Electronic Supplementary Information

Formation of Sandwiches, Macrocycles and Boxes supramolecular assemblies that were controlled by the distance of two oxygen atoms in hydrogen bonding donors

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Contents

1. X-Ray crystal structure analyses

The X-ray intensity data for **1_2●2**, **1●3** and **1_2●4_2** were collected on a standard Bruker SMART-1000 CCD Area Detector System equipped with a normal-focus molybdenum-target X-ray tube (λ = 0.71073 Å) operated at 2.0 kW (50 kV, 40 mA) and a graphite monochromator. The structures were solved by using direct methods and were refined by employing full-matrix leastsquares cycles on F^2 (Bruker, SHELXTL-97)..

2. Synthesis of 1_2●2, 1●3 and 1_2●4_2

To a solution of 1,8-Bis(4-pyridylethynyl)anthracene (3.8 mg, 0.1 mmol) in CH_2Cl_2 (3 mL) was slowly added a CH_2Cl_2 solution (1 mL) of hydroquinone **2**, resorcinol **3** and 1,5-dihydroxynaphthalene **4** respectively with stirring at room temperature, and yellow crystals of 1_2●2, 1●3 and 1_2●4_2 were then obtained by slow evaporation of the above mixture solution in 5 to 8 days.

3. Crystal structures data of 1_2●2, 1●3 and 1_2●4_2

1_2●2	
_space_group_crystal_system	'triclinic'
_space_group_IT_number	2
_space_group_name_H-M_alt	'P -1'
_space_group_name_Hall	'-P 1'
_cell_length_a	8.459(4)
_cell_length_b	10.258(5)
_cell_length_c	13.519(7)
_cell_angle_alpha	107.813(5)
_cell_angle_beta	96.028(6)
_cell_angle_gamma	91.195(6)
_cell_volume	1108.9(10)
_cell_formula_units_Z	2
_cell_measurement_reflns_used	3279
_cell_measurement_temperature	296.15

1●3	
_space_group_crystal_system	monoclinic
_space_group_IT_number	14
_space_group_name_H-M_alt	'P 21/c'
_space_group_name_Hall	'-P 2ybc'
_cell_length_a	5.6736(15)
_cell_length_b	25.031(6)
_cell_length_c	18.519(5)
_cell_angle_alpha	90
_cell_angle_beta	105.220(7)
_cell_angle_gamma	90
_cell_volume	2537.7(11)
_cell_formula_units_Z	4
_cell_measurement_temperature	298(2)

$1_2 \bullet 4_2$	
_space_group_crystal_system	triclinic
_space_group_IT_number	2
_space_group_name_H-M_alt	'P -1'
_space_group_name_Hall	'-P 1'
_space_group_symop_operation_xy	z
_cell_length_a	9.934(4)
_cell_length_b	11.169(4)
_cell_length_c	14.409(5)
_cell_angle_alpha	81.527(4)
_cell_angle_beta	72.017(4)
_cell_angle_gamma	66.137(4)
_cell_volume	1390.3(9)
_cell_formula_units_Z	2
_cell_measurement_temperature	296(2)