Electronic supplementary information

Separation of xylenes by enclathration

Luigi R. Nassimbeni,*[a] Nikoletta B. Báthori,[a] Leena Desiree Patel,[a] Hong Su[b] and Edwin Weber[c]

[a] *Crystal Engineering Unit, Department of Chemistry, Faculty of Applied Sciences, Cape Peninsula University of Technology, P.O. Box 652, 8000, South Africa.*
[b] *Centre for Supramolecular Chemistry Research, Department of Chemistry, University of Cape Town, Private Bag, Rondebosch 7701, South Africa.*
[c] *Institut für Organische Chemie, TU Bergakademie Freiberg, Leipziger Str. 29, Sachs, D-09596 Freiberg, Germany.*

Close contacts of the methyl group with the host molecules in all the structures

The interactions that occur between the methyl groups on the guest molecules with the neighbouring host molecules in each crystal structure are C-H-π interactions, which are presented in the Figures 1 to 4.

1. H1•0.5ox inclusion compound

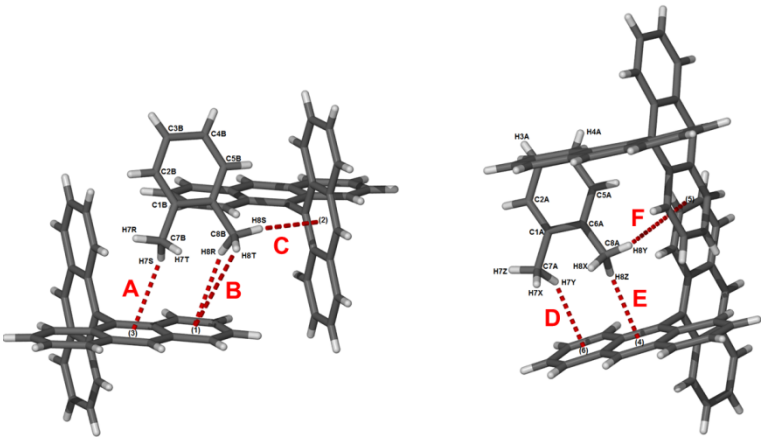

Figure 1S Close contacts that occur between methyl groups on the guest and host molecules in H1•0.5ox

Table 1S C-H-π interactions between methyl groups on guest with host in H1•0.5ox

	Geometry	Interaction (C-H•••c_g)	Intermolecular distance (Å)
A	Perpendicular y-shaped	C7B-H7S•••c_g(C15C,C16C,C21C,C22C,C23C,C28C)	2.94
B	Perpendicular y-shaped	C8B-H8R,T •••c_g(C16C-C21C)	3.03,3.84
C	Perpendicular y-shaped	C8B-H8S•••c_g(C1C,C2C,C7C,C8C,C9C,C14C)	2.90
D	Perpendicular y-shaped	C7A-H7Y •••c_g(C2F-C7F)	2.77
E	Perpendicular y-shaped	C8A-H8Z •••c_g(C1F,C2F,C7F,C8F,C9F,C14F)	2.75
F	Perpendicular y-shaped	C8A-H8Y•••c_g(C2E-C7E)	3.04

2. H1•0.5px inclusion compound

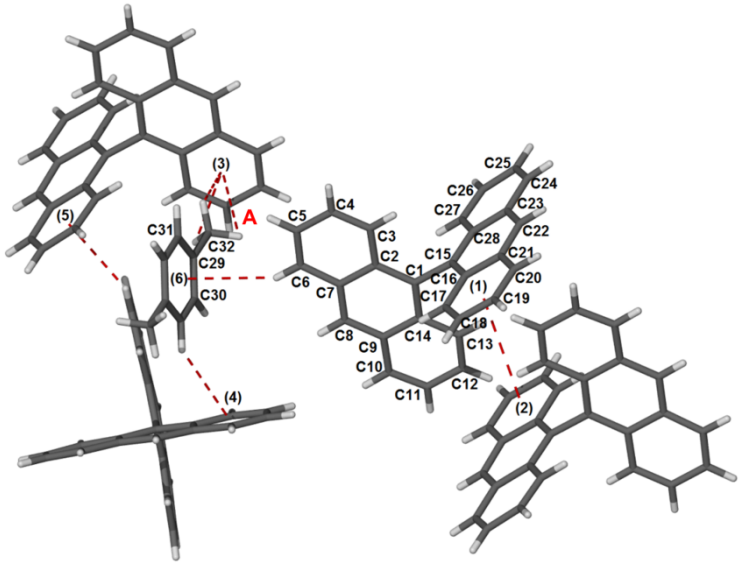

Figure 2S Close contacts that occur between methyl groups on the guest and host molecules in H1•0.5px

Table 2S C-H-π interactions between methyl groups on guest with host in H1•0.5px

	Geometry	**Interaction (C-H•••c_g & c_g•••c_g)**	**Intermolecular distance (Å)**
A	Perpendicular t-shaped	C32-H32A,B,C•••c_g(C2-C7)	3.23-3.57 Å.

3. H2•0.5px inclusion compound

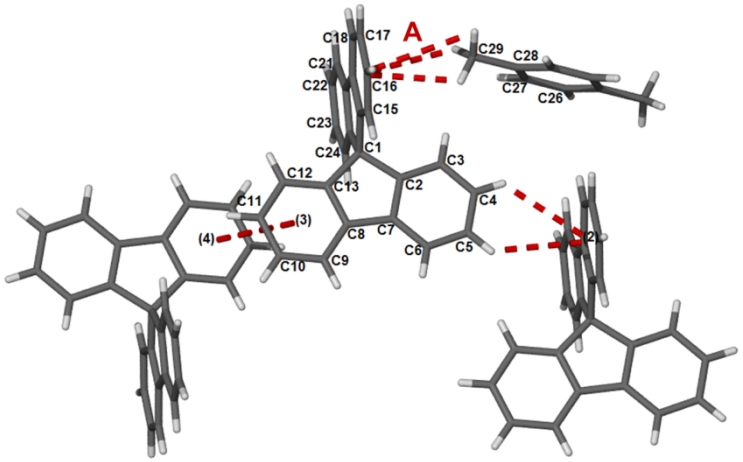

Figure 3S Close contacts that occur between methyl groups on the guest and host molecules in H2•0.5px

Table 3S C-H-π interactions between methyl groups on guest with host in H2•0.5px

	Geometry	**Interaction (C-H•••c_g)**	**Intermolecular distance (Å)**
A	Perpendicular t-shaped	C29-H29A,B,C•••c_g(C14-C20)	3.22-3.85

4. H3•ox inclusion compound

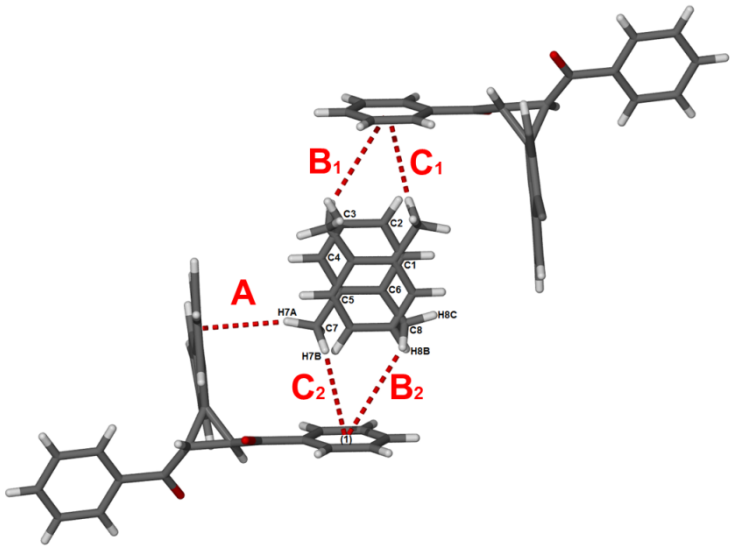

Figure 4S Close contacts that occur between methyl groups on the guest and host molecules in H3•ox

Table 4S C-H-π interactions between methyl groups on guest with host in H3•ox

	Geometry	Interaction (C-H•••c_g)	Intermolecular distance (Å)
A	Perpendicular y-shaped	C7-H7A•••c_g(C10-C15)	3.01
B	Perpendicular y-shaped	C8-H8B,T •••c_g(C19-C24)	3.62
C	Perpendicular y-shaped	C7B-H7B•••c_g(C19-C24)	3.15

H^1 NMR spectra for H1•0.5ox and H3•ox

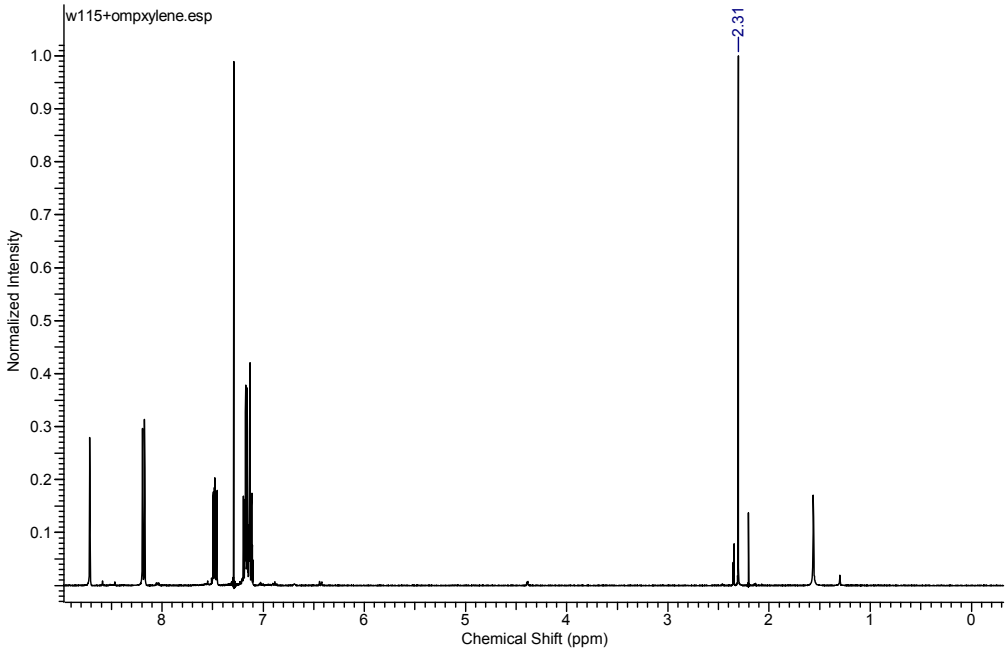

Figure 5S H^1 NMR spectrum for H2•0.5ox

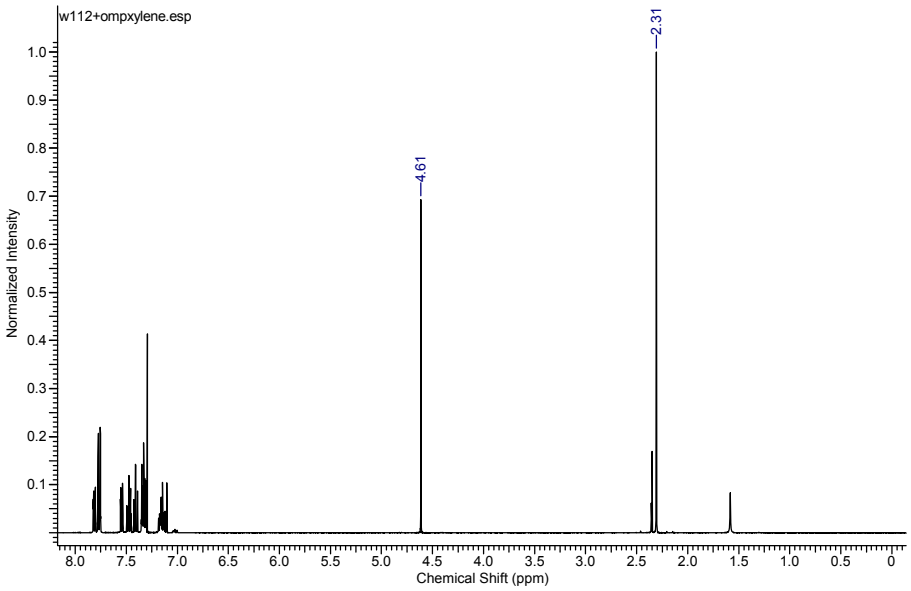

Figure 6S H^1 NMR spectrum for H3•ox