

Table S1: Summary of results obtained for PAHs used in previous studies

Compound	Refcode	%C...H	%C...C	Ratio (C-H/C-C)	Motif
Benzene (1)	BENZEN11	35.7	0	Infinite	HB
Biphenyl (5)	BIPHEN04	48.1	0	Infinite	HB
Quaterphenyl (12)	QUPHEN	56.7	0	Infinite	HB
Dibenzanthracene (11)	DBNTHR02	59.2	0.1	592.00	HB
Chrysene (8)	CRYSEN	58	0.4	145.00	HB
Picene (10)	ZZZOYC01	60.1	0.5	120.20	HB
Phenanthrene (4)	PHENAN08	51	0.5	102.00	HB
Naphthalene (2)	NAPHTA10	45.1	0.6	75.17	HB
Anthracene (3)	ANTCEN	49.1	1.8	27.28	HB
18-Annulene (19)	ANULEN	37.9	4.8	7.90	γ
Triphenylene (6)	TRIPHE11	41.7	8.7	4.79	HB
Benzo[c]phenanthrene (9)	BZPHAN	38	9.2	4.13	HB
1,2-Benzopyrene (38)	CEQGEL	41.9	10.5	3.99	Sandwich
Benzperylene (15)	BNPERY	44.3	11.8	3.75	Sandwich
Perylene (14)	PERLEN01	42.3	11.8	3.58	Sandwich
Pyrene (13)	PYRENE02	36.6	10.8	3.39	Sandwich
Quaterylene (17)	QUATER10	49.4	15.1	3.27	Sandwich
Diperinaphthyleneanthracene (32)	NAPANT01	40.4	13.8	2.93	β
Dibenzoperylene (20)	DBPERY	39.7	14.9	2.66	γ
Tetrabenzoperylene (29)	TBZPER	34	17.5	1.94	β
Kekulene (26)	KEKULN10	36.8	21.9	1.68	γ
Coronene (21)	CORONE	30.7	19.5	1.57	γ
Hexabenzocoronene (25)	HBZCOR01	36.2	24.8	1.46	γ
Benzopyrene (18)	BNPYRE10	25	19.3	1.30	γ
Ovalene (24)	OVALEN01	30.3	24.2	1.25	γ
Tribenzopyrene (27)	TBZPYR	21.2	22.1	0.96	β
Anthrabenzonaphthopentacene (31)	BOXGAW	15	31.4	0.48	β
Dibenzocoronene (42)	YOFCUR	16.2	34.9	0.46	β
Benzanthracene (7)	BEANTR	Structure incomplete (no H-atoms)			HB
Dinaphthoanthracene (16)	DNAPAN	Structure incomplete (no H-atoms)			Sandwich
Benzobisanthrene (22)	BEANTH	3D Coordinates available			γ
Dibenzocoronene (23)	DBZCOR	no H-atoms			γ
Violanthrene (28)	CORXAI10	no H-atoms			β
Diphenanthroperylene (30)	NAPPYR01	no H-atoms			β