Carboxylic-acid clathrate hosts of Diels-Alder adducts of phencyclone and 2-alkenoic acids. Role of bidentate C-H··O hydrogen bonds between the phenanthrene and carbonyl groups in host-host network

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ESI-1 Structures and compound number of the DA hosts
ESI-2a. Atomic number for 3ac·1,4-dioxane (1 : 1)
In an asymmetric unit, two halves of a dioxane molecule locate at (0.0, 0.5, 0.5) and (0.5, 0.5, 0.5) positions, in which the crystal center of symmetry is present at the molecular center of symmetry of dioxane.
ESI-2b. Packing diagram of 3ac·1,4-dioxane (1:1)

ESI-2c. Packing diagram of 3ac·1,4-dioxane (1:1)
ESI-2d.  a-Axis projection of 3ac-1,4-dioxane ( 1 : 1 )

ESI-2e.  Important distances in 3ac-1,4-dioxane ( 1 : 1 )
ESI-3a. Atomic number for 3αe-3-pentanone (1 : 1)
ESI-3b. Relative positioning of host and guest molecules for 3ae:3-pentanone (1:1)
ESI-3c. Space-filling model of 3ae·3-pentanone (1 : 1)
ESI-3d. Packing diagram of 3ae-3-pentanone
ESI-4a. Atomic number for 3bl-ethanol (1 : 1)
ESI-4b. Relative positioning of host and guest molecules for 3bl·ethanol (1 : 1)
ESI-4c. View of the guests surrounded by the phenyl rings of the hosts in 3bl·ethanol (1 : 1)
ESI-4d. Space-filling model of 3bl·ethanol (1 : 1)
ESI-5. The PM3-optimized structures for 3ad-ethanol and 3ad dimer.
PM3 for 3aa+benzene
Hf = 66.819192 kcal/mol

ESI-6. Virtual inclusion position of benzene
method          heat of formation
HF/3-21G        6.50 kcal/mol
HF/6-31G*       2.37          
HF/6-31+G**     2.10          
B3LYP/6-31G**   3.21          
B3LYP/6-31+G*   1.89          

H--O=C< distance  2.537Å        

ESI-7. Model bidentate interaction between phenanthrene and acetone
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