Electronic Supplementary Material (ESI) for Journal of Materials Chemistry

Supporting Information

Synthesis, Self-assembly, and Semiconducting Properties of Phenanthroline-fused Phthalocyanine derivatives

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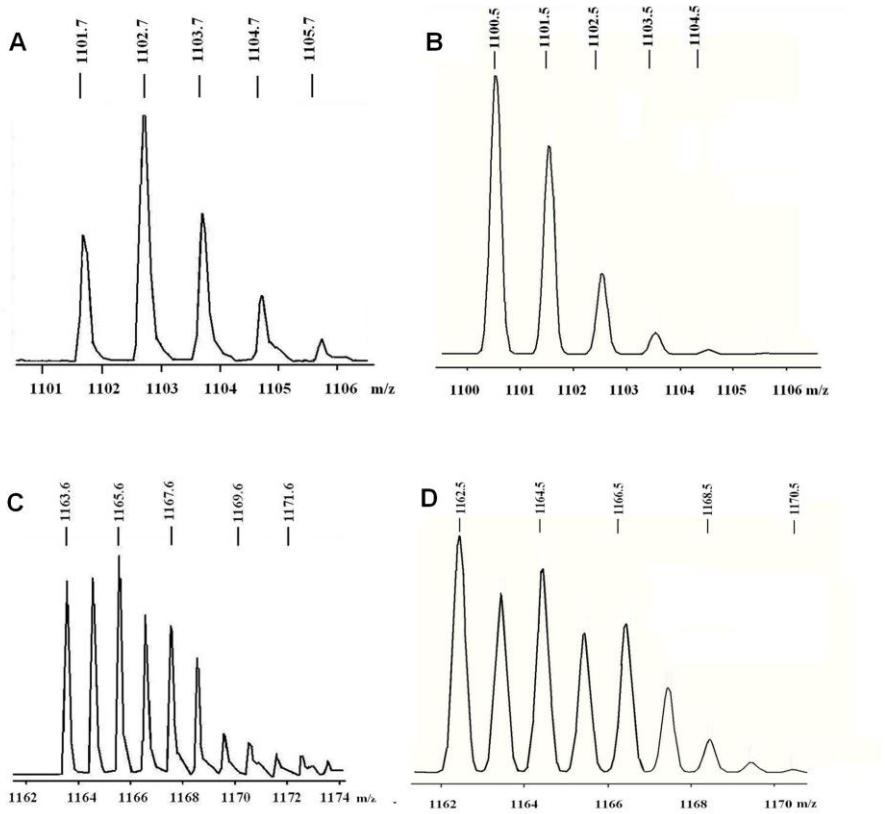

Fig. S1 (A) Experimental and (B) simulated isotopic patterns for the molecular ion of $H_2[Pc(OC_4H_9)_7(dicqn)]$ (**1**) shown in the MALDI-TOF mass spectrum; (C) Experimental and (D) simulated isotopic patterns for the molecular ion of $Zn[Pc(OC_4H_9)_7(dicqn)]$ (**2**) shown in the MALDI-TOF mass spectrum.

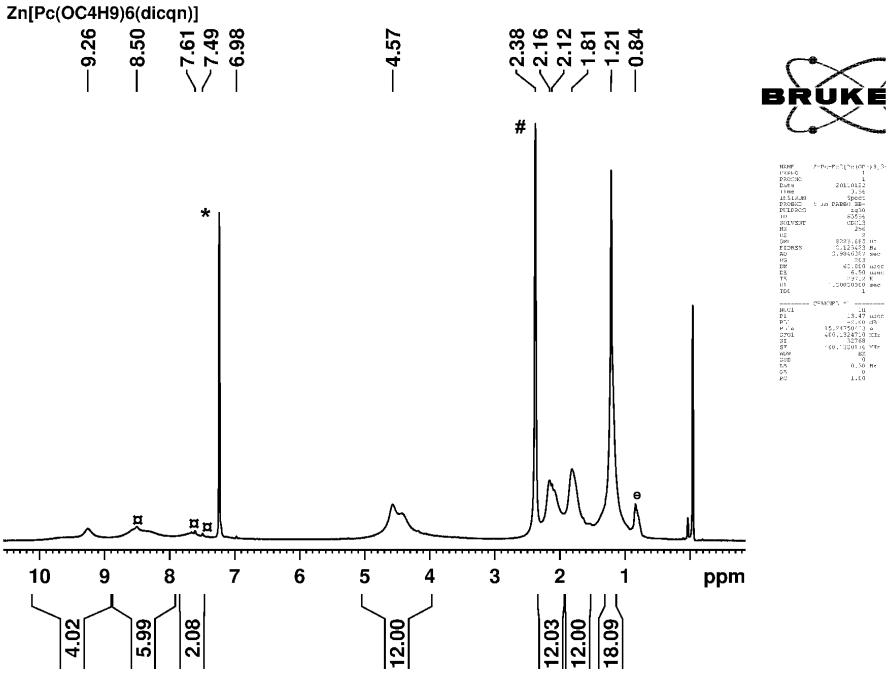

Fig. S2 ^{1}H NMR spectrum for Zn[Pc(OC_4H_9)$_6$(dicqn)] (**2**) in $CDCl_3$/[D_5]Pyridine (10:1). The signals due to residue C_5H_5N, $CHCl_3$, $(CH_3)_2CO$, and *n*-hexane are denoted as ¤, *, #, and Θ, respectively.

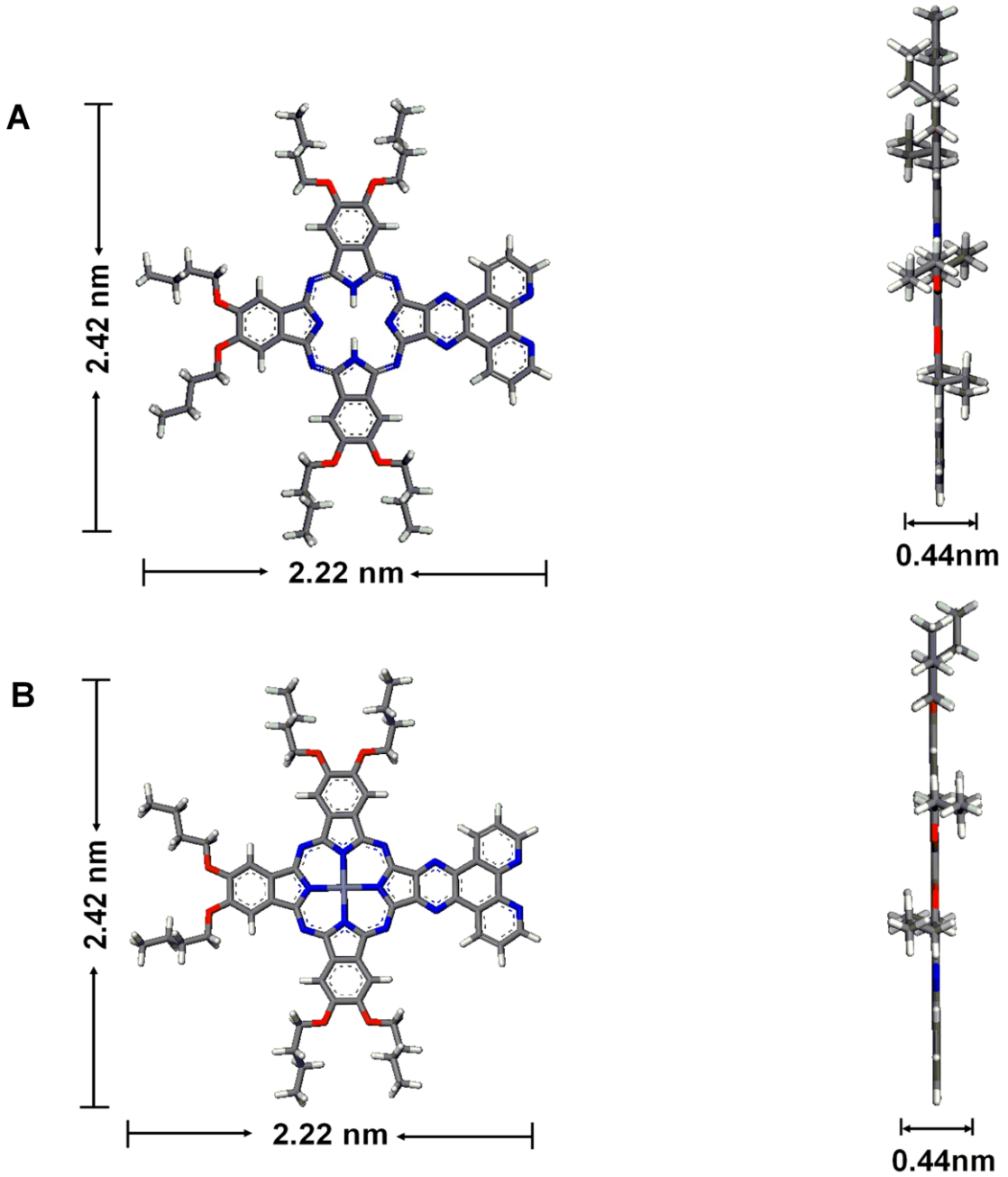

Fig. S3 The molecular dimension size of both **1** (A) and **2** (B) obtained on the basis of geometry optimization and energy minimized molecular structure using Gaussian 03 program at B3LYP/6-31G(d) level.

Table S1. Electronic absorption spectroscopic data for the compounds $H_2[Pc(OC_4H_9)_6(dicqn)]$ (**1**) and $Zn[Pc(OC_4H_9)_6(dicqn)]$ (**2**) dissolved in $CHCl_3$ and their self-assembled aggregates dispersed in methanol.

Compounds	λ_{max} / nm	
	$CHCl_3$	methanol
1	354, 458, 626, 664, 696	335, 445, 631
2	374, 629, 668, 698	372, 729