QUANTITATIVE STRUCTURE PROPERTY RELATIONSHIPS FOR ELECTRONIC PROPERTIES OF POLYCYCLIC AROMATIC HYDROCARBONS

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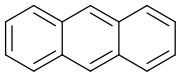
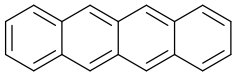
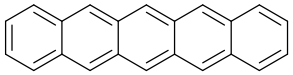
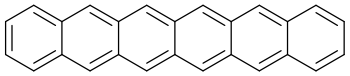
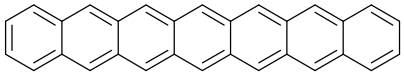
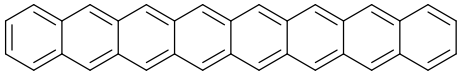
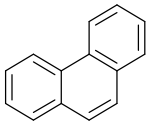
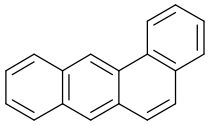
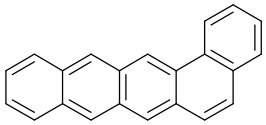
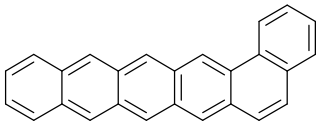
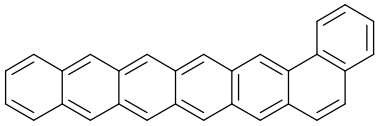
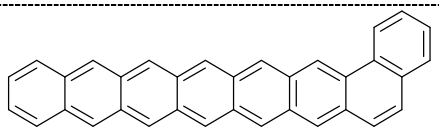
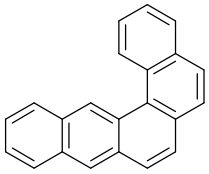
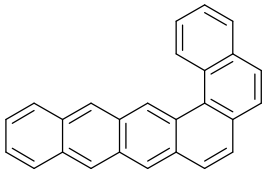
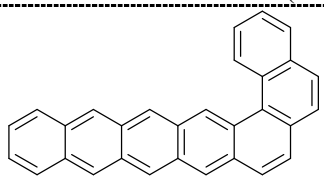
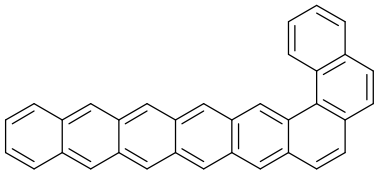
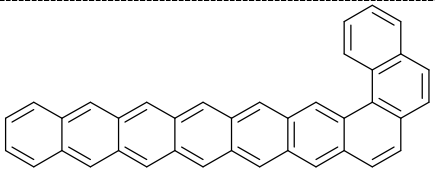
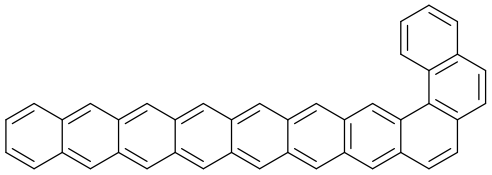
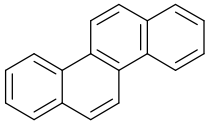
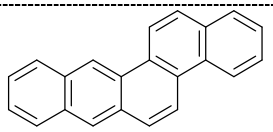
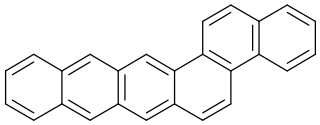
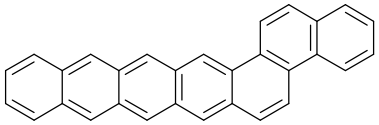
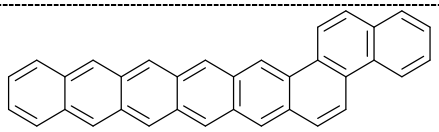
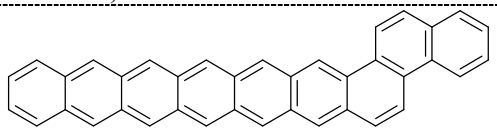
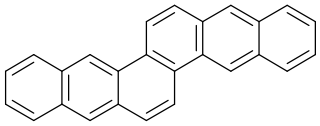
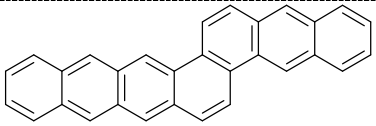
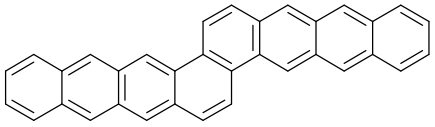
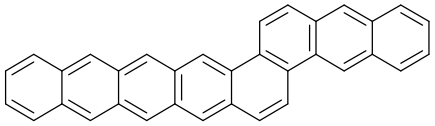
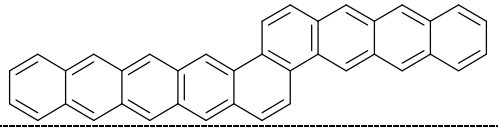
KEYWORDS quantitative structure-property relationships, polycyclic aromatic hydrocarbon, degree of π-orbital overlap, electronic properties.

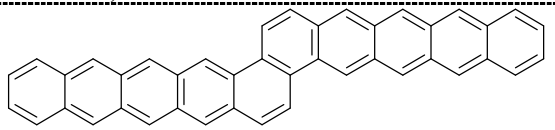
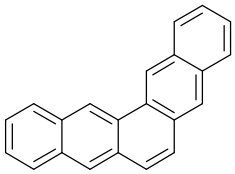
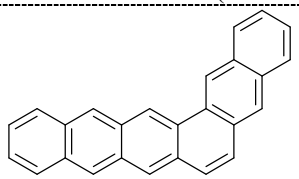
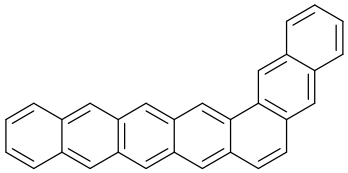
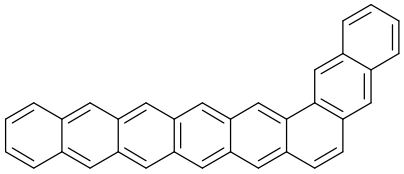
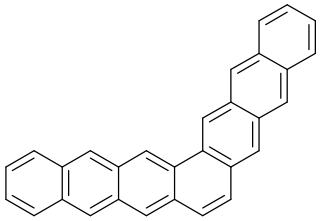
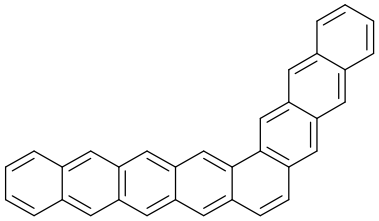
SUPPORTING INFORMATION

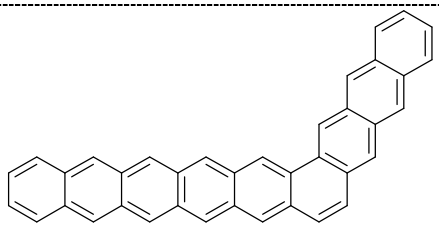
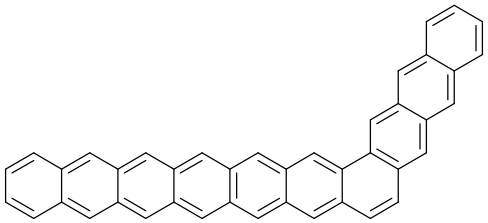
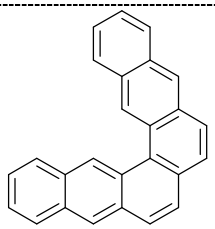
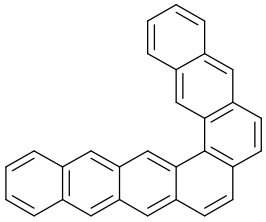
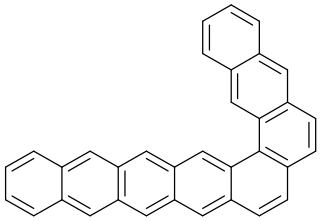
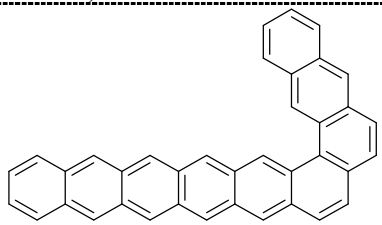
Table S1: PAH molecules used for determining DPO parameters

No	Structure	Band gap (eV)
A1	 C1=CC2=CC3=C(C=CC=C3)C=C2C=C1	3.545
A2	 C1=CC2=CC3=CC4=C(C=CC=C4)C=C3C=C2C=C1	2.747
A3	 C1=CC2=CC3=CC4=CC5=C(C=CC=C5)C=C4C=C3C=C2C=C1	2.188
A4	 C1=CC2=CC3=CC4=CC5=C(C=C6C=CC=CC6=C5)C=C4C=C3C=C2C=C1	1.780
A5	 C1=CC2=CC3=CC4=CC5=C(C=C6C=C7C=CC=CC7=CC6=C5)C=C4C=C3C=C2C=C1	1.472
A6	 C1=CC2=CC3=CC4=CC5=C(C=C4C=C3C=C2C=C1)C=C1C=C2C=C3C=CC=CC3=CC2=CC1=C5	1.235
B1	 C1=CC2=C(C=C1)C1=C(C=CC=C1)C=C2	4.674
B2	 C1=CC2=CC3=C(C=C2C=C1)C1=C(C=CC=C1)C=C3	3.720
B3	 C1=CC2=CC3=CC4=C(C=C3C=C2C=C1)C1=C(C=CC=C1)C=C4	2.920
B4	 C1=CC2=CC3=CC4=CC5=C(C=C4C=C3C=C2C=C1)C1=C(C=CC=C1)C=C5	2.336
B5	 C1=CC2=CC3=CC4=CC5=CC6=C(C=C5C=C4C=C3C=C2C=C1)C1=C(C=CC=C1)C=C6	1.902

B6		1.573
	C1=CC2=CC3=CC4=CC5=CC6=CC7=C(C=C6C=C5C=C4C=C3C=C2C=C1)C1=C(C=CC=C1)C=C7	
C1		3.411
	C1=CC2=CC3=C(C=C2C=C1)C1=C(C=CC2=CC=CC=C12)C=C3	
C2		2.755
	C1=CC2=CC3=CC4=C(C=C3C=C2C=C1)C1=C(C=CC2=CC=CC=C12)C=C4	
C3		2.239
	C1=CC2=CC3=CC4=CC5=C(C=C4C=C3C=C2C=C1)C1=C(C=CC2=CC=CC=C12)C=C5	
C4		1.841
	C1=CC2=CC3=CC4=CC5=CC6=C(C=C5C=C4C=C3C=C2C=C1)C1=C(C=CC2=CC=CC=C12)C=C6	
C5		1.533
	C1=CC2=CC3=CC4=CC5=CC6=CC7=C(C=C6C=C5C=C4C=C3C=C2C=C1)C1=C(C=CC2=CC=CC=C12)C=C7	
C6		1.290
	C1=CC2=CC3=CC4=CC5=CC6=CC7=CC8=C(C=C7C=C6C=C5C=C4C=C3C=C2C=C1)C1=C(C=CC2=CC=CC=C12)C=C8	
D1		4.207
	C1=CC2=C(C=C1)C1=C(C=C2)C2=C(C=CC=C2)C=C1	

D2	 C1=CC2=CC3=C(C=C2C=C1)C1=C(C=C3)C2=C(C=CC=C2)C=C1	3.469
D3	 C1=CC2=CC3=CC4=C(C=C3C=C2C=C1)C1=C(C=C4)C2=C(C=CC=C2)C=C1	2.782
D4	 C1=CC2=CC3=CC4=CC5=C(C=C4C=C3C=C2C=C1)C1=C(C=C5)C2=C(C=CC=C2)C=C1	2.247
D5	 C1=CC2=CC3=CC4=CC5=CC6=C(C=C5C=C4C=C3C=C2C=C1)C1=C(C=C6)C2=C(C=CC=C2)C=C1	1.840
D6	 C1=CC2=CC3=CC4=CC5=CC6=CC7=C(C=C6C=C5C=C4C=C3C=C2C=C1)C1=C(C=C7)C2=C(C=CC=C2)C=C1	1.527
D7	 C1=CC2=CC3=C(C=C2C=C1)C1=C(C=C3)C2=C(C=C1)C=C1C=CC=CC1=C2	3.117
D8	 C1=CC2=CC3=CC4=C(C=C3C=C2C=C1)C1=C(C=C4)C2=C(C=C1)C=C1C=CC=CC1=C2	2.635
D9	 C1=CC2=CC3=CC4=C(C=C3C=C2C=C1)C1=C(C=C4)C2=CC3=CC4=C(C=CC=C4)C=C3C=C2C=C1	2.404
D10	 C1=CC2=CC3=CC4=CC5=C(C=C4C=C3C=C2C=C1)C1=C(C=C5)C2=CC3=CC=CC=C3C=C2C=C1	2.173
D11		2.077

	C1=CC2=CC3=CC4=CC5=C(C=C4C=C3C=C2C=C1)C1=C(C=C5)C2=CC3=CC4=C(C=CC=C4)C=C3C=C2C=C1	
D12	 C1=CC2=CC3=CC4=CC5=C(C=C4C=C3C=C2C=C1)C1=C(C=C5)C2=CC3=CC4=C(C=C5C=CC=CC5=C4)C=C3C=C2C=C1	1.916
D13	 C1=CC2=CC3=C(C=C2C=C1)C1=CC2=CC=CC=C2C=C1C=C3	3.749
D14	 C1=CC2=CC3=CC4=C(C=C3C=C2C=C1)C1=CC2=CC=CC=C2C=C1C=C4	2.998
D15	 C1=CC2=CC3=CC4=CC5=C(C=C4C=C3C=C2C=C1)C1=CC2=CC=CC=C2C=C1C=C5	2.399
D16	 C1=CC2=CC3=CC4=CC5=CC6=C(C=C5C=C4C=C3C=C2C=C1)C1=CC2=CC=CC=C2C=C1C=C6	1.954
D17	 C1=CC2=CC3=CC4=C(C=C3C=C2C=C1)C1=CC2=CC3=CC=CC=C3C=C2C=C1C=C4	2.982
D18	 C1=CC2=CC3=CC4=CC5=C(C=C4C=C3C=C2C=C1)C1=CC2=CC3=CC=CC=C3C=C2C=C1C=C5	2.428

D19	 C1=CC2=CC3=CC4=CC5=CC6=C(C=C5C=C4C=C3C=C2C=C1)C1=CC2=CC3=CC=CC=C3C=C2C=C1C=C6	1.978
D20	 C1=CC2=CC3=CC4=CC5=CC6=CC7=C(C=C6C=C5C=C4C=C3C=C2C=C1)C1=CC2=CC3=CC=CC=C3C=C2C=C1C=C7	1.636
D21	 C1=CC2=CC3=C(C=C2C=C1)C1=C(C=C3)C=CC2=C1C=C1C=CC=CC1=C2	3.199
D22	 C1=CC2=CC3=CC4=C(C=C3C=C2C=C1)C1=C(C=CC2=C1C=C1C=CC=CC1=C2)C=C4	2.681
D23	 C1=CC2=CC3=CC4=CC5=C(C=C4C=C3C=C2C=C1)C1=C(C=CC2=C1C=C1C=CC=CC1=C2)C=C5	2.193
D24	 C1=CC2=CC3=CC4=CC5=CC6=C(C=C5C=C4C=C3C=C2C=C1)C1=C(C=CC2=C1C=C1C=CC=CC1=C2)C=C6	1.733

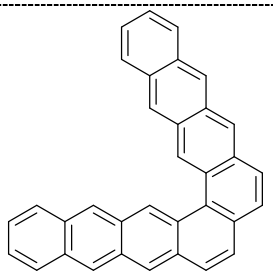
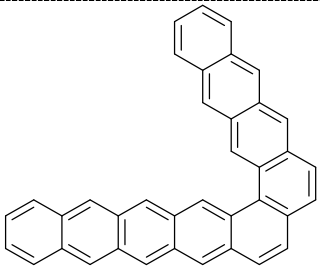
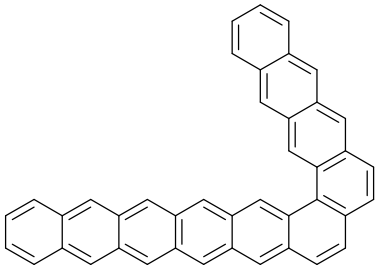
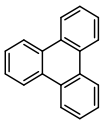
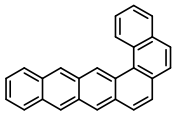
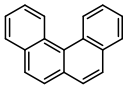
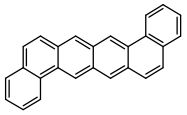
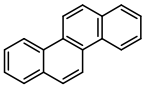
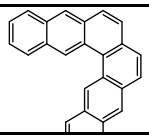
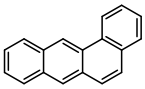
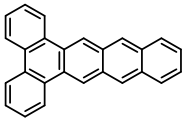
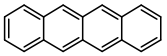
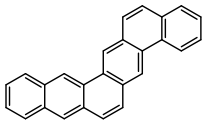
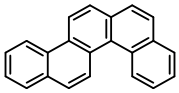
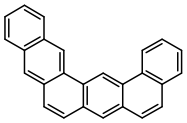
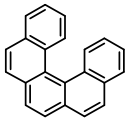
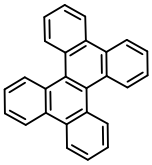
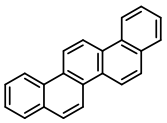
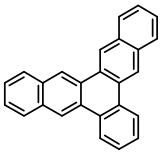
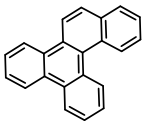
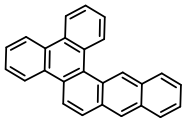
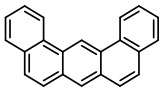
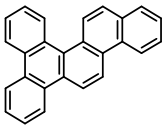
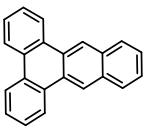
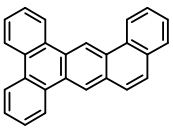
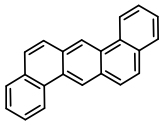
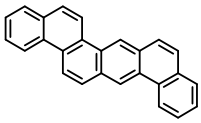
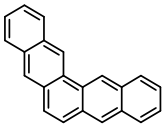
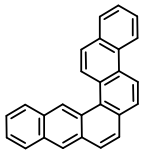
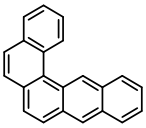
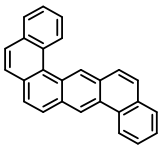
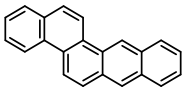
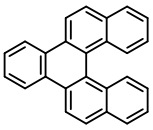
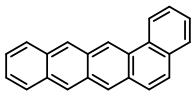
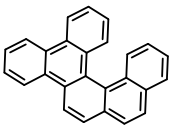
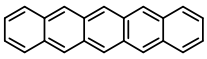
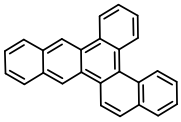
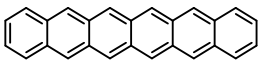
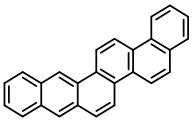
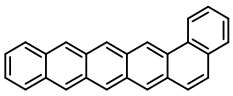
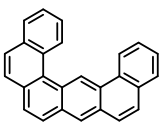
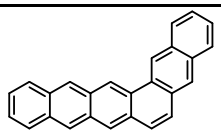
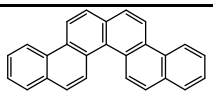
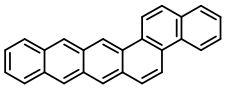
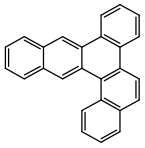
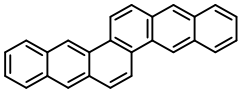
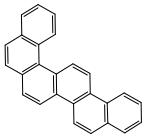
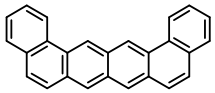
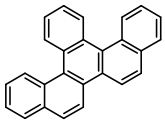
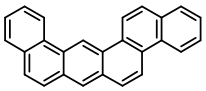
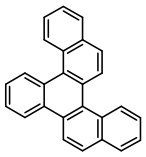
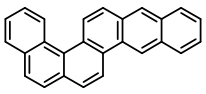
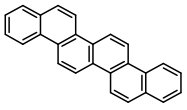
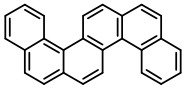
D25	 C1=CC2=CC3=CC4=C(C=C3C=C2C=C1)C1=C(C=C4)C=CC2=C1C=C1C=C3C=CC=CC3=CC1=C2	2.492
D26	 C1=CC2=CC3=CC4=CC5=C(C=C4C=C3C=C2C=C1)C1=C(C=CC2=C1C=C1C=C3C=CC=CC3=CC1=C2)C=C5	2.003
D27	 C1=CC2=CC3=CC4=CC5=CC6=C(C=C5C=C4C=C3C=C2C=C1)C1=C(C=CC2=C1C=C1C=C3C=CC=CC3=CC1=C2)C=C6	1.543

Table S2a: Egap, IP and EA properties (in eV) of PAH molecules having 4 to 6 fused rings.

Structure	Parameters		Structure	Parameters	
 **4.1**	Egap	8.173(4.837)	 **6.10**	Egap	6.536(2.755)
	IP	8.825(6.134)		IP	8.012(5.139)
	EA	0.652(1.297)		EA	1.476(2.384)
	$B_G(1)$	9		$B_G(1)$	14
	DPO	0.5		DPO	2.93
 **4.2**	Egap	7.746(4.168)	 **6.11**	Egap	6.834(3.084)
	IP	8.591(5.812)		IP	8.184(5.315)
	EA	0.845(1.644)		EA	1.350(2.231)
	$B_G(1)$	8		$B_G(1)$	16
	DPO	0.5		DPO	2.35
 **4.3**	Egap	7.698(4.207)		Egap	6.762(3.027)
	IP	8.596(5.799)		IP	8.116(5.271)
	EA	0.898(1.592)		EA	1.354(2.244)

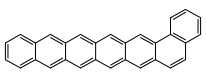
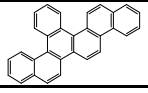
	$B_G(1)$	8	**6.12**	$B_G(1)$	15
	DPO	1.08		DPO	2.35
	Egap	7.400(3.720)		Egap	6.796(3.016)
	IP	8.450(5.599)		IP	8.169(5.294)
 **4.4**	EA	1.050(1.879)	 **6.13**	EA	1.373(2.278)
	$B_G(1)$	7		$B_G(1)$	17
	DPO	1.70		DPO	2.35
	Egap	6.563(2.747)		Egap	7.255(3.622)
	IP	8.028(5.131)		IP	8.392(5.549)
 **4.5**	EA	1.465(2.384)	 **6.14**	EA	1.137(1.927)
	$B_G(1)$	5		$B_G(1)$	17
	DPO	2.85		DPO	1.73
	Egap	7.695(4.201)		Egap	7.305(3.670)
	IP	8.590(5.813)		IP	8.423(5.593)
 **5.1**	EA	0.895(1.612)	 **6.15**	EA	1.118(1.923)
	$B_G(1)$	13		$B_G(1)$	17
	DPO	0.83		DPO	1.37
	Egap	7.660(4.122)		Egap	7.246(3.807)
	IP	8.530(5.768)		IP	8.300(5.570)
 **5.2**	EA	0.870(1.646)	 **6.16**	EA	1.054(1.763)
	$B_G(1)$	13		$B_G(1)$	24
	DPO	1.19		DPO	1.17
	Egap	7.643(4.19)		Egap	7.493(3.849)
	IP	8.575(5.779)		IP	8.517(5.739)
 **5.3**	EA	0.932(1.589)	 **6.17**	EA	1.024(1.890)
	$B_G(1)$	13		$B_G(1)$	19
	DPO	0.83		DPO	1.37
	Egap	7.511(4.042)		Egap	6.931(3.313)
	IP	8.469(5.723)		IP	8.192(5.384)
 **5.4**	EA	0.958(1.681)	 **6.18**	EA	1.261(2.071)
	$B_G(1)$	14		$B_G(1)$	19
	DPO	0.83		DPO	2.37
	Egap	7.495(3.887)		Egap	7.580(4.130)
	IP	8.507(5.692)		IP	8.517(5.772)
 **5.5**	EA	1.012(1.805)	 **6.19**	EA	0.937(1.643)
	$B_G(1)$	12		$B_G(1)$	23
	DPO	1.45		DPO	0.58
	Egap	7.490(3.853)		Egap	7.549(3.983)
	IP	8.504(5.695)		IP	8.540(5.756)
 **5.6**	EA	1.015(1.842)	 **6.20**	EA	0.991(1.773)
	$B_G(1)$	13		$B_G(1)$	22

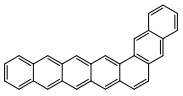
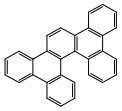
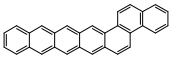
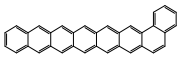
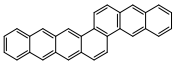
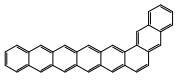
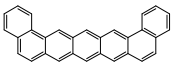
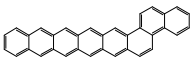
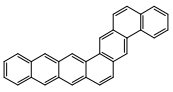
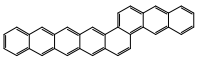
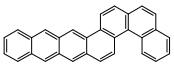
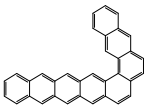
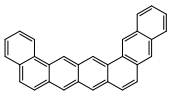
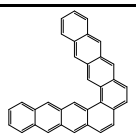
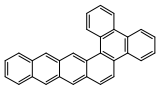
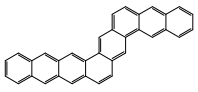
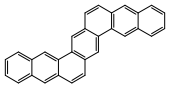
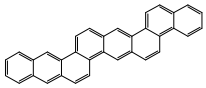
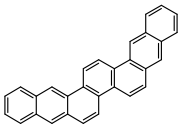
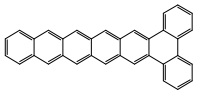
	DPO	1.45		DPO	1.2
 **5.7**	Egap	7.459(3.846)	 **6.21**	Egap	7.182(3.606)
	IP	8.485(5.654)		IP	8.356(5.544)
	EA	1.026(1.808)		EA	1.174(1.939)
	$B_G(1)$	12		$B_G(1)$	19
	DPO	1.33 (1.45)		DPO	1.78
 **5.8**	Egap	7.379(3.749)	 **6.22**	Egap	7.160(3.482)
	IP	8.446(5.593)		IP	8.322(5.493)
	EA	1.067(1.844)		EA	1.162(2.010)
	$B_G(1)$	10		$B_G(1)$	18
	DPO	1.62		DPO	1.95
 **5.9**	Egap	7.100(3.411)	 **6.23**	Egap	7.207(3.559)
	IP	8.281(5.448)		IP	8.344(5.530)
	EA	1.181(2.037)		EA	1.137(1.971)
	$B_G(1)$	11		$B_G(1)$	19
	DPO	2.03		DPO	1.78
 **5.10**	Egap	7.084(3.469)	 **6.24**	Egap	7.316(3.894)
	IP	8.300(5.478)		IP	8.367(5.637)
	EA	1.216(2.009)		EA	1.051(1.743)
	$B_G(1)$	11		$B_G(1)$	22
	DPO	2.03		DPO	1.17
 **5.11**	Egap	6.701(2.920)	 **6.25**	Egap	7.522(4.023)
	IP	8.109(5.226)		IP	8.467(5.733)
	EA	1.408(2.307)		EA	0.945(1.710)
	$B_G(1)$	9		$B_G(1)$	23
	DPO	2.60		DPO	1.17
 **5.12**	Egap	6.051(2.188)	 **6.26**	Egap	7.142(3.587)
	IP	7.782(4.870)		IP	8.310(5.531)
	EA	1.731(2.682)		EA	1.168(1.944)
	$B_G(1)$	6		$B_G(1)$	20
	DPO	3.70		DPO	1.78
 **6.1**	Egap	5.682(1.780)	 **6.27**	Egap	7.145(3.521)
	IP	7.609(4.680)		IP	8.340(5.518)
	EA	1.927(2.900)		EA	1.195(1.997)
	$B_G(1)$	7		$B_G(1)$	18
	DPO	4.50		DPO	1.95
 **6.2**	Egap	6.179(2.336)	 **6.28**	Egap	7.189(3.549)
	IP	7.857(4.952)		IP	8.337(5.523)
	EA	1.678(2.616)		EA	1.148(1.974)
	$B_G(1)$	11		$B_G(1)$	19
	DPO	3.45		DPO	1.78
	Egap	6.782(2.998)		Egap	7.398(3.901)

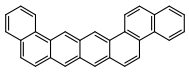
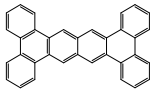
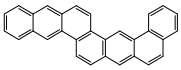
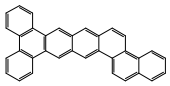
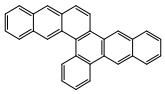
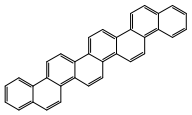
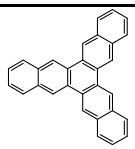
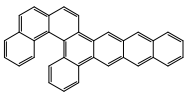
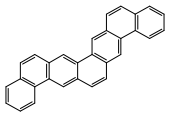
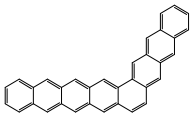
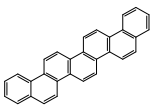
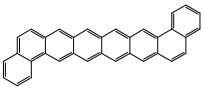
 **6.3**	IP	8.159(5.274)	 **6.29**	IP	8.455(5.683)
	EA	1.378(2.276)		EA	1.057(1.782)
	$B_G(1)$	13		$B_G(1)$	21
	DPO	2.52		DPO	1.17
 **6.4**	Egap	6.517(2.782)	 **6.30**	Egap	7.152(3.548)
	IP	8.026(5.165)		IP	8.305(5.501)
	EA	1.509(2.383)		EA	1.153(1.953)
	$B_G(1)$	14		$B_G(1)$	20
	DPO	2.93		DPO	1.78
 **6.5**	Egap	6.749(3.117)	 **6.31**	Egap	7.476(3.972)
	IP	8.140(5.316)		IP	8.477(5.707)
	EA	1.391(2.199)		EA	1.001(1.735)
	$B_G(1)$	15		$B_G(1)$	21
	DPO	2.35		DPO	1.17
 **6.6**	Egap	6.837(3.091)	 **6.32**	Egap	7.402(3.881)
	IP	8.186(5.321)		IP	8.418(5.678)
	EA	1.349(2.230)		EA	1.016(1.797)
	$B_G(1)$	16		$B_G(1)$	22
	DPO	2.35		DPO	0.58
 **6.7**	Egap	7.187(3.619)	 **6.33**	Egap	7.301(3.809)
	IP	8.361(5.558)		IP	8.368(5.620)
	EA	1.174(1.939)		EA	1.067(1.811)
	$B_G(1)$	19		$B_G(1)$	22
	DPO	1.78		DPO	1.17
 **6.8**	Egap	7.114(3.469)	 **6.34**	Egap	7.439(4.007)
	IP	8.310(5.479)		IP	8.481(5.703)
	EA	1.196(2.010)		EA	1.042(1.697)
	$B_G(1)$	18		$B_G(1)$	21
	DPO	1.95		DPO	1.17
 **6.9**	Egap	7.422(3.918)			
	IP	8.428(5.682)			
	EA	1.006(1.764)			
	$B_G(1)$	21			
	DPO	0.75			

** Egap, EA, and IP values in parentheses are calculated by DFT method while others by the PM7 method.*

Table S2b: Calculated Egap, IP and EA (in eV) properties for 7 to 8 fused PAHs rings.

Structure	Parameters		Structure	Parameters	
	Egap	5.788 (1.902)		Egap	7.347 (3.885)
	IP	7.671 (4.747)		IP	8.400 (5.683)

7.1	EA	1.883 (2.845)	**7.18**	EA	1.053 (1.798)
	DPO	4.25		DPO	0.92
 **7.2**	Egap	6.244 (2.399)	 **7.19**	Egap	7.596 (4.081)
	IP	7.898 (4.992)		IP	8.514 (5.801)
	EA	1.654 (2.593)		EA	0.918 (1.720)
	DPO	3.37		DPO	0.67
 **7.3**	Egap	6.059 (2.247)	 **8.1**	Egap	5.493 (1.573)
	IP	7.806 (4.916)		IP	7.533 (4.592)
	EA	1.747 (2.669)		EA	2.040 (3.019)
	DPO	3.78		DPO	5.00
 **7.4**	Egap	6.355 (2.635)	 **8.2**	Egap	5.840 (1.954)
	IP	7.952 (5.098)		IP	7.704 (4.780)
	EA	1.597 (2.463)		EA	1.864 (2.826)
	DPO	3.25		DPO	4.17
 **7.5**	Egap	6.308 (2.485)	 **8.3**	Egap	5.705 (1.840)
	IP	7.931 (5.034)		IP	7.638 (4.725)
	EA	1.623 (2.549)		EA	1.933 (2.885)
	DPO	3.20		DPO	4.58
 **7.6**	Egap	6.692 (2.924)	 **8.4**	Egap	5.972 (2.173)
	IP	8.122 (5.242)		IP	7.770 (4.885)
	EA	1.430 (2.318)		EA	1.798 (2.712)
	DPO	2.63		DPO	4.10
 **7.7**	Egap	6.555 (2.792)	 **8.5**	Egap	5.992 (2.140)
	IP	8.040 (5.164)		IP	7.758 (4.856)
	EA	1.485 (2.372)		EA	1.766 (2.716)
	DPO	2.85		DPO	3.89
 **7.8**	Egap	6.914 (3.169)	 **8.6**	Egap	6.162 (2.331)
	IP	8.234 (5.368)		IP	7.837 (4.945)
	EA	1.320 (2.199)		EA	1.675 (2.614)
	DPO	2.27		DPO	3.08
 **7.9**	Egap	6.425 (2.689)	 **8.7**	Egap	6.606 (2.831)
	IP	7.956 (5.100)		IP	8.083 (5.202)
	EA	1.531 (2.411)		EA	1.477 (2.371)
	DPO	3.27		DPO	2.73
 **7.10**	Egap	7.024 (3.346)	 **8.8**	Egap	6.709 (3.117)
	IP	8.282 (5.433)		IP	8.135 (5.327)
	EA	1.258 (2.087)		EA	1.426 (2.210)
	DPO	1.83		DPO	2.43
 **7.11**	Egap	7.156 (3.466)	 **8.9**	Egap	5.846 (1.955)
	IP	8.350 (5.528)		IP	7.709 (4.783)
	EA	1.194 (2.062)		EA	1.863 (2.828)
	DPO	1.92		DPO	4.00

 **7.12**	Egap	6.643 (2.941)	 **8.10**	Egap	7.021 (3.291)
	IP	8.098 (5.251)		IP	8.297 (5.460)
	EA	1.455 (2.310)		EA	1.276 (2.171)
	DPO	2.68		DPO	1.85
 **7.13**	Egap	6.828 (3.212)	 **8.11**	Egap	6.726 (3.027)
	IP	8.189 (5.370)		IP	8.149 (5.310)
	EA	1.361 (2.158)		EA	1.423 (2.283)
	DPO	2.10		DPO	2.43
 **7.14**	Egap	6.743 (3.131)	 **8.12**	Egap	7.315 (3.908)
	IP	8.114 (5.306)		IP	8.432 (5.660)
	EA	1.371 (2.175)		EA	1.117 (1.752)
	DPO	2.10		DPO	1.19
 **7.15**	Egap	7.580 (3.716)	 **8.13**	Egap	6.682 (2.939)
	IP	8.574 (5.709)		IP	8.097 (5.238)
	EA	0.994 (1.993)		EA	1.415 (2.299)
	DPO	1.28		DPO	2.60
 **7.16**	Egap	7.252 (3.667)	 **8.14**	Egap	6.279 (2.428)
	IP	8.395 (5.555)		IP	7.925 (5.013)
	EA	1.143 (1.888)		EA	1.646 (2.585)
	DPO	1.48		DPO	3.34
 **7.17**	Egap	7.417 (4.002)	 **8.15**	Egap	5.899 (2.029)
	IP	8.477 (5.692)		IP	7.735 (4.817)
	EA	1.060 (1.690)		EA	1.836 (2.788)
	DPO	1.08		DPO	4.00

** Egap, EA, and IP values in parentheses are calculated by DFT method while others by the PM7 method*