Supplementary data for the article:

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Supplementary Information

Strong C-H/O interactions between polycyclic aromatic hydrocarbons and water: influence of aromatic system size

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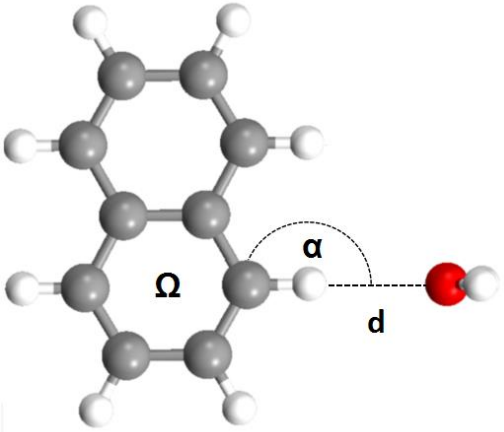
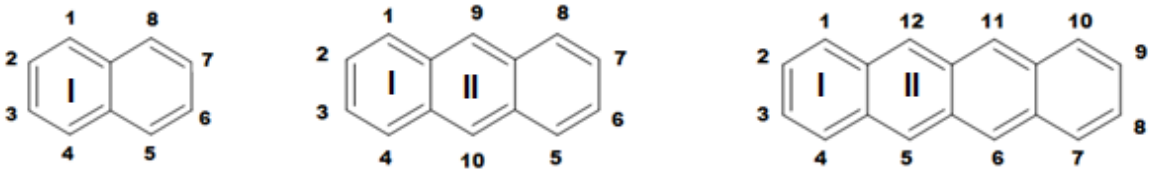


Figure S1. Graphical representation of the geometric parameters and mutual orientations of molecules in model systems



a) b) c)

Figure S2. Carbon atom numbering scheme for a) naphthalene, b) anthracene and c) tetracene used in this work. Hydrogen atoms were marked with respect to the number of the carbon atom they were attached to. Rings were marked with I and II.

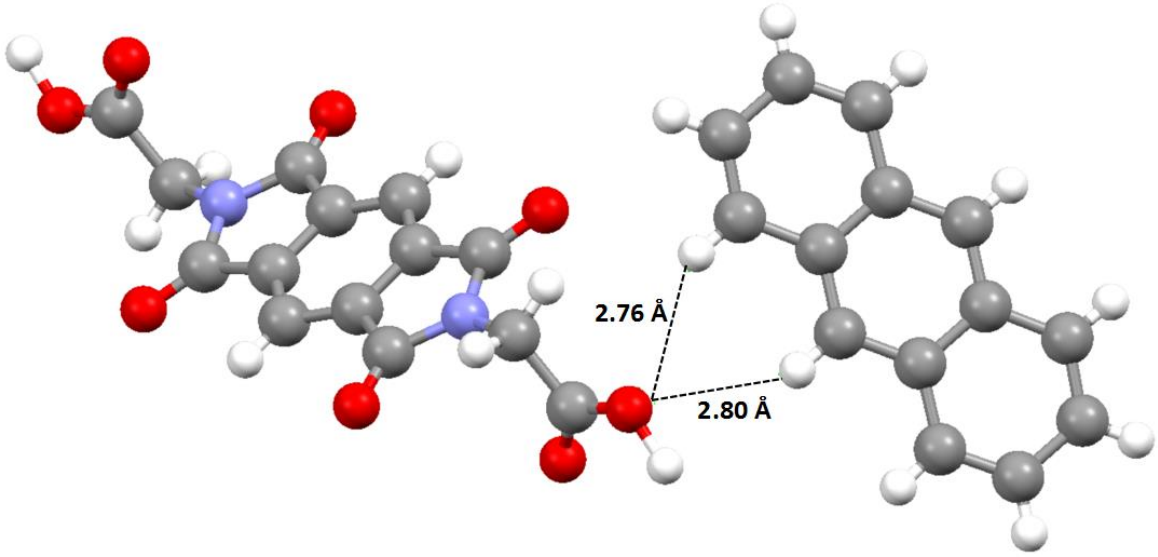


Figure S3. C-H/O contacts in crystal structure GENMES.[1] Oxygen atom forms bifurcated interaction with C-H9 and C-H1 fragments of anthracene.

Table S1. Calculated HOMA values for aromatic rings of benzene, naphthalene, anthracene and tetracene.

	HOMA values			
	Benzene	Naphthalene	Anthracene	Tetracene
Ring I	0.99	0.83	0.93	0.69
Ring II	-	-	0.89	0.67

References:

1. N.Barooah, R.J.Sarma, J.B.Baruah CCDC 290283: Experimental Crystal Structure Determination, 2014, DOI: 10.5517/cc9r1z1

Table S2. Coordinates of optimized benzene-water structure

C	0.00000	0.69696	0.29494
C	0.00000	-0.69696	0.29494
C	0.00000	-1.39319	-0.91255
C	0.00000	-0.69686	-2.12025
C	0.00000	0.69686	-2.12025
C	0.00000	1.39319	-0.91255
H	0.00000	1.22527	1.23792
H	0.00000	-1.22527	1.23792
H	0.00000	-2.47493	-0.91362
H	0.00000	-1.23748	-3.05710
H	0.00000	1.23748	-3.05710
H	0.00000	2.47493	-0.91362
O	0.00000	0.00000	3.71331
H	-0.75389	0.00000	4.30677
H	0.75389	0.00000	4.30677

Table S3. Coordinates of optimized naphthalene-water structure

C	-1.21790	0.80282	0.00000
C	0.00000	0.08125	0.00000
C	-0.03682	-1.34808	0.00000
C	-1.29199	-2.00095	0.00000
C	-2.46177	-1.27413	0.00000
C	-2.42367	0.13680	0.00000
C	1.25336	0.73929	0.00000
C	2.42324	0.01206	0.00000
C	2.38871	-1.39896	0.00000
C	1.18309	-2.06467	0.00000
H	-1.17821	1.88503	0.00000
H	-1.31899	-3.08395	0.00000
H	-3.41490	-1.78581	0.00000
H	-3.34917	0.69701	0.00000
H	1.26920	1.82209	0.00000
H	3.37634	0.52391	0.00000
H	3.31425	-1.95901	0.00000
H	1.15434	-3.14762	0.00000
O	0.12221	4.17497	0.00000
H	0.13595	4.76797	0.75435
H	0.13595	4.76797	-0.75435

Table S4. Coordinates of optimized anthracene-water structure

C	-2.44591	0.65524	0.00000
C	-1.13052	0.11457	0.00000
C	0.00000	0.93853	0.00000
C	1.28976	0.39773	0.00000
C	2.44826	1.22182	0.00000
C	3.70458	0.66951	0.00000
C	3.87009	-0.73908	0.00000
C	2.77544	-1.56683	0.00000
C	1.45817	-1.03277	0.00000
C	0.32629	-1.85377	0.00000
C	-0.96443	-1.31588	0.00000
C	-2.12359	-2.13846	0.00000
C	-3.37841	-1.58261	0.00000
C	-3.54023	-0.17342	0.00000
H	-2.55983	1.73225	0.00000
H	-0.13420	2.01475	0.00000
H	2.31925	2.29737	0.00000
H	4.57611	1.31035	0.00000
H	4.86605	-1.16124	0.00000
H	2.90097	-2.64293	0.00000
H	0.45256	-2.93145	0.00000
H	-1.99924	-3.21469	0.00000
H	-4.25114	-2.22191	0.00000
H	-4.53620	0.24909	0.00000
O	-1.52017	4.18272	0.00000
H	-1.60496	4.76966	0.75448
H	-1.60496	4.76966	-0.75448

Table S5. Coordinates of optimized tethracene-water structure

C	-1.02753	-3.68839	0.00000
C	-0.34315	-2.43985	0.00000
C	-1.03029	-1.22619	0.00000
C	-0.34445	0.00000	0.00000
C	-1.03029	1.22619	0.00000
C	-0.34316	2.43985	0.00000
C	1.10047	2.44213	0.00000
C	1.78677	1.22828	0.00000
C	1.10612	0.00000	0.00000
C	1.78677	-1.22828	0.00000
C	1.10047	-2.44213	0.00000
C	1.78273	-3.69141	0.00000
C	1.08723	-4.87269	0.00000
C	-0.33377	-4.87069	0.00000
C	-1.02753	3.68839	0.00000
C	-0.33377	4.87069	0.00000
C	1.08723	4.87269	0.00000
C	1.78273	3.69141	0.00000
H	-2.11082	-3.68526	0.00000
H	-2.11494	-1.21871	0.00000
H	-2.11494	1.21871	0.00000
H	2.87192	1.23183	0.00000
H	2.87192	-1.23183	0.00000
H	2.86617	-3.69225	0.00000
H	1.62118	-5.81344	0.00000
H	-0.86941	-5.81055	0.00000
H	-2.11082	3.68526	0.00000
H	-0.86941	5.81055	0.00000
H	1.62118	5.81344	0.00000
H	2.86617	3.69225	0.00000
O	-4.41815	-0.00001	0.00000
H	-5.01118	-0.00001	0.75455
H	-5.01118	-0.00001	-0.75455