

SUPPORTING INFORMATION

Crystal-to-Crystal Guest-Exchange of Large Organic Molecules within a 3D-Coordination Network

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CONTENTS

Experimental Details

Figure S1. Photographs of guest-exchange process for **4b**.

Figure S2-S5. ORTEP drawing for **4a-4d**.

Figure S6-S11. UV-vis spectral change in guest exchange process.

Figure S12-S14. The HOMO-LUMOs of **4a-c**.

Experimental Details

General Methods: Reagents and solvents were obtained from commercial suppliers and used without further purification. The diffuse reflectance UV-vis spectra were obtained using Shimazdu UV-3150 equipped with an integrating sphere and were converted from reflection to absorbance by the Kubelka-Munk method. Single crystal X-ray diffraction data were collected on a Siemens SMART/CCD diffractmeter equipped with a 80 K.

Typical Procedure of guest exchange: The crystal of **2** (4 mg) was immersed in a cyclohexane (or hexnane) solution (0.8 ml) and the solution was saturated by adding excess amount of a guest molecules (**3a-d**) in each case. After 24 h, the crystal was removed from the solution and the X-ray analysis was revealed the inclusion complexes (**4a-d**). The crystallographic details were described in the cif files.

Anal Calcd for $C_{75}H_{66}I_6N_{12}Zn_3 \{[(ZnI_2)_3(1)_2] \cdot 1.5(3a) \cdot 2(\text{cyclohexane})\}$ (**4a**): C, 43.04; H, 3.18; N, 8.03. Found C, 42.82; H, 3.09; N, 7.89.

Anal Calcd for $C_{62.4}H_{48}I_6N_{12}Zn_3 \{[(ZnI_2)_3(1)_2] \cdot 1.2(3b) \cdot 0.8(\text{cyclohexane})\}$ (**4b**): C, 38.96; H, 2.52; N, 8.74. Found C, 38.95; H, 2.66; N, 8.47.

Anal Calcd for $C_{62.4}H_{48}I_6N_{12}Zn_3 \{[(ZnI_2)_3(1)_2] \cdot (3c) \cdot 2(\text{cyclohexane})\}$ (**4c**): C, 40.78; H, 3.02; N, 8.39. Found C, 40.59; H, 2.85; N, 8.06.

Anal Calcd for $C_{57.6}H_{42}I_6N_{12}O_{1.2}P_{1.2}Zn_3 \{[(ZnI_2)_3(1)_2] \cdot 1.2(3d)\}$ (**4d**): C, 36.10; H, 2.21; N, 8.77. Found C, 36.04; H, 2.56; N, 8.66.

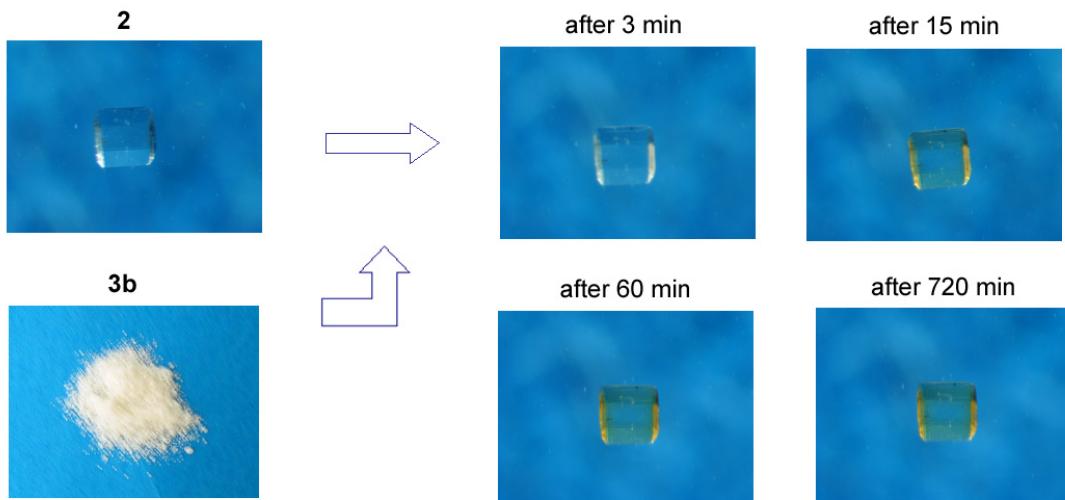


Figure S1. Photographs of guest-exchange process for **4b**.

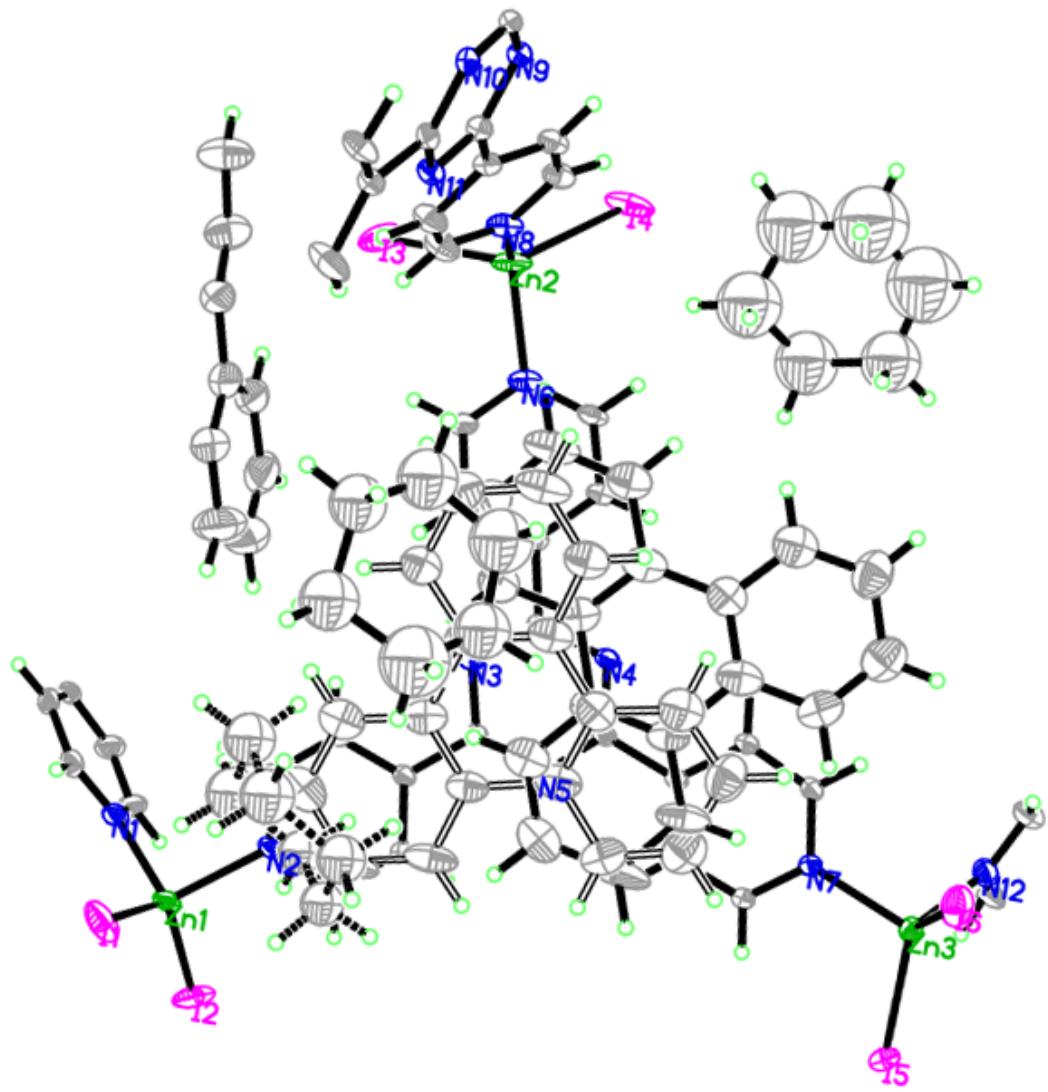


Figure S2. ORTEP drawing for the triphenylene inclusion complex (**4a**). The atoms are represented by 30% probable thermal ellipsoids.

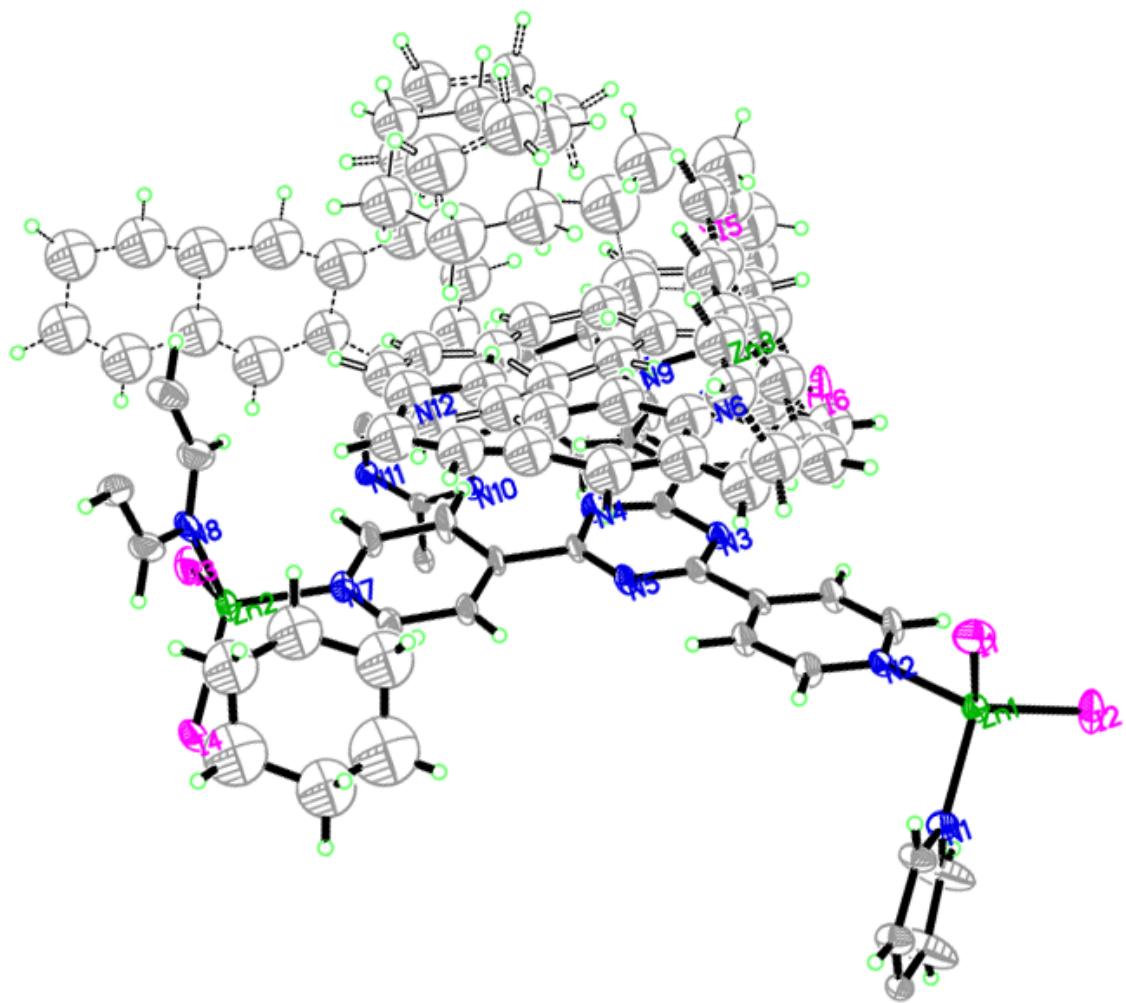


Figure S3. ORTEP drawing for the anthracene inclusion complex (**4b**). The atoms are represented by 30% probable thermal ellipsoids.

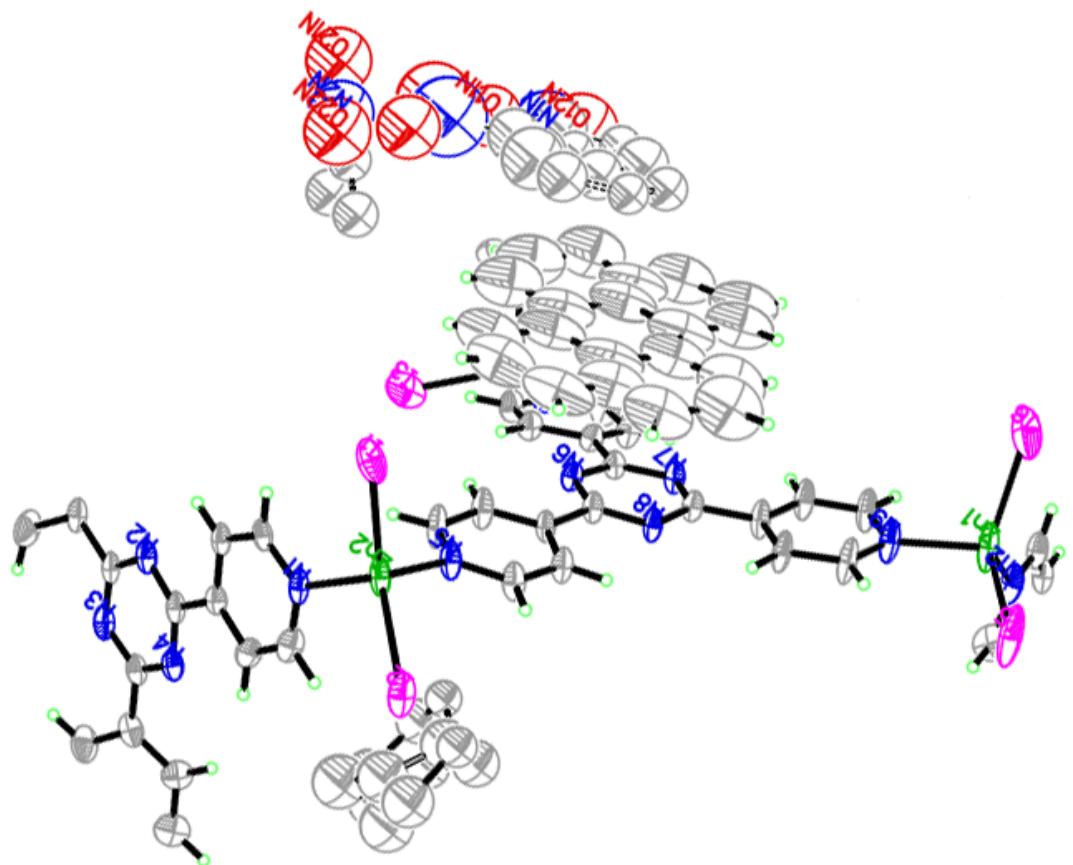


Figure S4. ORTEP drawing for the perylene inclusion complex (**4c**). The atoms are represented by 30% probable thermal ellipsoids.

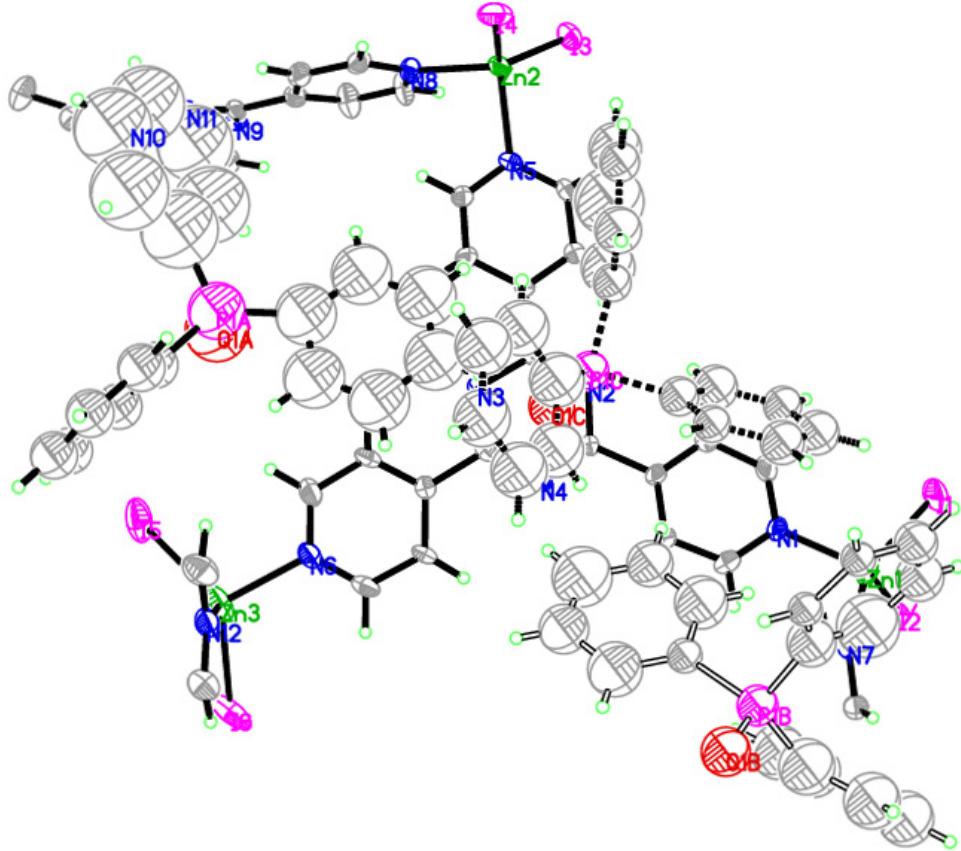


Figure S5. ORTEP drawing for the triphenylphosphine oxide inclusion complex (**4b**). The atoms are represented by 30% probable thermal ellipsoids.

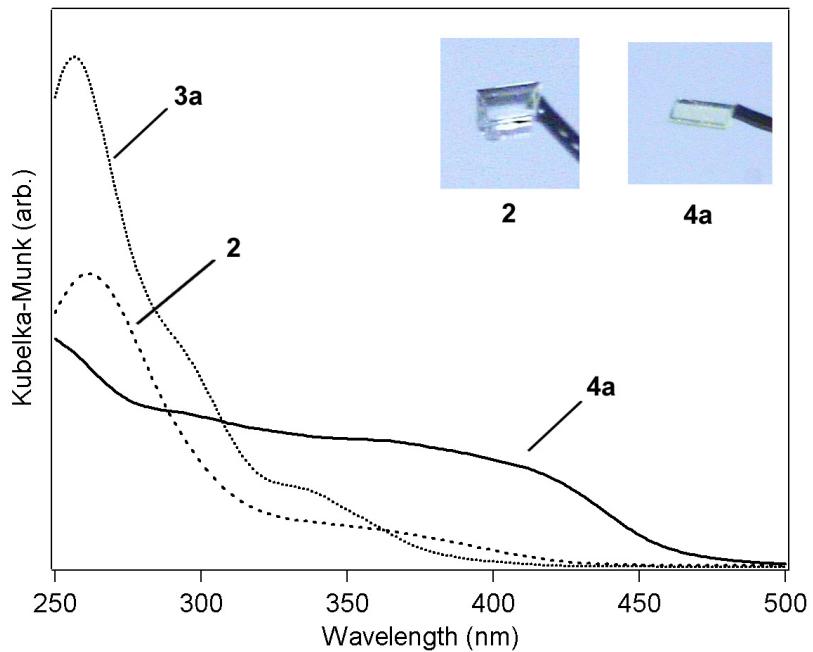


Figure S6. Diffuse reflectance UV-vis spectra of **2**, **3a**, and **4a**.

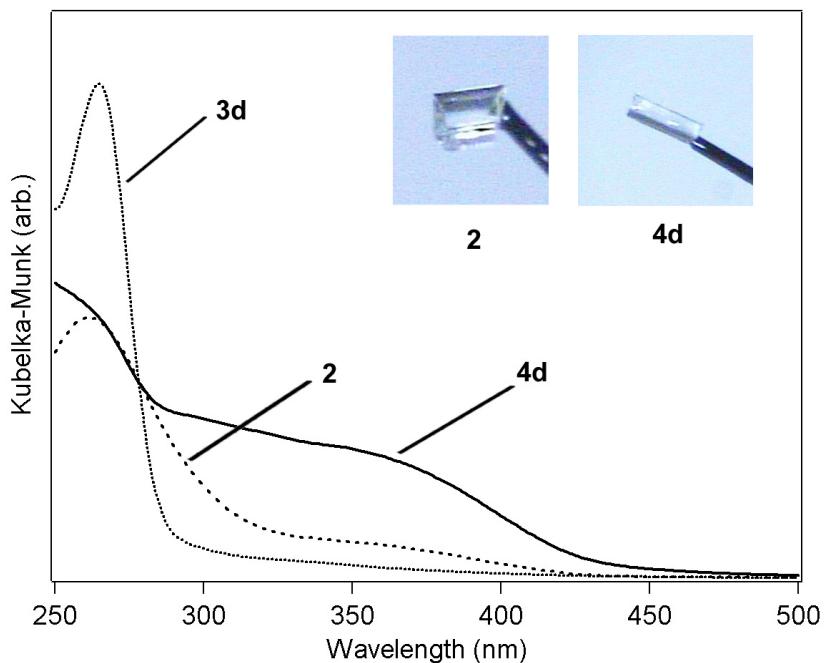


Figure S7. Diffuse reflectance UV-vis spectra of **2**, **3d**, and **4d**.

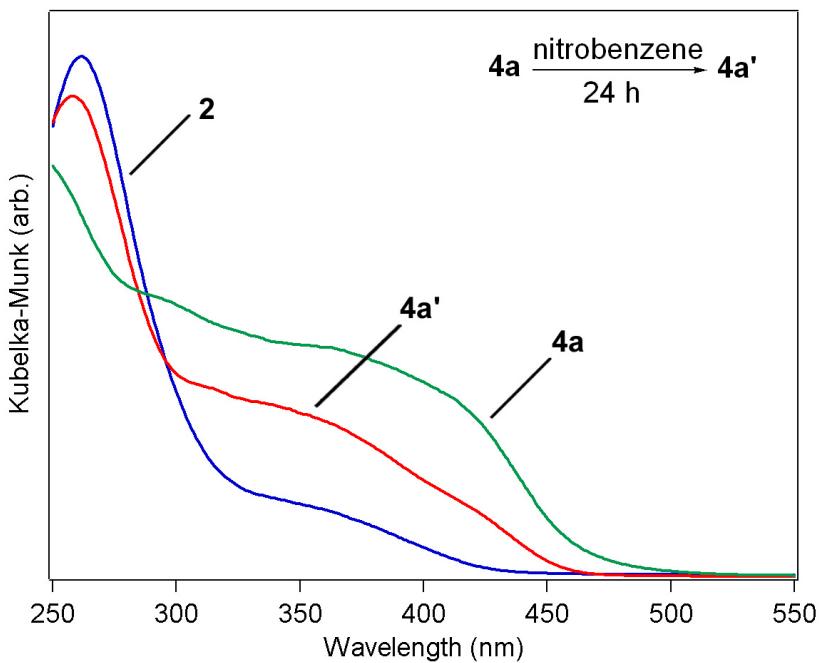


Figure S8. Diffuse reflectance UV-vis spectra of **2**, **4a**, and **4a'**.

2: nitrobenzene included complex; **4a**: triphenylene included complex; **4a'**: **4a** was immersed in nitrobenzene for 24h.

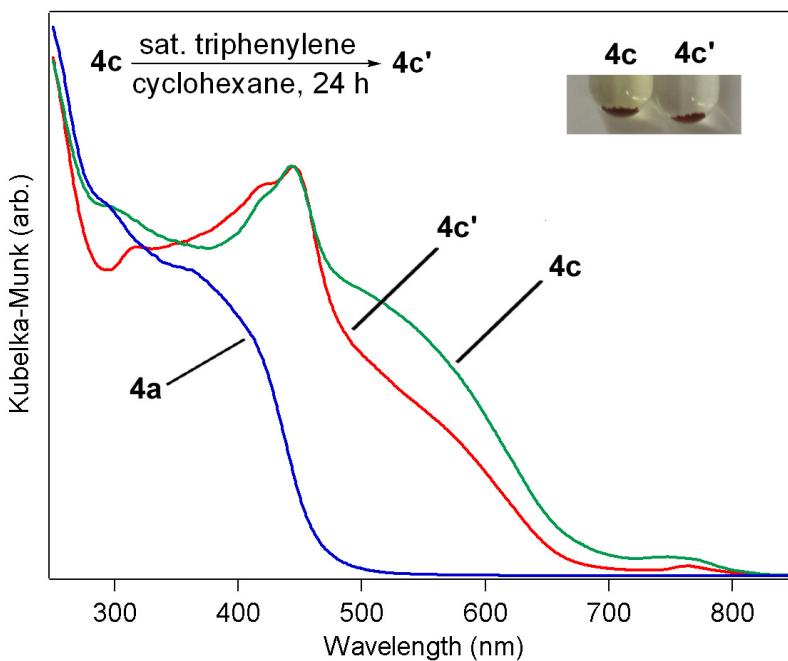


Figure S9. Diffuse reflectance UV-vis spectra of **4a**, **4c** and **4c'**.

4c: perylene included complex; **4c'**: **4c** was immersed in a saturated solution of triphenylene for 24h.; **4a** triphenylene included complex.

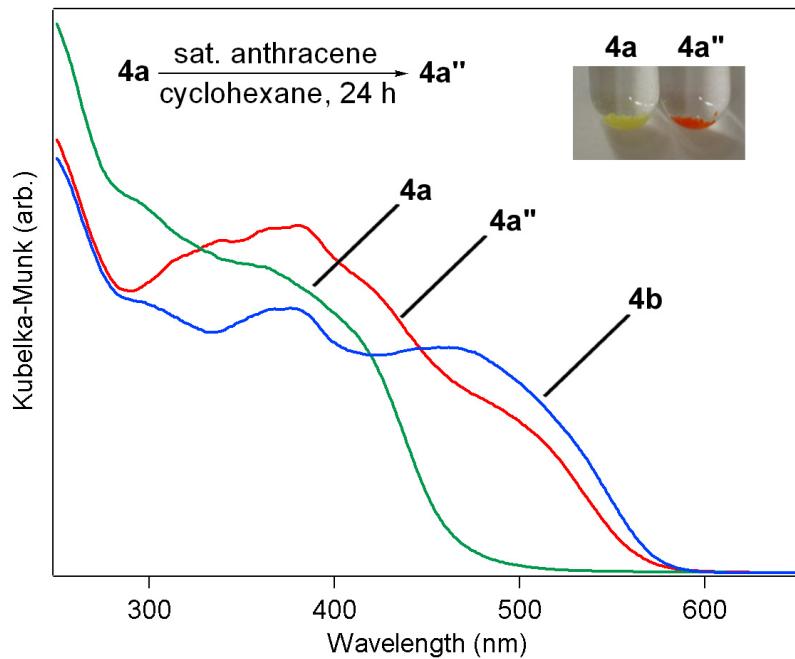


Figure S10. Diffuse reflectance UV-vis spectra of **4a**, **4a''** and **4b**.

4a: triphenylene included complex; **4a''**: **4a** was immersed in a saturated solution of anthracene for 24h.; **4b**: anthracene included complex.

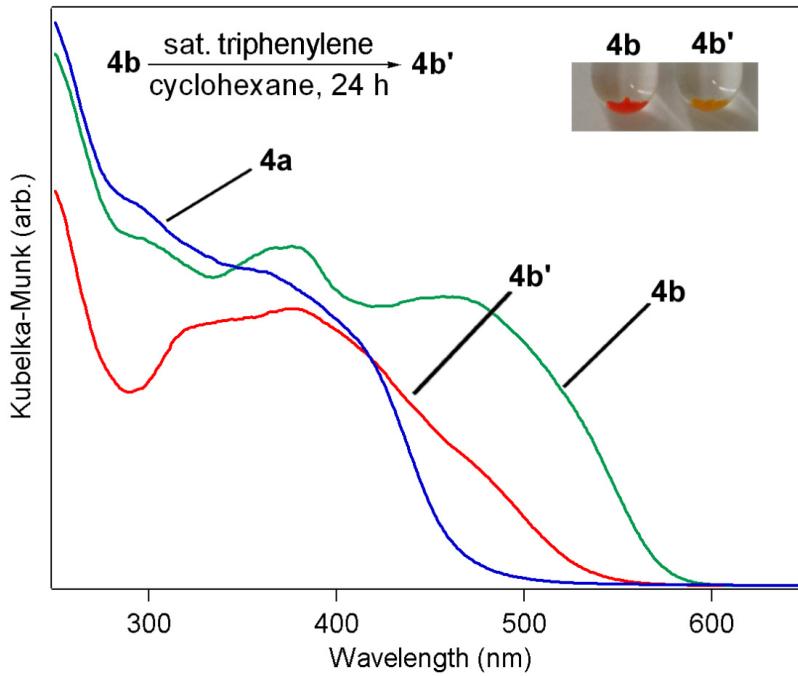


Figure S11. Diffuse reflectance UV-vis spectra of **4a**, **4b** and **4b'**.

4b: anthracene included complex; **4b'**: **4b** was immersed in a saturated solution of triphenylene for 24h.; **4a**: triphenylene included complex.

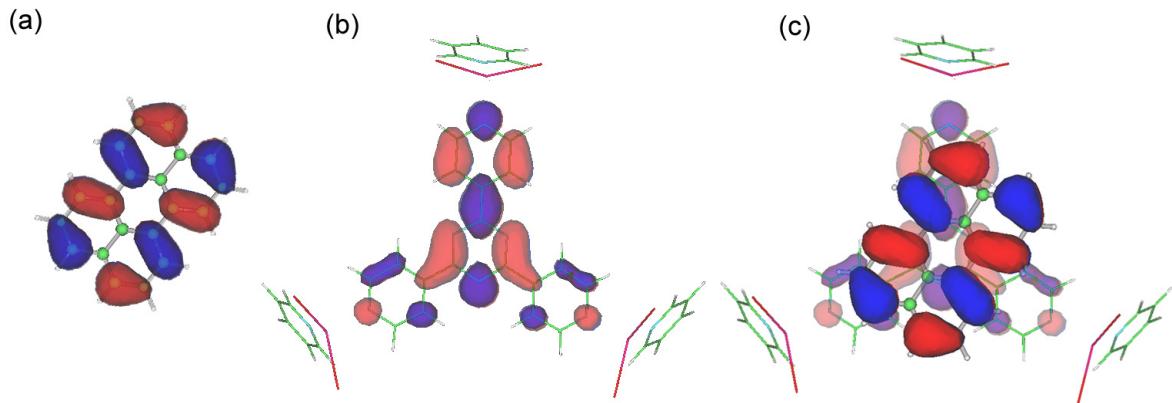


Figure S12. The HOMO of **3c**. (b) The LUMO of the simplified model framework of **2**. (c) Superposition of the HOMO and the LUMO.

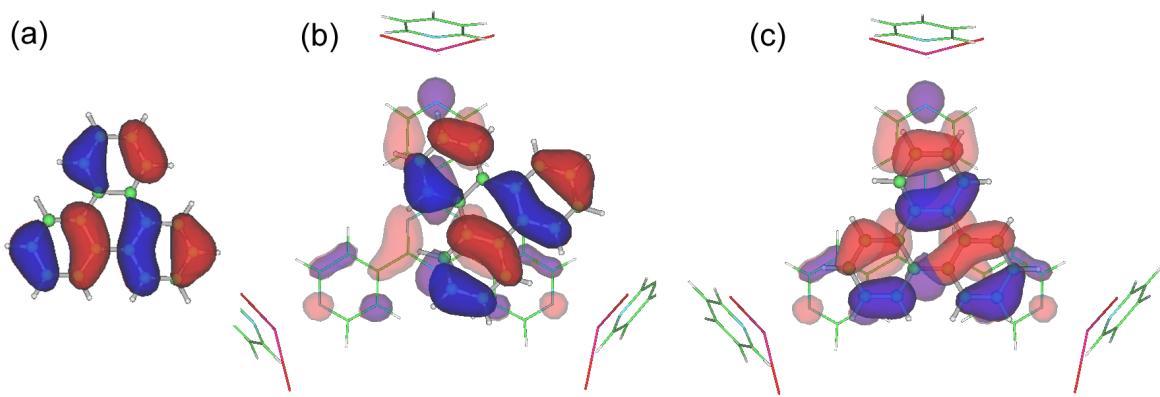


Figure S13. (a) The HOMO of **3a**. (b) Superposition of the HOMO of **3a** and the LUMO of the simplified model framework of **2** in the position **B**. (c) Superposition of the HOMO and the LUMO in the position **C**.

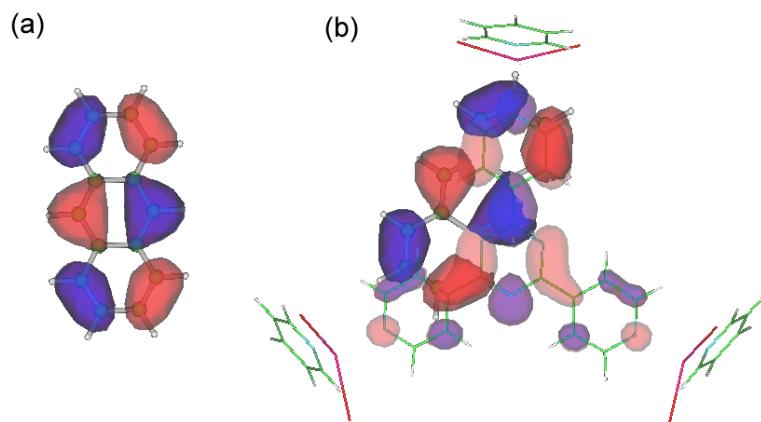


Figure S14. (a) The HOMO of **3b**. (b) Superposition of the HOMO of **3b** and the LUMO of the simplified model framework of **2**.