Supporting Information

for

The Photophysical Behavior of Open-shell First-row Transition Metal Octabutoxynaphthalocyanines: $CoNc(OBu)_8$ and $CuNc(OBu)_8$ as a Case Study

Alexandra V. Soldatova, Junhwan Kim, Angela Rosa,* Giampaolo Ricciardi,* Malcolm E. Kenney,* and Michael A. J. Rodgers*

Table S1. Selected Geometrical Parameters (Å, deg) Calculated for the Ground State (1^2B_2) and the 1^2A_2 and 1^2B_1 Excited States of $CuNc(OMe)_8$.

Parameter	GS	1^2A_2[a]	1^2B_1[a]
$Cu–N_p$	1.964	2.011	2.005
$C_\alpha–N_p$	1.374	1.365	1.363
$C_\alpha–C_®$	1.458	1.466	1.468
$C_®–C_®$	1.436	1.438	1.433
$C_o–O$	1.368	1.365	1.363
$C_\alpha–N_b$	1.327	1.334	1.335
$C_\alpha–N_p–C_\alpha$	109.3	109.7	110.1
$C_\alpha–N_b–C_\alpha$	124.1	125.0	124.9
O···O	3.911	3.973	4.010
$C_{Me}–O–C_o–C_\beta$	63.0	61.1	58.5
$(C_\alpha–N_p–N_p–C_\alpha)_{ad}$[b]	11.3	16.9	15.3

[a]geometry optimizations of the excited states were performed under the D_{2d} symmetry constraint; [b]dihedral angle between adjacent pyrrole ring planes.

Table S2. Selected Geometrical Parameters (Å, deg) Calculated for the Ground State (1^2A_1) and the 1^2B_1 Excited State of $CoNc(OMe)_8$.

Parameter	GS	1^2B_1[a]
$Co–N_p$	1.920	1.911/1.912
$C_\alpha–N_p$	1.381	1.385/1.382
$C_\alpha–C_®$	1.453	1.450/1.453
$C_®–C_®$	1.432	1.433/1.431
$C_o–O$	1.368	1.368/1.367
$C_\alpha–N_b$	1.322	1.321/1.322
$C_\alpha–N_p–C_\alpha$	107.9	107.7/107.5
$C_\alpha–N_b–C_\alpha$	122.8	122.5
O···O	3.880	3.877
$C_{Me}–O–C_o–C_\beta$	63.1	63.7/62.4
$(C_\alpha–N_p–N_p–C_\alpha)_{ad}$[b]	11.2	11.2

[a]Jahn–Teller distorted C_{2v} structure; [b]dihedral angle between adjacent pyrrole ring planes.