]			Exp[d]		Wavefunction=[e]
--	1	---	---	---	---	---	Ground state
Q	2	14.9	669	(0.60)	12.9	778	95% a → -s; 4% s → -a; …
Q	3	15.4	651	(0.46)	13.7	730	89% a → -a; 10% s → -s; …

B1	8	26.6	376	(0.26)	23.4	428	50% H□3 ($1b_{1u}$) → -s; 17% s → -a; …
B1	13	29.4	340	(0.02)	24.7	405	68% H□3 ($1b_{1u}$) → -s; 13% H□2 ($1e_g$) → -a; …
B2	21	33.5	299	(0.26)	29.9	334	40% s → -a; 27% H□5 ($2a_{1u}$) → -s; 19% H□6^N ($1b_{2g}^N$) → -s; …
B2	23	34.5	290	(0.15)	32.7	306	19% H□16 → -s; 16% H□5 ($2a_{1u}$) → -a; 13% H□8 ($2a_{2u}$) → -s; 10% H□6^N ($1b_{2g}^N$) → -s; 8% s → -s; …
3a							
Band[a]	#[b]	Calc[c]			Exp[d]		Wavefunction=[e]
--	1	---	---	---	---	---	Ground state
Q	2	14.8	675	(0.51)	13.3	754	95% a → -s; 3% s → -a; …
Q	3	15.3	654	(0.47)	13.7	731	95% a → -a; 4% s → -s; …
B1	23	31.7	315	(0.24)	29.7	337	25% s → -s; 16% d_{z2} → -s; 12% H□5 ($2e_g$) → -a; …
B1	23	32.0	313	(0.19)	30.6	327	27% s →-a; 17% H□9 ($3e_g$) → -s; 15% H□4 ($2a_{1u}$) → s; …

a − Band assignment described in the text. b − The number of the state assigned in terms of ascending energy within the TD-DFT calculation. c − Calculated band energies ($10^3.cm^{-1}$), wavelengths (nm) and oscillator strengths in parentheses (f). d − Observed energies ($10^3.cm^{-1}$) and wavelengths (nm) in **Figure 1**. e − The wave functions based on the eigenvectors predicted by TD-DFT. One-electron transitions associated with Michl's perimeter model are highlighted in bold. H and L refer to the HOMO and LUMO, respectively, while N refers to □-MOs associated primarily with the lone pairs of the aza-nitrogens, and A and B refer to the □- and □-spin electrons. When the H and L nomenclature is used the symmetry label for the corresponding MO in the π-systems of D_{4h} MPc complexes is provided in parentheses where applicable.