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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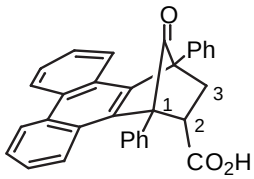
ESI data



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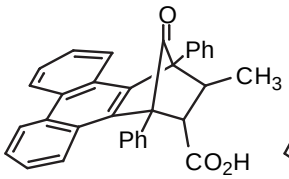

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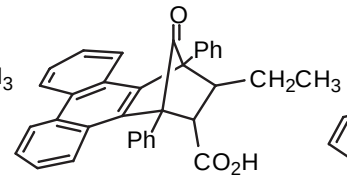

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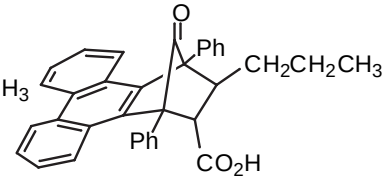

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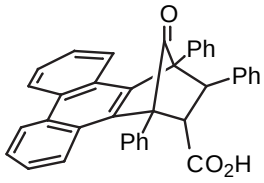

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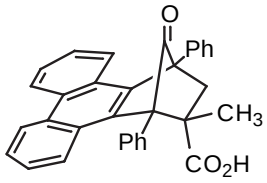

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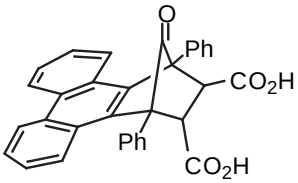

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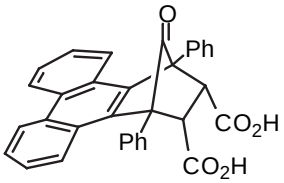

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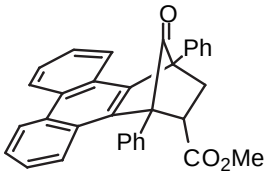

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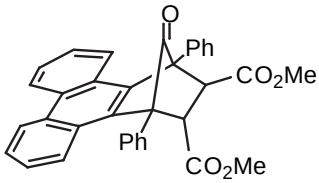

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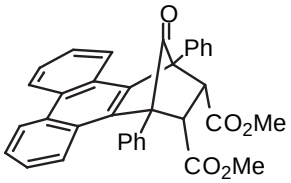

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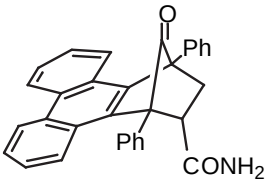

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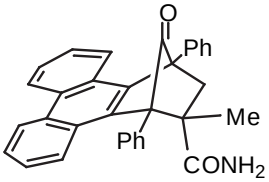

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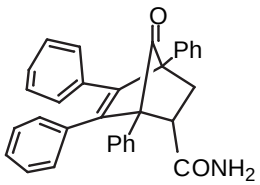
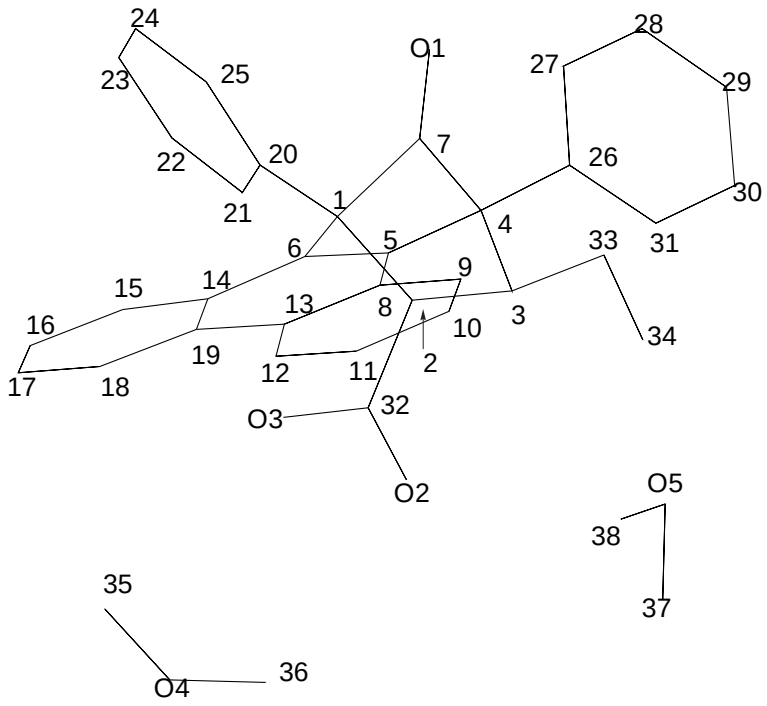
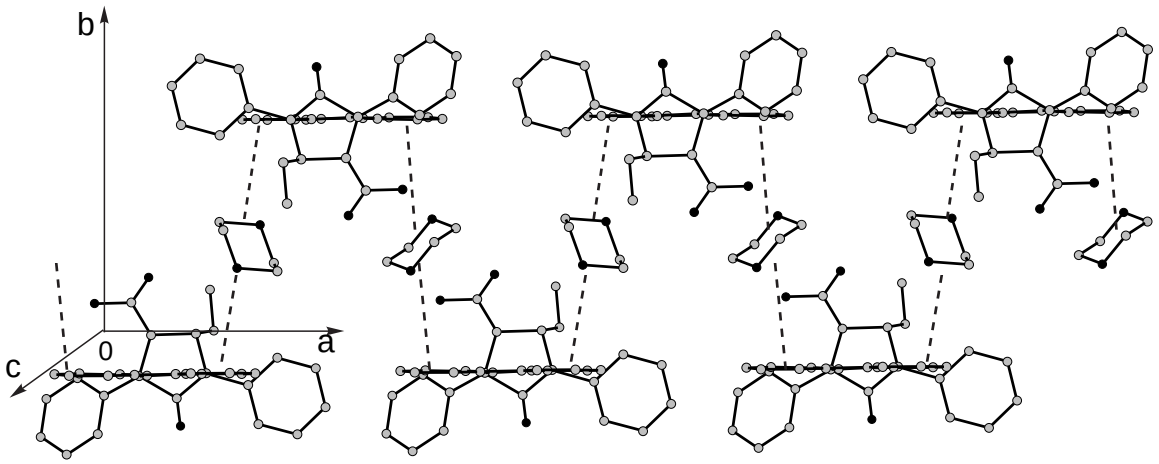


3bl

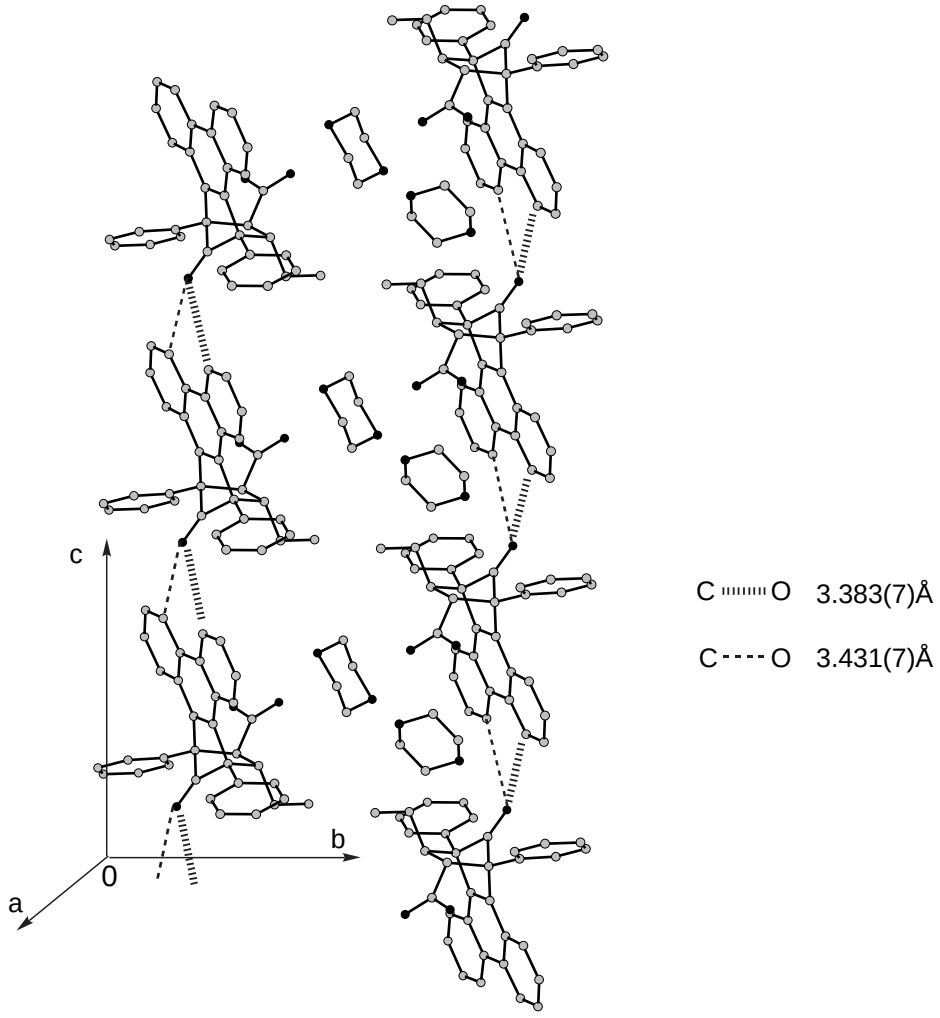
ESI-1 Structures and compound number of the DA hosts



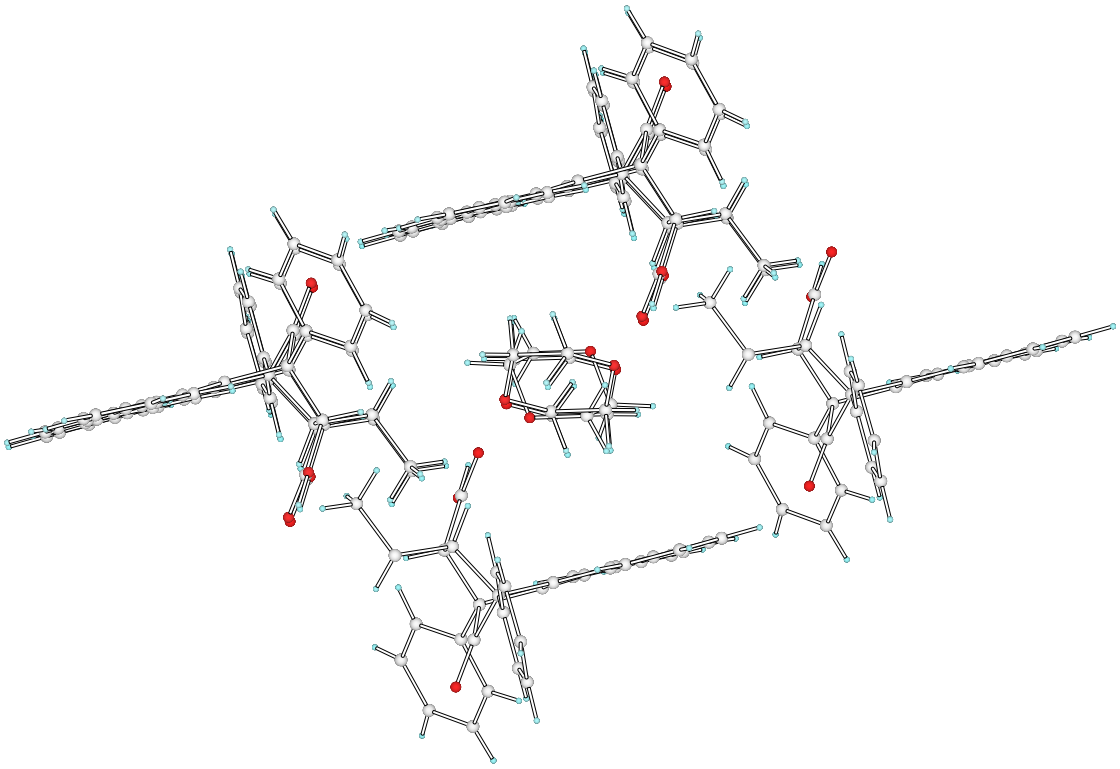
ESI-2a. Atomic number for 3ac·1,4-dioxane (1 : 1)
In an asymmetric unit, two halves of a dioxane molecule locate at (0.0, 0.5, 0.5) and (0.5, 0.5, 0.5) positions, in which the crystal center of symmetry is present at the molecular center of symmetry of dioxane.



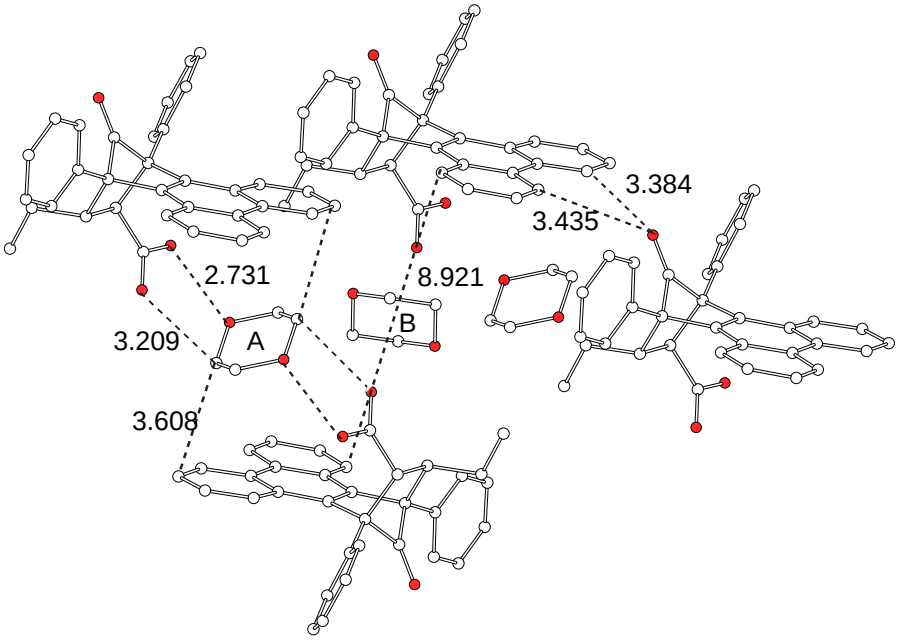
ESI-2b. Packing diagram of 3ac·1,4-dioxane (1 : 1)



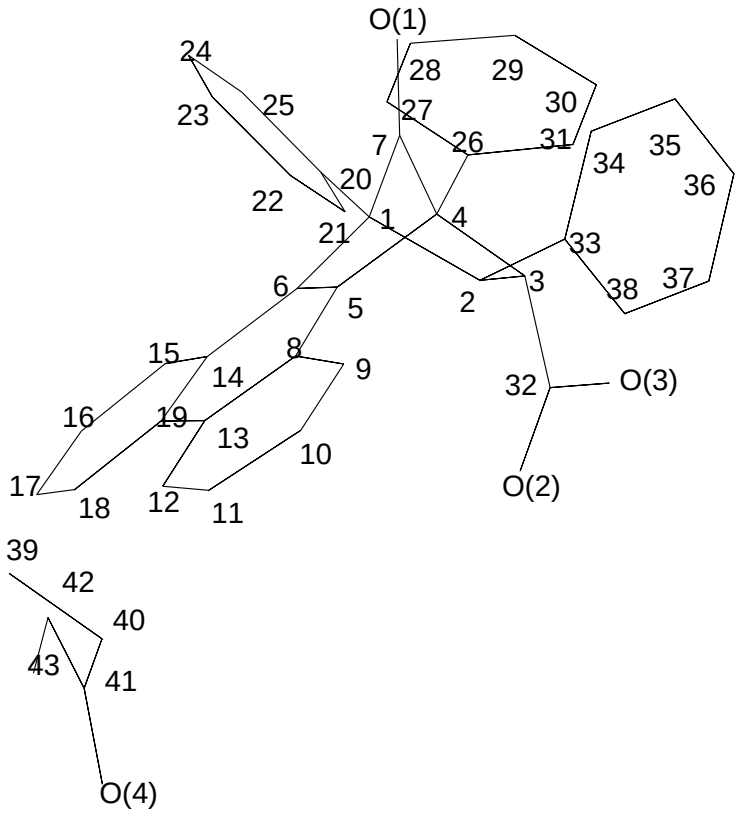
ESI-2c. Packing diagram of 3ac·1,4-dioxane (1 : 1)



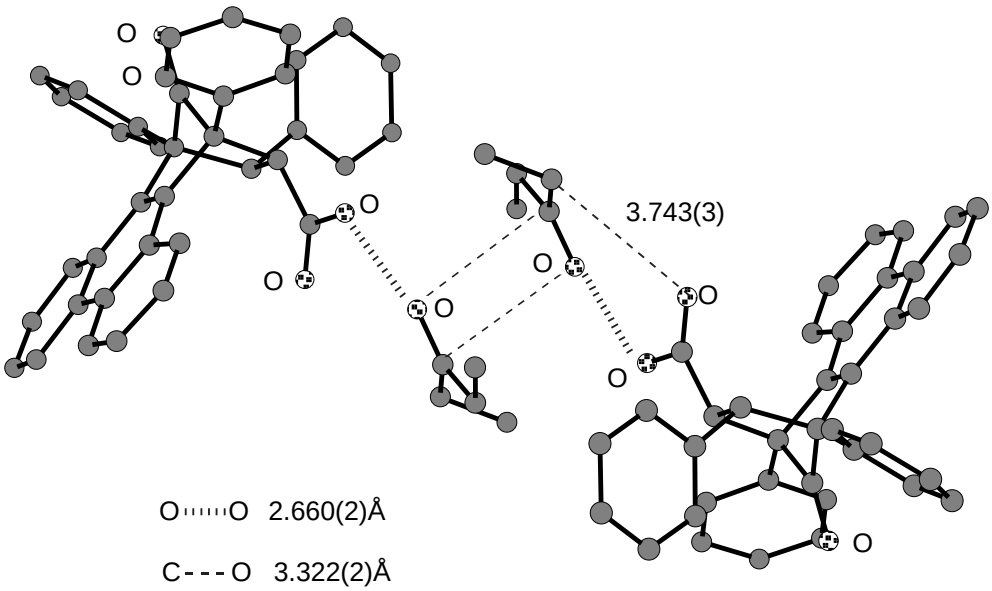
ESI-2d. a-Axis projection of 3ac·1,4-dioxane (1 : 1)



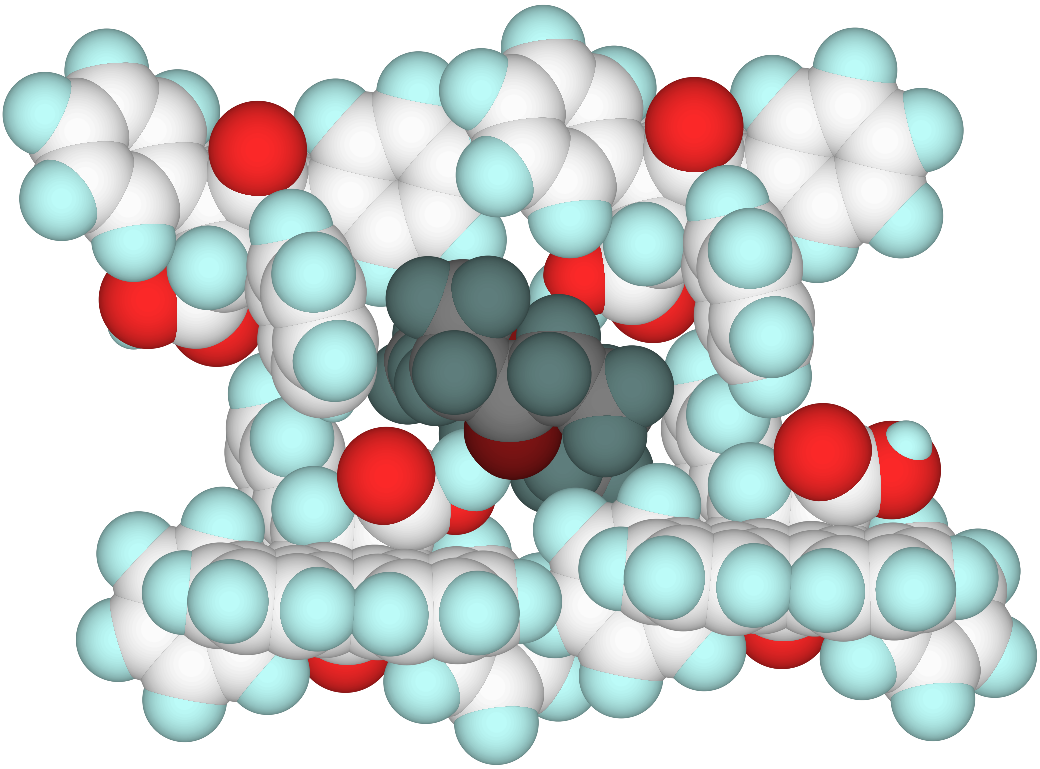
ESI-2e. Important distances in 3ac·1,4-dioxane (1 : 1)



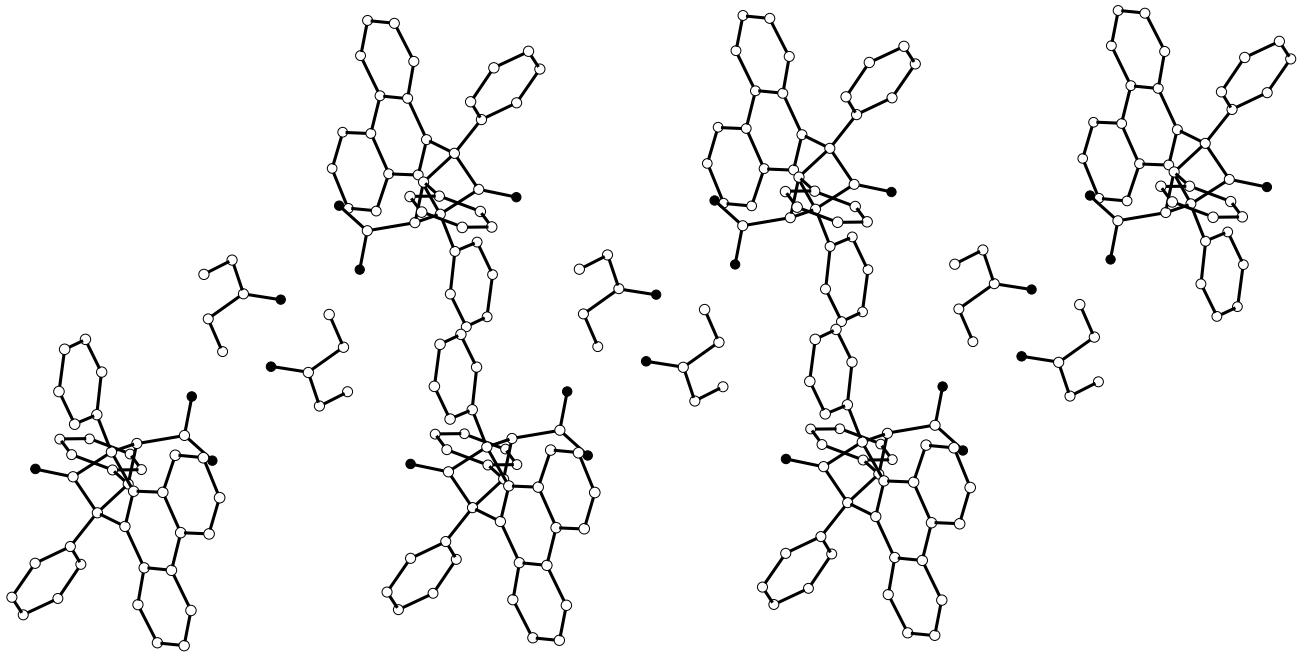
ESI-3a. Atomic number for 3ae·3-pentanone (1 : 1)



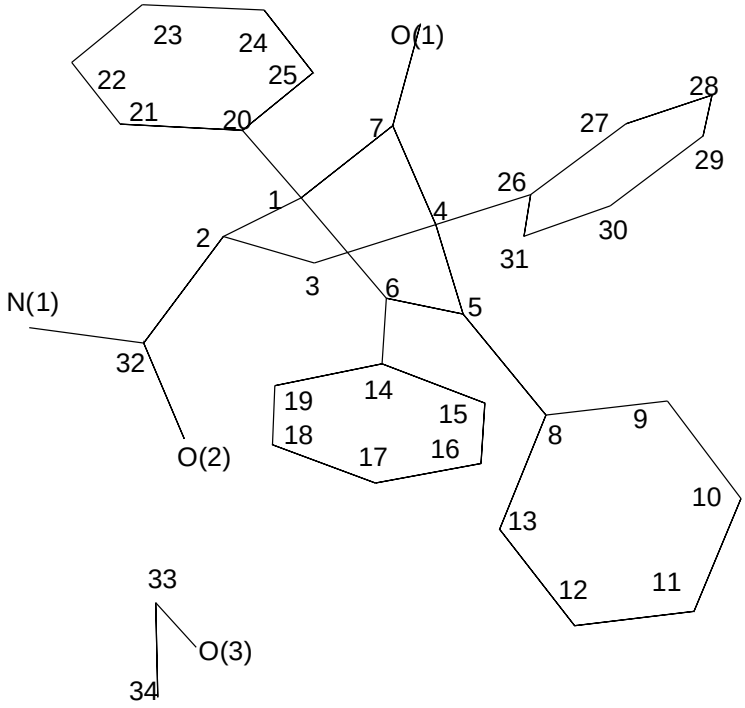
ESI-3b. Relative positioning of host and guest molecules for 3ae·3-pentanone (1 : 1)



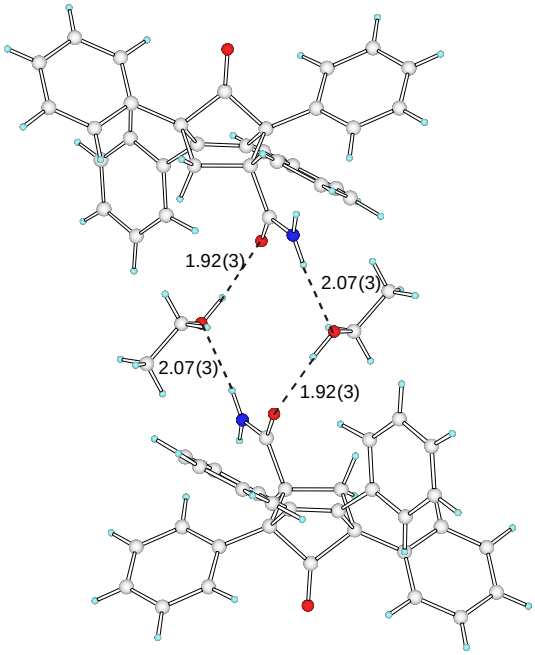
ESI-3c. Space-filling model of 3ae·3-pentanone (1 : 1)



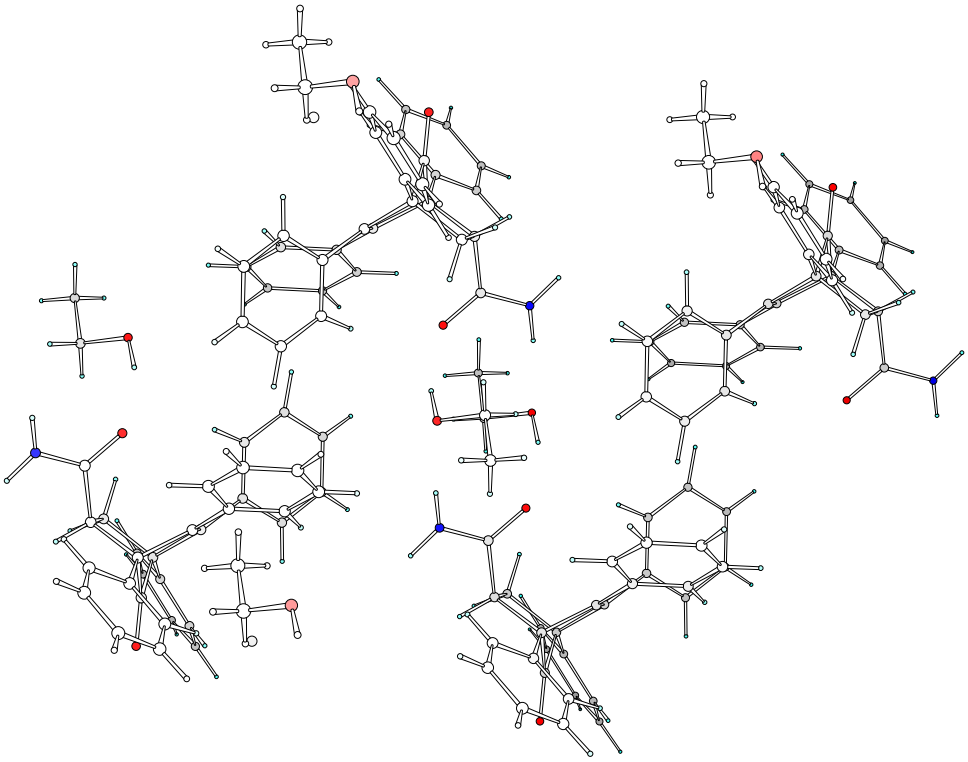
ESI-3d. Packing diagram of 3ae·3-pentanone



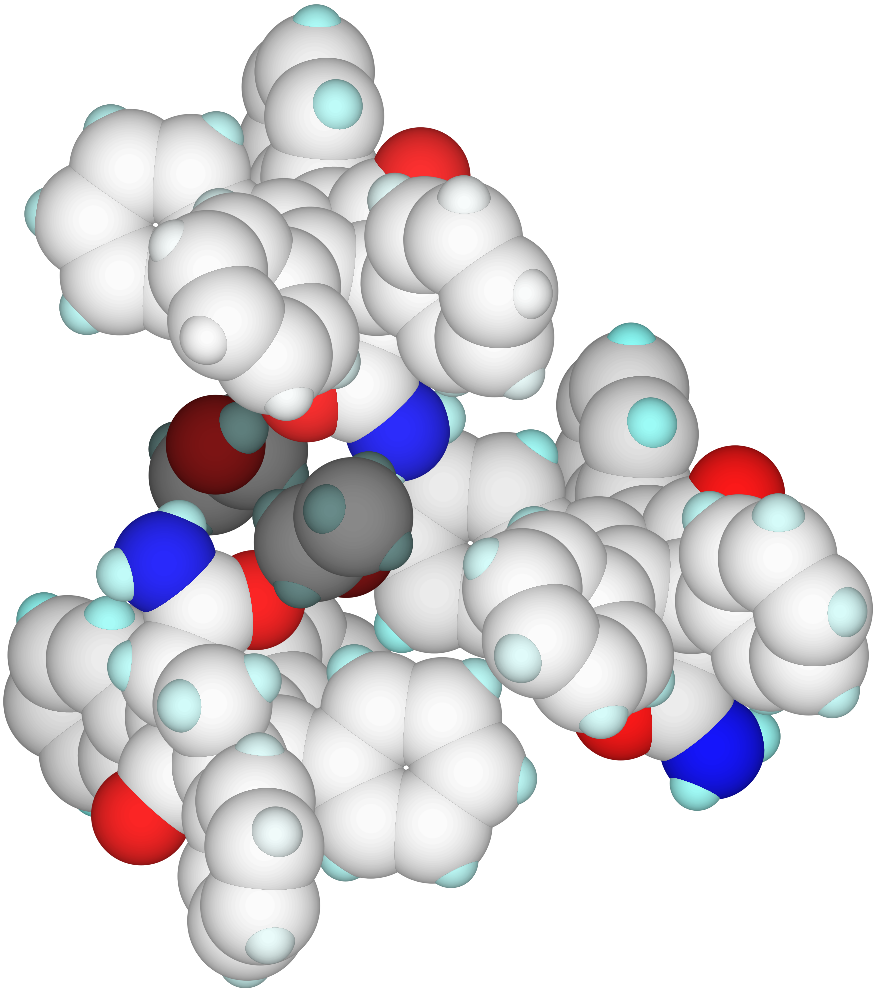
ESI-4a. Atomic number for 3bl·ethanol (1 : 1)



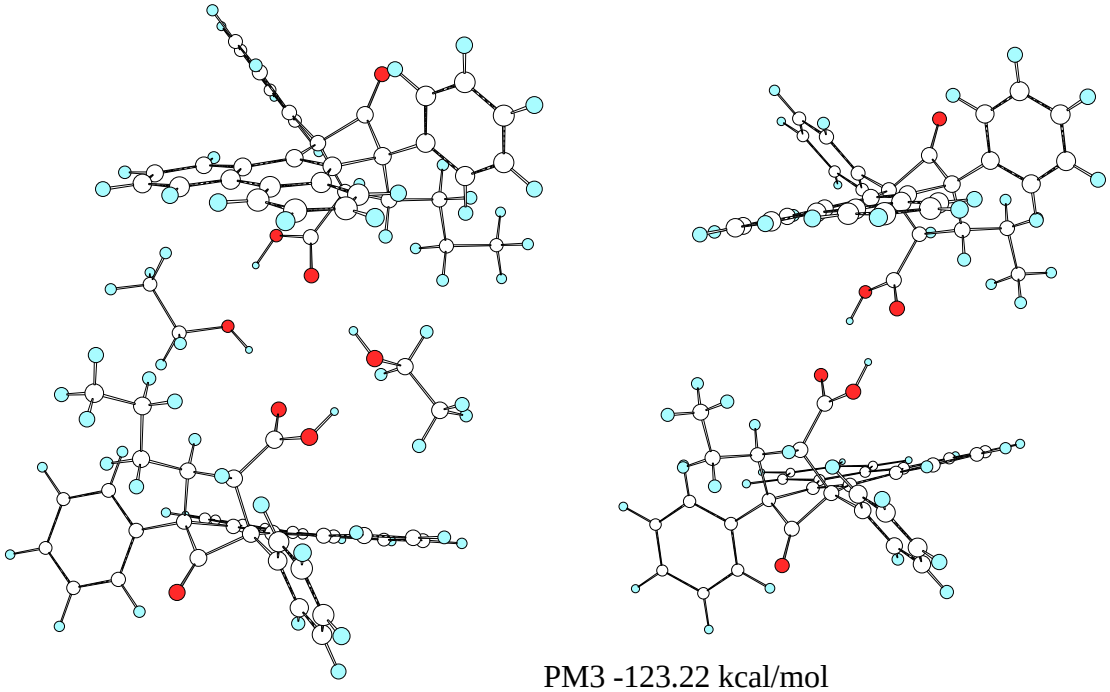
ESI-4b. Relative positioning of host and guest molecules for 3bl·ethanol (1 : 1)



ESI-4c. View of the guests surrounded by the phenyl rings of the hosts in 3bl·ethanol (1 : 1)

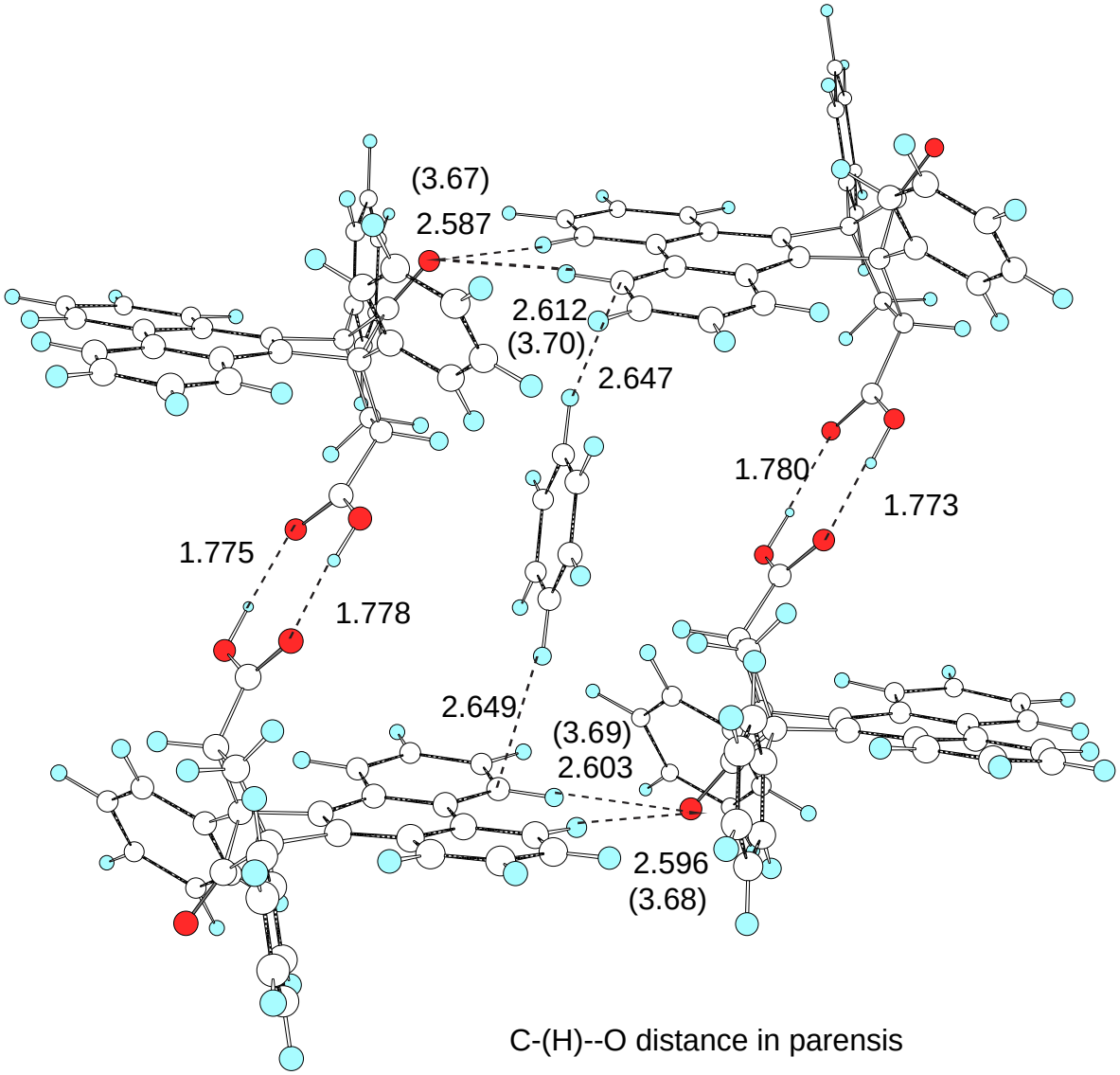


ESI-4d. Space-filling model of 3bl·ethanol (1 : 1)



PM3 -123.22 kcal/mol

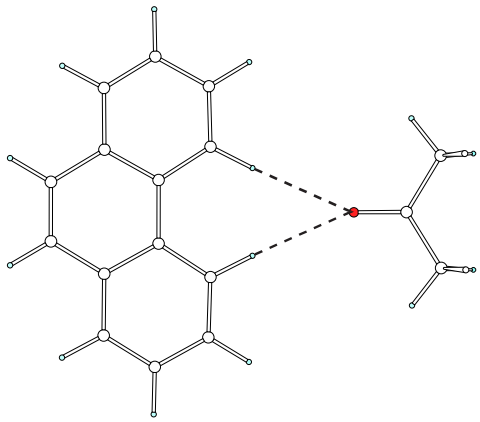
ESI-5. The PM3-optimized structures for 3ad·ethanol and 3ad dimer.



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

EOF