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	Structural Information (indication of number or					Topological Information (Number of Edge Group and Ring Types)									Results	
Molecule Name	Carbons	Hydrogens	Rings	5-membered Rings	Aliphatics	Armchair	Zigzag	Free Edge	Bay	Fjord	Aromatic Sextets	Empty Rings	Dbl(1)	Dbl(2)	HOMO-LUMO Gap (eV)	BE Avg (kJ/mol)
benzene	6	6	1	0	N	0	0	6	0	0	1	0	0	0	8.0444	
ethynylbenzene	8	6	1	0	Y	0	0	7	0	0	1	0	0	0	5.4968	
styrene	8	8	1	0	Y	0	0	7	0	0	1	0	0	0	5.4447	
1_3-diethynylbenzene	10	6	1	0	Y	0	0	8	0	0	1	0	0	0	5.2591	
1_4-diethynyl-2-vinylbenzene	12	8	1	0	Y	0	0	9	0	0	1	0	0	0	4.51	
1_3-diethynyl-5-vinylbenzene	12	8	1	0	Y	0	0	9	0	0	1	0	0	0	5.0386	
naphthalene	10	8	2	0	N	0	2	6	0	0	1	0	0	1	4.6722	
1_1'-biphenyl	12	10	2	0	Y	0	0	12	0	0	2	0	0	0	5.2148	-38.05
1-vinylnaphthalene	12	10	2	0	Y	0	2	7	0	0	1	0	0	1	4.1595	
2-vinylnaphthalene	12	10	2	0	Y	0	2	7	0	0	1	0	0	1	4.2733	
acenaphthylene	12	8	3	1	N	0	3	5	0	0	1	0	1	1	4.1133	
5-vinylacenaphthylene	14	10	3	1	Y	0	3	6	0	0	1	0	1	1	3.748	
4-vinylacenaphthylene	14	10	3	1	Y	0	3	5	0	0	1	0	1	1	3.8584	
4-	14	8	3	0	Y	0	3	6	0	0	1	0	1	1	3.891	
3-	14	8	3	1	Y	0	3	6	0	0	1	0	1	1	3.8822	
anthracene	14	10	3	0	N	0	4	6	0	0	1	0	0	2	3.5087	-48.71
phenanthrene	14	10	3	0	N	1	2	7	0	0	2	0	1	0	4.3985	-44.49
2-phenylnaphthalene	16	12	3	0	Y	0	2	12	0	0	2	0	0	1	4.3678	-38.47
1-ethynyl-8-vinylacenaphthylene	16	10	3	1	Y	0	3	7	0	0	1	0	1	1	3.5406	
3-ethynyl-8-vinylacenaphthylene	16	10	3	1	Y	0	3	7	0	0	1	0	1	1	3.5764	
4_7-divinylacenaphthylene	16	12	3	1	Y	0	3	7	0	0	1	0	1	1	3.8056	
4_6-divinylacenaphthylene	16	12	3	1	Y	0	3	7	0	0	1	0	1	1	3.5599	
cyclopenta[fg]acenaphthylene	14	8	4	2	N	0	4	4	0	0	1	0	2	1	3.8592	
3-vinylcyclopenta[fg]acenaphthylene	16	10	4	2	Y	0	4	5	0	0	1	0	2	1	3.0188	
3-ethynylcyclopenta[fg]acenaphthylene	16	8	4	2	Y	0	4	5	0	0	1	0	2	1	3.1296	-57.26
aceanthrylene	16	10	4	1	N	1	3	6	0	0	1	0	1	2	3.2852	-59.18
acephenanthrylene	16	10	4	1	N	1	3	6	0	0	2	0	2	0	3.7223	
pyrene	16	10	4	0	N	0	4	6	0	0	2	0	2	0	3.9302	
3-ethynyl-8-vinylcyclopenta[fg]acenaphthylene	18	10	4	2	Y	0	4	6	0	0	1	0	2	1	2.9235	
3-ethynyl-4-vinylcyclopenta[fg]acenaphthylene	18	10	4	2	Y	0	4	6	0	0	1	0	2	1	2.8557	
3_8-divinylcyclopenta[fg]acenaphthylene	18	12	4	2	Y	0	4	6	0	0	1	0	2	1	2.8489	
2-ethylpyrene	18	14	4	0	Y	0	4	6	0	0	2	0	2	0	3.9106	
2-vinylpyrene	18	12	4	0	Y	0	4	7	0	0	2	0	2	0	3.8623	
tetraphene	18	12	4	0	N	1	4	7	0	0	2	0	1	1	4.5382	-66.11
chrysene	18	12	4	0	N	2	2	8	0	0	2	0	1	1	3.9613	-68.25
tetracene	18	12	4	0	N	0	6	6	0	0	1	0	0	3	2.7412	-62.34
triphenylene	18	12	4	0	N	3	0	9	0	0	3	1	0	0	4.9796	-70.88
2-propylpyrene	19	16	4	0	Y	0	4	6	0	0	2	0	2	0	3.9098	
(E)-2-(buta-1_3-dien-1-yl)pyrene	20	14	4	0	Y	0	4	8	0	0	2	0	2	0	3.9362	
2-butylpyrene	20	18	4	0	Y	0	4	6	0	0	2	0	2	0	3.9104	
benzo[ghi]fluoranthene	18	10	5	1	N	1	3	6	0	0	2	1	1	1	3.8173	-69.03
benzo[mno]aceanthrylene	18	10	5	1	N	0	5	5	0	0	1	0	2	2	1.9979	-67.93
cyclopenta[hi]aceanthrylene	18	10	5	2	N	2	2	6	0	0	1	0	2	2	3.0495	
cyclopenta[fg]aceanthrylene	18	12	5	2	N	2	2	6	0	0	1	1	0	3	2.9921	
cyclopenta[hi]acephenanthrylene	18	10	5	2	N	2	2	6	0	0	2	0	3	0	3.754	
cyclopenta[cd]pyrene	18	10	5	1	N	0	5	5	0	0	2	0	3	0	3.6927	-67.22
5-vinylcyclopenta[hi]aceanthrylene	20	12	5	2	Y	2	2	7	0	0	1	0	2	2	2.8518	

	Structural Information (indication of number or					Topological Information (Number of Edge Group and Ring Types)									Results	
Molecule Name	Carbons	Hydrogens	Rings	5-membered Rings	Aliphatics	Armchair	Zigzag	Free Edge	Bay	Fjord	Aromatic Sextets	Empty Rings	Dbl(1)	Dbl(2)	HOMO-LUMO Gap (eV)	BE Avg (kJ/mol)
benzo[pqr]tetraphene	20	12	5	0	N	1	4	7	0	0	2	0	2	1	3.3821	-77.91
benzo[e]pyrene	20	12	5	0	N	2	2	8	0	0	3	1	1	0	3.9104	-76.82
perylene	20	12	5	0	N	2	2	8	0	0	2	1	0	2	3.1423	-79.29
2_10-divinylcyclopenta[hi]aceanthrylene	22	14	5	2	Y	2	2	8	0	0	1	0	2	2	1.9312	
benzo[c]chrysene	22	14	5	0	N	1	3	9	1	0	3	0	2	0	4.2388	
dibenzo[c_g]phenanthrene	22	14	5	0	N	0	4	9	1	0	3	0	2	0	4.0461	
benzo[k]tetraphene	22	14	5	0	N	2	4	8	0	0	3	0	2	0	3.6261	-79.73
benzo[f]tetraphene	22	14	5	0	N	3	2	9	0	0	3	1	0	1	4.6564	-86.94
benzo[m]tetraphene	22	14	5	0	N	2	4	8	0	0	3	0	2	0	4.3454	-80.43
pentaphene	22	14	5	0	N	1	6	7	0	0	2	0	1	2	3.5374	-78.53
benzo[a]tetracene	22	14	5	0	N	1	6	7	0	0	2	0	1	2	2.8524	-77.76
benzo[g]chrysene	22	14	5	0	N	2	1	10	1	0	3	1	0	1	3.7974	
picene	22	14	5	0	N	3	2	9	0	0	3	0	2	0	3.8325	-81.28
pentacene	22	14	5	0	N	0	8	6	0	0	1	0	0	4	2.2042	-75.17
3-vinylcyclopenta[fg]aceanthrylene	20	12	6	2	Y	2	2	7	0	0	1	0	2	2	2.8597	
8-vinylcyclopenta[fg]aceanthrylene	20	12	6	2	Y	2	2	7	0	0	1	0	2	2	2.761	
dicyclopenta[cd_fg]pyrene	20	10	6	2	N	1	4	5	0	0	2	0	4	0	3.4412	
dibenzo[ghi_mno]fluoranthene	20	10	6	1	N	0	5	5	0	0	2	1	2	1	4.4919	-78.46
dicyclopenta[cd_mn]pyrene	20	10	6	2	N	0	6	4	0	0	2	0	4	0	3.6318	-80.96
3-vinyldicyclopenta[cd_fg]pyrene	22	12	6	2	Y	1	4	6	0	0	2	0	4	0	3.1664	
cyclopenta[cd]perylene	22	12	6	1	N	2	3	7	0	0	2	1	1	2	2.9143	-86.94
benzo[l]cyclopenta[cd]pyrene	22	12	6	1	N	2	3	7	0	0	3	1	2	0	3.3761	-89.26
benzo[pqr]cyclopenta[gh]tetraphene	22	12	6	1	N	2	3	7	0	0	2	0	3	1	2.4294	-87.96
indeno[5_6_7_1-pqra]tetraphene	22	12	6	1	N	1	5	6	0	0	2	0	3	1	3.1312	-85.44
benzo[pqr]cyclopenta[de]tetraphene	22	12	6	1	N	1	5	6	0	0	2	0	3	1	2.5959	-85.17
benzo[pqr]cyclopenta[ij]tetraphene	22	12	6	1	N	2	3	7	0	0	2	0	3	1	2.7594	-84.44
indeno[1_2_3-cd]pyrene	22	12	6	1	N	2	3	7	0	0	3	1	2	0	3.0118	-84.56
indeno[6_7_1_2-ghij]tetraphene	22	12	6	1	N	1	5	6	0	0	2	0	3	1	2.2059	-86.28
dicyclopenta[de_op]tetracene	22	12	6	2	N	3	2	7	0	0	1	0	2	3	2.1565	
7-vinyldicyclopenta[cd_mn]pyrene	22	16	6	2	N	0	6	5	0	0	2	0	4	0	3.3967	
indeno[1_2_3-cd]fluoranthene	22	12	6	2	N	4	0	8	0	0	3	2	0	1	3.2844	-76.45
naphtho[7_8_1_2_3-nopqr]tetraphene	22	12	6	0	N	0	6	6	0	0	2	0	3	1	3.1009	-87.92
benzo[ghi]perylene	22	12	6	0	N	1	4	7	0	0	3	1	2	0	3.4394	-85.25
8-vinyldicyclopenta[de_op]tetracene	24	14	6	2	Y	3	2	8	0	0	1	0	2	3	2.1177	
dibenzo[de_mn]tetracene	24	14	6	0	N	2	4	8	0	0	2	0	2	2	2.5656	-91.98
benzo[rst]pentaphene	24	14	6	0	N	2	4	8	0	0	3	0	3	0	3.2962	-93.14
naphtho[2_1_8-qra]tetracene	24	14	6	0	N	1	6	7	0	0	2	0	2	2	2.8116	-90.19
benzo[pqr]picene	24	14	6	0	N	2	4	8	0	0	3	0	3	0	3.3103	-92.41
naphtho[1_2_3_4-pqr]tetraphene	24	14	6	0	N	1	3	9	1	0	3	1	1	1	3.2999	
dibenzo[m_pqr]tetraphene	24	14	6	0	N	0	5	8	1	0	3	0	3	0	3.3587	

	Structural Information (indication of number or					Topological Information (Number of Edge Group and Ring Types)									Results	
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dibenzo[ij_no]tetraphene	24	14	6	0	N	1	3	9	1	0	3	1	1	1	3.5193	
dibenzo[c_pqr]tetraphene	24	14	6	0	N	2	4	8	0	0	2	0	2	2	2.9044	-91.95
dibenzo[de_qr]tetracene	24	14	6	0	N	2	4	8	0	0	3	1	1	1	3.8675	-94.02
dibenzo[f_pqr]tetraphene	24	14	6	0	N	3	2	9	0	0	3	1	1	1	3.431	-89.64
benzo[b]perylene	24	14	6	0	N	3	2	9	0	0	3	1	1	1	3.1062	-92.6
benzo[a]perylene	24	14	6	0	N	1	3	9	1	0	2	1	0	3	2.6582	
dibenzo[fg_op]tetracene	24	14	6	0	N	4	0	10	0	0	4	2	0	0	3.9006	-100.91
dibenzo[a_c]tetraphene	26	16	6	0	N	2	3	10	1	0	3	1	0	2	3.1595	
naphtho[1_2-a]tetraphene	26	16	6	0	N	0	6	9	0	1	3	0	2	1	3.5646	
dibenzo[a_m]tetraphene	26	16	6	0	N	1	5	9	1	0	3	0	2	1	4.0711	
benzo[a]pentaphene	26	16	6	0	N	2	6	8	0	0	3	0	2	1	3.8165	-92.54
naphtho[1_2-	26	16	6	0	N	0	5	8	1	0	2	0	1	3	2.6532	
naphtho[2_1-c]chrysene	26	16	6	0	N	1	4	10	0	1	3	0	2	1	3.942	
naphtho[2_3-a]tetraphene	26	16	6	0	N	0	7	8	1	0	2	0	1	3	3.615	
benzo[s]picene	26	16	6	0	N	1	2	11	2	0	3	0	2	1	3.8738	
dibenzo[a_l]tetracene	26	16	6	0	N	2	6	8	0	0	3	0	2	1	2.9623	-91.47
dibenzo[c_l]chrysene	26	16	6	0	N	0	4	10	2	0	3	0	2	1	3.5577	
benzo[b]picene	26	16	6	0	N	3	4	9	0	0	3	0	2	1	3.3817	-92.7
4b_6a_14a_14b-tetrahydronaphtho[2_1-a]tetracene	26	16	6	0	N	2	6	8	0	0	2	0	2	2	2.6943	-91.14
dibenzo[a_k]tetraphene	26	16	6	0	N	1	5	9	1	0	3	0	2	1	4.0159	
naphtho[2_1-c]tetraphene	26	16	6	0	N	1	5	9	1	0	3	0	2	1	3.2892	
dibenzo[c_f]tetraphene	26	16	6	0	N	2	3	10	1	0	3	1	0	2	3.3492	
dibenzo[a_f]tetraphene	26	16	6	0	N	2	3	10	1	0	3	1	0	2	3.3272	
naphtho[2_1-a]tetraphene	26	16	6	0	N	1	5	9	1	0	3	0	2	1	3.2911	
dibenzo[c_p]chrysene	26	16	6	0	N	1	2	11	2	0	3	1	0	2	3.5365	
dibenzo[c_g]chrysene	26	16	6	0	N	2	2	11	0	1	4	1	1	0	4.0148	
benzo[f]picene	26	16	6	0	N	3	1	11	1	0	4	1	1	0	3.7457	
benzo[a]picene	26	16	6	0	N	2	3	10	1	0	3	0	2	1	4.0989	
naphtho[1_2-g]chrysene	26	16	6	0	N	2	2	11	0	1	3	1	0	2	3.5765	
naphtho[1_2-c]chrysene	26	16	6	0	N	2	3	10	1	0	3	0	2	1	3.5791	
naphtho[2_3-c]tetraphene	26	16	6	0	N	2	6	8	0	0	2	0	1	3	2.9257	-91.25
dibenzo[a_j]tetracene	26	16	6	0	N	2	6	8	0	0	3	0	2	1	2.9553	-90.89
benzo[c]picene	26	16	6	0	N	4	2	10	0	0	3	0	2	1	3.6604	-94.09
benzo[h]pentaphene	26	16	6	0	N	3	4	9	0	0	3	1	0	2	3.7548	-96.87
dibenzo[a_c]tetracene	26	16	6	0	N	3	4	9	0	0	3	1	0	2	4.2054	-93.86
dibenzo[f_k]tetraphene	26	16	6	0	N	4	2	10	0	0	4	1	1	0	4.3126	
dibenzo[c_k]tetraphene	26	16	6	0	N	3	4	9	0	0	3	0	2	1	3.3401	-92.88
dibenzo[c_m]tetraphene	26	16	6	0	N	3	4	9	0	0	3	0	2	1	4.0575	-93.71
benzo[c]pentaphene	26	16	6	0	N	2	6	8	0	0	3	0	2	1	3.4064	-91.62
hexaphene	26	16	6	0	N	1	8	7	0	0	2	0	1	3	2.9379	-89.5
benzo[a]pentacene	26	16	6	0	N	1	8	7	0	0	2	0	1	3	2.3119	-89.5
dibenzo[g_p]chrysene	26	16	6	0	N	2	0	12	2	0	4	1	1	0	3.631	
hexacene	26	16	6	0	N	0	10	6	0	0	1	0	0	5	1.8105	-87.02
tricyclopenta[cd_fg_jk]pyrene	22	10	7	3	N	1	5	4	0	0	2	0	5	0	3.1657	-89.9
3-vinyltricyclopenta[cd_fg_jk]pyrene	24	12	7	2	Y	1	5	5	0	0	2	0	5	0	3.3413	
indeno[5_6_7_1-pqra]perylene	24	12	7	1	N	1	5	6	0	0	3	1	3	0	2.8394	-99.25
cyclopenta[gh]naphtho[7_8_1_2_3-nopqr]tetraphene	24	12	7	1	N	1	5	6	0	0	2	1	2	2	2.253	-98.82
benzo[ghi]cyclopenta[cd]perylene	24	12	7	1	N	1	5	6	0	0	3	1	3	0	3.1468	-94.87
cyclopenta[ij]naphtho[7_8_1_2_3-nopqr]tetraphene	24	12	7	1	N	1	5	6	0	0	2	0	4	1	2.873	-97.31

Molecule Name	Structural Information (indication of number or					Topological Information (Number of Edge Group and Ring Types)									Results	
	Carbons	Hydrogens	Rings	5-membered Rings	Aliphatics	Armchair	Zigzag	Free Edge	Bay	Fjord	Aromatic Sextets	Empty Rings	Dbl(1)	Dbl(2)	HOMO-LUMO Gap (eV)	BE Avg (kJ/mol)
cyclopenta[de]naphtho[7_8_1_2_3-nopqr]tetraphene	24	12	7	1	N	0	7	5	0	0	2	0	4	1	2.2898	-95.58
benzo[ij]indeno[5_4_3_2_1-nopqr]tetraphene	24	12	7	1	N	2	3	7	0	0	3	2	1	1	2.9538	-97.33
tricyclopenta[de_hi_op]tetracene	24	12	7	3	N	2	2	7	1	0	1	0	3	3	2.419	
tricyclopenta[de_hi_mn]tetracene	24	12	7	3	N	1	4	6	1	0	1	0	3	3	2.6533	
coronene	24	12	7	0	N	0	6	6	0	0	3	1	3	0	4.4196	-98.9
naphtho[7_8_1_2_3-pqrst]pentaphene	26	14	7	0	N	1	6	7	0	0	3	0	4	0	3.0388	-102.47
dibenzo[a_ghi]perylene	26	14	7	0	N	0	5	8	1	0	3	1	2	1	2.9803	
anthra[2_1_9_8-opqra]tetracene	26	14	7	0	N	1	6	7	0	0	2	0	3	2	2.6407	-103.48
benzo[f]naphtho[7_8_1_2_3-nopqr]tetraphene	26	14	7	0	N	2	4	8	0	0	3	1	2	1	3.129	-108.9
naphtho[8_1_2-bcd]perylene	26	14	7	0	N	2	4	8	0	0	3	1	2	1	2.9011	-105.33
dibenzo[b_ghi]perylene	26	14	7	0	N	2	4	8	0	0	3	1	2	1	3.229	-106.6
dibenzo[cd_lm]perylene	26	14	7	0	N	2	4	8	0	0	3	0	4	0	3.0262	-104.21
naphtho[1_2_3_4-ghi]perylene	26	14	7	0	N	3	2	9	0	0	3	2	0	2	3.1605	-110.79
dibenzo[b_pqr]perylene	26	14	7	0	N	3	2	9	0	0	4	2	1	0	3.4777	-99.4
dibenzo[f_tuv]picene	28	16	7	0	N	2	3	10	1	0	4	1	2	0	3.2782	
tribenzo[f_m_pqr]tetraphene	28	16	7	0	N	2	3	10	1	0	4	1	2	0	3.394	
dibenzo[f_pqr]picene	28	16	7	0	N	2	3	10	1	0	4	1	2	0	3.3418	
naphtho[2_1-b]perylene	28	16	7	0	N	2	3	10	1	0	3	1	1	2	2.959	
benzo[c]naphtho[8_1_2-fgh]tetraphene	28	16	7	0	N	2	3	10	1	0	3	1	1	2	3.1803	
tribenzo[a_fg_op]tetracene	28	16	7	0	N	3	1	11	1	0	4	2	0	1	3.5708	
benzo[de]naphtho[3_2_1-mn]tetracene	28	16	7	0	N	1	5	9	1	0	2	0	2	3	2.3855	
dibenzo[a_k]perylene	28	16	7	0	N	2	3	10	1	0	3	1	1	2	2.6221	
naphtho[2_1_8-def]picene	28	16	7	0	N	2	3	10	1	0	4	1	2	0	3.5414	
dibenzo[de_uv]pentaphene	28	16	7	0	N	1	5	9	1	0	3	1	1	2	3.0077	
benzo[c]naphtho[8_1_2-mno]tetraphene	28	16	7	0	N	1	5	9	1	0	3	0	3	1	3.1668	
tribenzo[c_m_pqr]tetraphene	28	16	7	0	N	1	5	9	1	0	3	0	3	1	2.9338	
naphtho[2_1_8-uva]pentaphene	28	16	7	0	N	0	7	8	1	0	3	0	3	1	3.1621	
dibenzo[a_rst]pentaphene	28	16	7	0	N	1	5	9	1	0	3	0	3	1	3.1509	
dibenzo[a_pqr]picene	28	16	7	0	N	1	5	9	1	0	3	0	3	1	3.1023	
phenanthro[9_10_1-qra]tetracene	28	16	7	0	N	1	5	9	1	0	3	1	1	2	2.7229	
naphtho[2_1-a]perylene	28	16	7	0	N	2	3	10	1	0	3	1	1	2	2.6954	
naphtho[1_2_3_4-rst]pentaphene	28	16	7	0	N	0	4	10	2	0	3	1	1	2	3.1877	
dibenzo[fg_qr]pentacene	28	16	7	0	N	4	2	10	0	0	4	1	2	0	3.0965	-109.92
dibenzo[pq_uv]pentaphene	28	16	7	0	N	0	6	9	0	1	2	0	2	3	2.0872	
dibenzo[de_op]pentacene	28	16	7	0	N	2	6	8	0	0	2	0	2	3	2.3899	-102.91
dibenzo[fg_ij]pentaphene	28	16	7	0	N	4	2	10	0	0	4	1	2	0	3.0516	-110.53
dibenzo[de_uv]pentacene	28	16	7	0	N	2	6	8	0	0	3	1	1	2	3.4552	-103.53
tribenzo[a_hi_mn]tetracene	28	16	7	0	N	3	4	9	0	0	4	1	2	0	3.6133	-106.18
dibenzo[c_pqr]picene	28	16	7	0	N	3	4	9	0	0	3	0	3	1	3.1695	-104.73
tribenzo[a_de_mn]tetracene	28	16	7	0	N	3	4	9	0	0	2	0	2	3	2.2574	-107.12
dibenzo[b_tuv]picene	28	16	7	0	N	3	4	8	0	0	3	0	3	1	2.9435	-105.81

	Structural Information (indication of number or					Topological Information (Number of Edge Group and Ring Types)									Results	
Molecule Name	Carbons	Hydrogens	Rings	5-membered Rings	Aliphatics	Armchair	Zigzag	Free Edge	Bay	Fjord	Aromatic Sextets	Empty Rings	Dbl(1)	Dbl(2)	HOMO-LUMO Gap (eV)	BE Avg (kJ/mol)
naphtho[2_1_8-fgh]pentaphene	28	16	7	0	N	3	4	9	0	0	3	1	1	2	3.4512	-108.5
naphtho[8_1_2-cde]pentaphene	28	16	7	0	N	2	6	8	0	0	3	0	3	1	3.1132	-103.44
dibenzo[c_rst]pentaphene	28	16	7	0	N	3	4	9	0	0	3	0	3	1	3.1141	-105.85
benzo[a]naphtho[2_1_8-hij]tetracene	28	16	7	0	N	2	6	8	0	0	3	0	3	1	2.8845	-103.34
benzo[a]naphtho[8_1_2-cde]tetracene	28	16	7	0	N	3	4	9	0	0	3	1	1	2	2.8817	-107.26
dibenzo[de_qr]pentacene	28	16	7	0	N	3	4	9	0	0	3	0	3	1	2.5874	-105.81
benzo[vwx]hexaphene	28	16	7	0	N	2	6	8	0	0	3	0	3	1	2.843	-104.18
anthra[2_1_9-qra]tetracene	28	16	7	0	N	2	6	8	0	0	2	0	2	3	2.4696	-104.1
benzo[a]naphtho[8_1_2-lmn]tetracene	28	16	7	0	N	2	6	8	0	0	3	0	3	1	2.9043	-103.83
naphtho[1_2_3_4-pqr]picene	28	16	7	0	N	4	2	10	0	0	4	1	2	0	3.3887	-109.96
naphtho[1_2-b]perylene	28	16	7	0	N	4	2	10	0	0	3	1	1	2	2.9428	-107.53
tribenzo[c_f_pqr]tetraphene	28	16	7	0	N	2	3	10	1	0	3	1	1	2	2.9042	
dibenzo[fg_uv]pentaphene	28	16	7	0	N	1	5	9	1	0	2	1	0	4	2.2379	
benzo[fg]naphtho[1_2_3-op]tetracene	28	16	7	0	N	3	1	11	1	0	4	2	0	1	3.3674	
dibenzo[a_e]perylene	28	16	7	0	N	2	3	10	1	0	3	1	1	2	2.7052	
benzo[a]naphtho[8_1_2-fgh]tetraphene	28	16	7	0	N	2	3	10	1	0	3	1	1	2	3.1716	
benzo[m]naphtho[1_2_3_4-pqr]tetraphene	28	16	7	0	N	1	4	10	0	1	4	1	2	0	3.2392	
benzo[no]naphtho[1_2_3-ij]tetraphene	28	16	7	0	N	0	4	10	2	0	3	1	1	2	3.1592	
benzo[ij]naphtho[3_2_1-no]tetraphene	28	16	7	0	N	1	4	10	0	1	3	1	1	2	3.1708	
benzo[de]naphtho[1_2_3-qr]tetracene	28	16	7	0	N	1	5	9	1	0	3	1	1	2	3.1306	
benzo[a]naphtho[8_1_2-mno]tetraphene	28	18	7	0	N	0	6	9	0	1	3	0	3	1	3.1249	
naphtho[1_2-a]perylene	28	16	7	0	N	1	4	10	0	1	3	1	1	2	2.5953	
tribenzo[a_ij_no]tetraphene	28	16	7	0	N	1	4	10	0	1	4	1	2	0	3.4418	
dibenzo[b_e]perylene	28	16	7	0	N	2	3	10	1	0	3	1	1	2	3.0991	
dibenzo[a_f]perylene	28	16	7	0	N	0	4	10	2	0	2	1	0	4	2.2245	
dibenzo[a_o]perylene	28	16	7	0	N	1	4	10	0	1	2	1	0	4	2.3678	
tribenzo[f_ij_no]tetraphene	28	16	7	0	N	1	2	11	2	0	4	1	2	0	3.381	
dibenzo[h_rst]pentaphene	28	16	7	0	N	4	2	10	0	0	3	1	1	2	3.3332	-112.79
dibenzo[fg_st]pentacene	28	16	7	0	N	4	2	10	0	0	4	2	0	1	3.8391	-110.15
dibenzo[de_kl]pentaphene	28	16	7	0	N	3	4	9	0	0	2	0	2	3	2.1113	-104.45
dibenzo[a_n]perylene	28	16	7	0	N	2	3	10	1	0	3	1	1	2	2.6646	
dibenzo[c_m]picene	30	18	7	0	N	5	2	11	0	0	4	0	3	0	3.593	-105.58
heptacene	30	18	7	0	N	7	0	12	6	0	1	0	0	6	1.5128	-98.32
tribenzo[f_k_m]tetraphene	30	18	7	0	N	6	0	12	0	0	5	2	0	0	4.1953	-111.41
tetracyclopenta[cd_fg_jk_mn]pyrene	24	10	8	4	N	2	4	4	0	0	2	0	6	0	2.6955	
1-ethynyltetracyclopenta[cd_fg_jk_mn]pyrene	26	10	8	4	Y	2	4	5	0	0	2	0	6	0	2.6197	-108.32
cyclopenta[bc]coronene	26	12	8	0	N	0	7	5	0	0	3	1	4	0	3.2794	-109.74
diindeno[1_2_3_4-defg:1'_2'_3'_4'-mnop]chrysene	26	12	8	2	N	4	0	8	0	0	4	3	1	0	3.5709	-101.7
tetraceno[2_1_12_11_10-mnopqra]tetracene	28	14	8	0	N	0	8	6	0	0	2	0	4	2	2.4585	-112.1
phenanthro[2_1_10_9_8_7-pqrstuv]pentaphene	28	14	8	0	N	1	6	7	0	0	3	0	5	0	2.8316	-117.06

Molecule Name	Structural Information (indication of number or					Topological Information (Number of Edge Group and Ring Types)									Results	
	Carbons	Hydrogens	Rings	5-membered Rings	Aliphatics	Armchair	Zigzag	Free Edge	Bay	Fjord	Aromatic Sextets	Empty Rings	Dbl(1)	Dbl(2)	HOMO-LUMO Gap (eV)	BE Avg (kJ/mol)
phenanthro[2_3_4_5-pqrab]perylene	28	14	8	0	N	2	4	8	0	0	4	2	2	0	3.7235	-120.04
benzo[ghi]naphtho[8_1_2-bcd]perylene	28	14	8	0	N	1	6	7	0	0	3	1	3	1	2.9095	-113.68
benzo[cd]naphtho[3_2_1_8-pqra]perylene	28	14	8	0	N	2	4	8	0	0	3	2	1	2	2.8601	-120.75
benzo[pqr]naphtho[8_1_2-bcd]perylene	28	14	8	0	N	2	4	8	0	0	4	2	2	0	3.2227	-123.14
benzo[a]coronene	28	14	8	0	N	2	4	8	0	0	4	2	2	0	3.3506	-115.91
phenanthro[1_10_9_8-opqra]perylene	28	14	8	0	N	2	4	8	0	0	2	2	0	4	2.1343	-123.21
benzo[a]naphtho[2_1_8-cde]perylene	30	16	8	0	N	2	3	10	1	0	3	1	2	2	2.6073	
benzo[ghi]naphtho[2_1-a]perylene	30	16	8	0	N	1	5	9	1	0	4	1	3	0	2.9883	
benzo[ghi]naphtho[2_1-b]perylene	30	16	8	0	N	1	5	9	1	0	4	1	3	0	3.1588	
benzo[pqr]naphtho[2_1_8-def]picene	30	16	8	0	N	1	5	9	1	0	4	1	3	0	3.2302	
tetrabenzo[de_hi_mn_qr]tetracene	30	16	8	0	N	0	4	10	2	0	4	1	3	0	3.1589	
dibenzo[de_mn]naphtho[2_1_8-qra]tetracene	30	16	8	0	N	1	5	9	1	0	2	0	3	3	2.0956	
dibenzo[gh_m]naphtho[3_2_1_8-pqra]tetraphene	30	16	8	0	N	1	5	9	1	0	3	1	2	2	2.9618	
benzo[pqr]naphtho[1_2-b]perylene	30	16	8	0	N	2	2	10	1	0	4	2	1	1	3.1999	
benzo[a]naphtho[8_1_2-klm]perylene	30	16	8	0	N	1	5	9	1	0	3	1	2	2	2.4717	
benzo[de]naphtho[8_1_2_3-stuv]picene	30	16	8	0	N	1	5	9	1	0	3	0	4	1	2.9602	
tribenzo[a_ghi_k]perylene	30	16	8	0	N	2	3	10	1	0	4	2	1	1	3.0263	
benzo[a]naphtho[1_2_3_4-ghi]perylene	30	16	8	0	N	2	3	10	1	0	3	2	0	3	2.733	
tribenzo[a_ghi_n]perylene	30	16	8	0	N	1	5	9	1	0	3	1	2	2	2.8099	
benzo[lm]naphtho[1_8-ab]perylene	30	16	8	0	N	2	3	10	1	0	3	1	2	2	2.5863	
benzo[ghi]naphtho[1_2-a]perylene	30	16	8	0	N	0	6	9	0	1	4	1	3	0	2.8815	
benzo[a]naphtho[7_8_1_2_3-pqrst]pentaphene	30	16	8	0	N	0	7	8	1	0	3	0	4	1	2.8784	
tetrapheno[5_6_7_8-opqra]tetracene	30	16	8	0	N	1	5	9	1	0	3	1	2	2	2.6126	
benzo[uv]naphtho[2_1_8_7-defg]pentaphene	30	16	8	0	N	0	7	8	1	0	3	1	2	2	2.5251	
anthra[8_9_1_2-lmnop]benzo[a]tetracene	30	16	8	0	N	0	7	8	1	0	3	0	4	1	2.6768	
benzo[pqr]naphtho[2_1-b]perylene	30	16	8	0	N	2	3	10	1	0	4	2	1	1	3.243	
phenanthro[1_2_3_4-ghi]perylene	30	16	8	0	N	2	3	10	1	0	4	1	3	0	3.1351	
tribenzo[a_cd_lm]perylene	30	16	8	0	N	2	3	10	1	0	4	1	3	0	2.9889	
dinaphtho[8_1_2-lmn:2'_1'_8'-qra]tetracene	30	16	8	0	N	0	7	8	1	0	3	0	4	1	2.8316	
dibenzo[c_gh]naphtho[3_2_1_8-pqra]tetraphene	30	16	8	0	N	4	2	10	0	0	4	2	1	1	3.1616	-118.65
benzo[pqr]naphtho[8_1_2-cde]picene	30	16	8	0	N	2	6	8	0	0	3	0	4	1	2.7527	-115.55
tetraceno[2_1_12_11-opqra]tetracene	30	16	8	0	N	2	6	8	0	0	2	0	3	3	2.2673	-117.08
phenanthro[3_4_5_6-fghij]pentaphene	30	16	8	0	N	3	4	9	0	0	4	1	3	0	3.1516	-121.02
anthra[1_2_3_4-ghi]perylene	30	16	8	0	N	3	4	9	0	0	3	2	0	3	2.7805	-120.66

	Structural Information (indication of number or					Topological Information (Number of Edge Group and Ring Types)									Results	
Molecule Name	Carbons	Hydrogens	Rings	5-membered Rings	Aliphatics	Armchair	Zigzag	Free Edge	Bay	Fjord	Aromatic Sextets	Empty Rings	Dbl(1)	Dbl(2)	HOMO-LUMO Gap (eV)	BE Avg (kJ/mol)
benzo[ghi]naphtho[1_2-b]perylene	30	16	8	0	N	3	4	9	0	0	4	1	3	0	3.1391	-119.12
benzo[rst]naphtho[2_1_8-fgh]pentaphene	30	16	8	0	N	4	2	10	0	0	4	2	1	1	3.0947	-123.88
benzo[qr]naphtho[2_1_8_7-defg]pentacene	30	16	8	0	N	3	4	9	0	0	4	1	3	0	2.9138	-119.23
benzo[h]naphtho[7_8_1_2_3-pqrst]pentaphene	30	16	8	0	N	3	3	9	0	0	4	1	3	0	3.0681	-124.83
benzo[ij]naphtho[2_1_8_7-defg]pentaphene	30	16	8	0	N	3	4	9	0	0	4	1	3	0	2.8307	-119.44
benzo[kl]naphtho[2_1_8_7-defg]pentaphene	30	16	8	0	N	2	6	8	0	0	3	0	4	1	2.3107	-115.81
anthra[2_1_9_8-defgh]pentaphene	30	16	8	0	N	2	6	8	0	0	3	1	2	2	3.1305	-118.13
benzo[st]naphtho[2_1_8_7-defg]pentacene	30	16	8	0	N	3	4	9	0	0	4	2	1	1	3.3377	-119.59
phenanthro[9_10_1_2_3-pqrst]pentaphene	30	16	8	0	N	3	4	9	0	0	4	1	3	0	3.041	-117.5
benzo[c]naphtho[7_8_1_2_3-pqrst]pentaphene	30	16	8	0	N	2	6	8	0	0	3	0	4	1	2.8868	-114.51
phenanthro[2_3_4_5-tuvab]picene	30	16	8	0	N	2	6	8	0	0	3	0	4	1	2.6844	-116.27
anthra[8_9_1_2-cdefg]benzo[a]tetracene	30	16	8	0	N	3	4	9	0	0	3	1	2	2	2.6768	-120.81
benzo[uv]naphtho[2_1_8_7-defg]pentacene	30	16	8	0	N	2	6	8	0	0	3	1	2	2	2.8311	-116.56
benzo[op]naphtho[2_1_8_7-defg]pentacene	30	16	8	0	N	2	6	8	0	0	3	0	4	1	2.5171	-114.56
naphtho[7_8_1_2_3-tuvwx]hexaphene	30	16	8	0	N	2	5	8	0	0	3	0	4	1	2.695	-117.44
naphtho[3_2_1_8_7-vwxyz]hexaphene	30	16	8	0	N	1	8	7	0	0	3	0	4	1	2.7202	-114.99
benzo[b]naphtho[1_2_3_4-pqr]perylene	30	16	8	0	N	3	1	11	1	0	4	2	1	1	3.1163	
tribenzo[b_e_ghi]perylene	30	16	8	0	N	2	3	10	1	0	4	2	1	1	3.2531	
tribenzo[a_e_ghi]perylene	30	16	8	0	N	2	3	10	1	0	4	2	1	1	3.0583	
benzo[a]naphtho[2_1_8-lmn]perylene	30	16	8	0	N	1	5	9	1	0	3	1	2	2	2.5538	
tribenzo[a_ghi_o]perylene	30	16	8	0	N	0	6	9	0	1	3	1	2	2	2.7515	
pyranthrene	30	16	8	0	N	2	6	8	0	0	3	0	4	1	2.8529	-118.16
anthra[2_1_9_8-stuva]pentacene	30	16	8	0	N	1	8	7	0	0	2	0	4	2	2.2461	-114.43
benzo[qr]naphtho[2_1_8_7-fghi]pentacene	30	16	8	0	N	4	2	10	0	0	4	2	1	1	3.2419	-117.95
tribenzo[de_ij_rst]pentaphene	30	16	8	0	N	4	2	10	0	0	4	2	1	1	2.9048	-121.55
dibenzo[de_st]pentacen	30	16	8	0	N	3	4	9	0	0	3	1	1	2	2.7501	-118.04
tribenzo[de_kl_rst]pentaphene	30	16	8	0	N	4	2	10	0	0	3	2	0	3	2.4876	-117.78
tribenzo[fg_ij_rst]pentaphene	30	16	8	0	N	5	0	11	0	0	5	3	0	0	3.5076	-126.19
anthra[1_2_3_4-rst]pentaphene	32	18	8	0	N	0	6	10	2	0	3	1	1	3	3.2346	-117.78
dibenzo[hi_uv]hexacene	32	18	8	0	N	4	4	10	0	0	4	2	0	2	3.9374	
octacene	34	20	8	0	N	8	0	14	6	0	1	0	0	7	1.2804	-107.97
dicyclopenta[bc_hi]coronene	28	12	9	0	N	0	8	4	0	0	3	1	5	0	3.8307	-119.17
dibenzo[mn_qr]fluoreno[2_1_9_8_7-defghi]tetracene	30	14	9	1	N	1	4	8	1	0	4	2	3	0	3.1359	-100.76
dibenzo[e_ghi]indeno[1_2_3_4-pqra]perylene	30	14	9	1	N	3	3	8	0	0	4	3	1	1	2.5741	-126.5
dibenzo[bc_kl]coronene	30	14	9	0	N	0	8	6	0	0	3	0	6	0	2.6347	-128.77
dibenzo[bc_ef]coronene	30	14	9	0	N	1	6	7	0	0	3	2	2	2	2.5156	
naphtho[8_1_2-abc]coronene	30	14	9	0	N	1	6	7	0	0	4	2	3	0	3.0912	-122.49

Molecule Name	Structural Information (indication of number or					Topological Information (Number of Edge Group and Ring Types)									Results	
	Carbons	Hydrogens	Rings	5-membered Rings	Aliphatics	Armchair	Zigzag	Free Edge	Bay	Fjord	Aromatic Sextets	Empty Rings	Dbl(1)	Dbl(2)	HOMO-LUMO Gap (eV)	BE Avg (kJ/mol)
benzo[4_10]anthra[3_2_1_9_8-rstuva]pentaphene	32	16	9	0	N	1	5	9	1	0	4	2	2	1	2.9952	
anthra[2_1_9_8_7-defghi]benzo[uv]pentacene	32	16	9	0	N	2	6	8	0	0	3	1	3	2	2.5784	-129.86
tetraceno[2_1_12_11_10-qrstuva]pentacene	32	16	9	0	N	1	8	7	0	0	2	0	4	3	2.1186	-127.5
naphtho[1_2-a]coronene	32	16	9	0	N	1	5	9	1	0	4	2	2	1	3.8129	
dibenzo[a_ghi]naphtho[2_1_8-cde]perylene	32	16	9	0	N	2	3	10	1	0	4	2	2	1	2.9127	
dibenzo[a_ghi]naphtho[8_1_2-klm]perylene	32	16	9	0	N	1	5	9	1	0	4	2	2	1	2.839	
benzo[e]phenanthro[2_3_4_5-pqrab]perylene	32	16	9	0	N	1	5	9	1	0	4	2	2	1	3.042	
dibenzo[a_cd]naphtho[8_1_2_3-fghi]perylene	32	16	9	0	N	2	3	10	1	0	4	2	2	1	2.8554	
pyreno[5_4_3_2_1-pqrst]pentaphene	32	16	9	0	N	1	5	9	1	0	4	1	4	0	2.8605	
benzo[de]phenaleno[1_2_3_4_5-rstuv]pentaphene	32	16	9	0	N	1	5	9	1	0	3	2	1	3	2.562	
anthra[3_2_1_9-pqra]benzo[cd]perylene	32	16	9	0	N	1	5	9	1	0	3	2	1	3	2.4513	
dibenzo[a_ghi]naphtho[2_1_8-lmn]perylene	32	16	9	0	N	0	7	8	1	0	3	1	3	2	2.5943	
benzo[3_4]phenanthro[2_1_10_9_8_7-pqrstuv]pentaphene	32	16	9	0	N	1	5	8	1	0	4	1	4	0	2.8043	
benzo[lm]phenanthro[5_4_3-abcd]perylene	32	16	9	0	N	1	5	9	1	0	4	1	4	0	2.7835	
dinaphtho[1_8-ab:8'_1'_2'_3'-fghi]perylene	32	16	9	0	N	1	5	9	1	0	3	1	3	2	2.4657	
dibenzo[ghi_lm]naphtho[1_8-ab]perylene	32	16	9	0	N	1	5	9	1	0	3	1	3	2	2.4443	
anthra[2_1_9_8_7-defghi]benzo[op]pentacene	32	16	9	0	N	2	6	8	0	0	3	1	3	2	2.563	-117.38
dibenzo[a_d]coronene	32	16	9	0	N	2	3	10	1	0	4	2	2	1	3.1412	
dinaphtho[2_1_8_7-defg:2'_1'_8'_7'-opqr]pentacene	32	16	9	0	N	2	6	8	0	0	4	1	4	0	2.7832	-128.79
naphtho[2_3-a]coronene	32	16	9	0	N	2	6	8	0	0	4	2	2	1	2.973	-129.54
benzo[h]phenanthro[2_1_10_9_8_7-pqrstuv]pentaphene	32	16	9	0	N	3	4	9	0	0	4	1	4	0	2.8507	-136.84
dinaphtho[2_1_8_7-defg:2'_1'_8'_7'-ijkl]pentaphene	32	16	9	0	N	2	6	8	0	0	4	1	4	0	2.6215	-128.81
dibenzo[ij_rst]naphtho[2_1_8_7-	32	16	9	0	N	4	2	10	0	0	5	3	1	0	3.2386	-134.81
dibenzo[fg_ij]naphtho[7_8_1_2_3-pqrst]pentaphene	32	16	9	0	N	4	2	10	0	0	5	3	1	0	3.7331	-137.76
anthra[2_1_9_8_7-defghi]benzo[st]pentacene	32	16	9	0	N	3	4	9	0	0	4	2	2	1	3.0543	-133.63
dibenzo[cd_n]naphtho[3_2_1_8-pqra]perylene	32	16	9	0	N	4	2	10	0	0	4	3	0	2	2.9086	-138.36
dinaphtho[2_1_8-fgh:3'_2'_1'_8'_7'-rstuv]pentaphene	32	16	9	0	N	3	4	8	0	0	4	2	2	1	2.8284	-135.58
anthra[2_1_9_8-defgh]benzo[rst]pentaphene	32	16	9	0	N	3	4	9	0	0	4	2	2	1	2.8102	-133.94
dibenzo[cd_k]naphtho[3_2_1_8-pqra]perylene	32	16	9	0	N	3	4	9	0	0	3	2	1	3	2.5302	-134.56

Molecule Name	Structural Information (indication of number or					Topological Information (Number of Edge Group and Ring Types)									Results	
	Carbons	Hydrogens	Rings	5-membered Rings	Aliphatics	Armchair	Zigzag	Free Edge	Bay	Fjord	Aromatic Sextets	Empty Rings	Dbl(1)	Dbl(2)	HOMO-LUMO Gap (eV)	BE Avg (kJ/mol)
dibenzo[de_ij]naphtho[3_2_1_8_7-rstuv]pentaphene	32	16	9	0	N	3	4	9	0	0	4	2	2	1	2.9509	-133.5
anthra[2_1_9_8_7-defghi]benzo[qr]pentacene	32	16	9	0	N	3	4	9	0	0	4	2	2	1	2.934	-132.97
dinaphtho[2_1_8-fgh:7'_8'_1'_2'_3'-pqrst]pentaphene	32	16	9	0	N	3	4	9	0	0	4	2	2	1	2.8453	-134.66
benzo[10_5]anthra[3_2_1_9_8-rstuva]pentaphene	32	16	9	0	N	2	6	8	0	0	4	1	4	0	2.8025	-130.91
benzo[def]pyranthrene	32	16	9	0	N	2	6	8	0	0	3	0	5	1	2.6318	-130.19
phenanthro[2_1_10_9_8_7-tuvwxyz]hexaphene	32	16	9	0	N	2	6	8	0	0	3	0	5	1	2.6147	-129.86
anthra[7_8_9_1_2_3-rstuvwx]hexaphene	32	16	9	0	N	1	8	7	0	0	3	0	5	1	2.5006	-127.24
benzo[e]phenanthro[1_10_9_8-opqra]perylene	32	16	9	0	N	3	4	9	0	0	3	2	1	3	2.1385	-138.05
dibenzo[de_kl]naphtho[7_8_1_2_3-pqrst]pentaphene	32	16	9	0	N	3	4	9	0	0	4	2	2	1	2.678	-129.62
dibenzo[de_ij]naphtho[7_8_1_2_3-pqrst]pentaphene	32	16	9	0	N	3	4	9	0	0	4	2	2	1	2.9004	-126.59
dinaphtho[8_1_2-cde:7'_8'_1'_2'_3'-pqrst]pentaphene	32	16	9	0	N	2	6	8	0	0	3	0	5	1	2.5708	-127.12
benzo[fg]phenaleno[1_2_3_4_5-rstuv]pentaphene	32	16	9	0	N	1	5	9	1	0	2	2	0	5	1.8976	
dibenzo[a_g]coronene	32	16	9	0	N	4	2	10	0	0	5	3	1	0	3.3191	-129.25
tetrapheno[10_11_12_1_2-defghij]pentaphene	32	16	9	0	N	2	6	8	0	0	4	1	4	0	2.8723	-132.49
dinaphtho[2_1_8_7-defg:2'_1'_8'_7'-qrst]pentacene	32	16	9	0	N	3	4	9	0	0	4	2	2	1	3.056	-129.22
dibenzo[a_j]coronene	32	16	9	0	N	4	2	10	0	0	4	3	0	2	3.1618	-132.82
tetraceno[2_1_12_11-stuva]pentacene	34	18	9	0	N	2	8	8	0	0	2	0	3	4	1.9631	-126.76
benzo[uv]naphtho[2_1_8_7-fghi]hexacene	34	18	9	0	N	4	3	10	0	0	4	2	1	2	3.1464	-130.99
anthra[9_1_2-hij]hexaphene	36	20	9	0	N	2	7	10	1	0	3	1	1	4	2.5543	-130.23
anthra[1_2_3-uv]benzo[fg]pentaphene	36	20	9	0	N	1	8	10	0	1	2	1	0	6	1.87	
tetrabenzo[c_h_m_rst]pentaphene	36	20	9	0	N	6	2	12	0	0	4	1	2	2	3.1232	-131.32
tetrabenzo[a_c_hi_qr]pentacene	36	20	9	0	N	7	0	13	0	0	6	3	0	0	3.7769	-132.57
nonacene	38	22	9	0	N	9	0	16	6	0	1	0	0	8	1.0952	-116.76
diacenaphtho[3_2_1_8-cdefg:3'_2'_1'_8'-lmnop]chrysene	30	12	10	2	N	2	4	6	0	0	4	3	3	0	3.8821	
tricyclopenta[bc_hi_no]coronene	30	12	10	3	N	0	9	3	0	0	3	1	6	0	3.6752	-128.72
di-as-indaceno[3_4_5_6-cdefg:3'_4'_5'_6'-lmnop]chrysene	30	12	10	4	N	4	2	6	0	0	2	1	5	2	2.7015	
12-vinyl-9_10-dihydrocyclopenta[qr]indeno[1_7_6_5-lmno]-as-indaceno[3_4_5_6-cdefg]chrysene	32	16	10	4	Y	6	4	6	0	0	2	1	6	1	2.564	
1-vinyldicyclopenta[hi_qr]diindeno[1_7_6_5-cdef:1'_7'_6'_5'-lmno]chrysene	32	14	10	4	Y	2	5	5	0	0	2	0	7	1	2.1304	

Molecule Name	Structural Information (indication of number or					Topological Information (Number of Edge Group and Ring Types)									Results	
	Carbons	Hydrogens	Rings	5-membered Rings	Aliphatics	Armchair	Zigzag	Free Edge	Bay	Fjord	Aromatic Sextets	Empty Rings	Dbl(1)	Dbl(2)	HOMO-LUMO Gap (eV)	BE Avg (kJ/mol)
4-vinyl-2a_2b-dihydrodi-as-indaceno[3_4_5_6-cdefg:3'_4'_5'_6'-lmnop]chrysene	32	14	10	4	Y	4	2	7	0	0	2	2	4	2	2.6691	
cyclopenta[kl]diindeno[1_7_6_5-fghi:5'_6'_7'_1'-tuva]picene	32	14	10	3	N	3	5	6	0	0	3	0	7	0	1.7117	
aceanthryleno[8_7_6_5-opqra]dicyclopenta[de_hi]tetracene	32	14	10	3	N	2	4	7	1	0	2	1	4	3	1.4127	
dicyclopenta[de_gh]diindeno[1_7-lm:5'_6'_7'_1'-pqra]tetraphene	32	14	10	4	N	2	4	6	1	0	3	0	7	0	2.7377	-120.28
ovalene	32	14	10	0	N	0	8	6	0	0	4	2	4	0	2.869	-139.66
benzo[p]naphtho[8_1_2-abc]coronene	34	16	10	0	N	1	5	8	1	0	4	2	3	1	2.877	
benzo[ghi]tetrapheno[1_12_11-abcde]perylene	34	16	10	0	N	1	5	9	1	0	4	2	3	1	2.7106	
benzo[m]naphtho[8_1_2abc]coronene	34	16	10	0	N	3	4	9	0	0	5	3	2	0	3.124	-129.76
pentaceno[2_1_14_13_12_11-opqrstuva]pentacene	34	18	10	0	N	0	10	6	0	0	2	0	6	2	2.162	
benzo[bc]naphtho[1,2,3-ef]coronene	34	16	10	0	N	0	7	7	1	0	3	2	2	3	2.2583	
anthra[9,1,2-abc]coronene	34	16	10	0	N	0	7	8	1	0	4	2	3	1	2.9426	
dibenzo[ij_rst]phenanthro[9_10_1_2-defg]pentaphene	36	18	10	0	N	6	0	12	0	0	6	4	0	0	3.2598	-148.99
dibenzo[fg_ij]phenanthro[9_10_1_2_3-pqrst]pentaphene	36	18	10	0	N	6	0	12	0	0	6	4	0	0	3.7511	-153.23
tribenzo[fgh_pqr_za1b1]trinaphthylene	36	18	10	0	N	6	0	12	0	0	6	4	0	0	3.9264	-150.47
dibenzo[a1b1_jk]octacene	40	22	10	0	N	4	8	10	0	0	4	2	0	4	2.9277	
decacene	42	24	10	0	N	10	0	18	6	0	1	0	0	9	2.3098	-124.82
tetracyclopenta[bc_ef_hi_no]coronene	32	12	11	4	N	2	6	4	0	0	3	1	7	0	2.5629	-133.15
acenaphtho[5_4-l]dicyclopenta[de_ij]indeno[5_6_7_1-pqra]tetraphene	32	16	11	4	N	2	7	6	1	0	3	0	7	1	2.5409	
cyclopenta[bc]ovalene	34	14	11	1	N	0	9	5	0	0	4	2	5	0	2.4111	-146.91
tetrabenzo[bc_ef_kl_no]coronene	36	16	11	0	N	2	6	8	0	0	2	3	0	6	1.5778	-159.27
benzo[a]ovalene	36	16	11	0	N	2	6	8	0	0	5	3	3	0	2.886	-146.13
benzo[4,10]anthra[1,9,8-abcd]coronene	36	16	11	0	N	3	4	9	0	0	5	3	3	0	2.8974	
dinaphtho[8,1,2-abc:2',1',8'-efg]coronene	36	16	11	0	N	3	4	9	0	0	5	3	3	0	2.8396	
dinaphtho[8,1,2-abc:2',1',8'-nop]coronene	36	16	11	0	N	0	7	8	1	0	4	2	3	1	2.6628	
dibenzo[ef,hi]naphtho[8,1,2-abc]coronene	36	16	11	0	N	3	4	9	0	0	4	3	2	2	2.4662	
tetrabenzo[bc,ef,hi,kl]coronene	36	16	11	0	N	3	4	9	0	0	4	3	2	2	2.8508	
tetrabenzo[a_d_j_m]coronene	40	20	11	0	N	4	0	14	2	0	5	3	1	2	2.9704	
dibenzo[kl_rst]benzo[10_5]anthra[9_1_2-cde]pentaphene	40	20	11	0	N	6	2	12	0	0	4	3	0	4	2.1118	-150.82
tetrabenzo[c1d1_de_no_st]heptacene	42	22	11	0	N	4	8	10	0	0	5	2	2	2	2.7201	
pentacyclopenta[bc_ef_hi_kl_no]coronene	34	12	12	5	N	4	3	5	0	0	3	1	8	0	3.0118	-136.64
dicyclopenta[bc_st]ovalene	36	14	12	2	N	1	8	5	0	0	4	2	6	0	2.1661	-154.31

Molecule Name	Structural Information (indication of number or					Topological Information (Number of Edge Group and Ring Types)									Results	
	Carbons	Hydrogens	Rings	5-membered Rings	Aliphatics	Armchair	Zigzag	Free Edge	Bay	Fjord	Aromatic Sextets	Empty Rings	Dbl(1)	Dbl(2)	HOMO-LUMO Gap (eV)	BE Avg (kJ/mol)
naphtho[2'_1'_8'_7':4_10_5]anthra[1_9_8-abcd]coronene	38	16	12	0	N	2	6	8	0	0	5	3	4	0	2.9667	-167.06
naphtho[2_1_8-uva]ovalene	38	16	12	0	N	2	6	8	0	0	5	3	4	0	2.6801	-157.59
naphtho[8,1,2-abc]ovalene	38	16	12	0	N	1	8	7	0	0	5	3	4	0	3.4037	
dibenzo[bc,uv]ovalene	38	16	12	0	N	2	6	8	0	0	5	3	4	0	2.6193	
dibenzo[hi,uv]ovalene	38	16	12	0	N	2	6	8	0	0	5	3	4	0	2.6719	
naphtho[2,1,8-bcd]ovalene	38	16	12	0	N	1	8	8	0	0	4	2	5	1	2.4458	
dibenzo[hi,st]ovalene	38	16	12	0	N	2	6	8	0	0	4	3	3	2	2.3178	
dibenzo[bc,st]ovalene	38	16	12	0	N	1	8	7	0	0	4	2	5	1	2.1921	
dibenzo[bc,ef]ovalene	38	16	12	0	N	1	8	7	0	0	3	3	2	4	1.9167	
tetrabenzo[def_lm_qrs_yz]pyranthrene	40	18	12	0	N	4	4	10	0	0	6	4	2	0	2.8283	-166.62
hexacyclopenta[bc_ef_hi_kl_no_qr]coronene	36	12	13	6	N	6	0	6	0	0	3	1	9	0	3.4687	-158.75
tricyclopenta[bc_hi_mn]ovalene	38	14	13	3	N	1	9	4	0	0	4	2	7	0	2.1116	-170.33
phenanthro[3,4,5,6-bcdef]ovalene	38	16	13	0	N	0	10	6	0	0	4	3	4	2	2.2712	
benzo[bc]naphtho[2_1_8_7-stuv]ovalene	40	16	13	0	N	1	8	7	0	0	5	3	5	0	2.4871	-163.65
phenanthro[3_4_5_6-bcdef]ovalene	40	16	13	0	N	0	10	6	0	0	4	3	4	2	2.2712	-176.26
hexabenzo[bc_ef_hi_kl_no_qr]coronene	42	18	13	0	N	6	0	12	0	0	7	6	0	0	3.6253	-193.23
dibenzo[a_jk]phenanthro[8_9_10_1_2-cdefgh]pyranthrene	44	20	13	0	N	6	2	12	0	0	7	5	1	0	3.008	
tetracyclopenta[bc_hi_mn_st]ovalene	40	14	14	4	N	2	8	4	0	0	4	2	8	0	2.0064	-182.05
dinaphtho[2_1_8_7-hijk:2'_1'_8'_7'-stuv]ovalene	42	16	14	0	N	0	10	6	0	0	5	3	6	0	2.5508	-166.71
tribenzo[a_jk_v]phenanthro[8_9_10_1_2-cdefgh]pyranthrene	48	22	14	0	N	8	0	14	0	0	8	6	0	0	2.9897	
dibenzo[kl_rst]dibenzo[8_9:13_14]pentapheno[5_4_3-cde]pentaphene	50	24	14	0	N	8	2	14	0	0	5	4	0	5	1.8573	-179.62
pentacyclopenta[bc_ef_hi_mn_st]ovalene	42	14	15	5	N	4	5	5	0	0	4	2	9	0	2.7143	-190.43
benzo[d]dinaphtho[2_1_8_7-hijk:2'_1'_8'_7'-stuv]ovalene	46	18	15	0	N	2	8	8	0	0	6	4	5	0	2.5857	-202.35
difluorantheno[4_3_2-abc:2'_3'_4'-klm]coronene	48	20	15	2	N	6	4	10	0	0	7	5	3	0	2.555	
benzo[1_2_3-bc:4_5_6-b'c']dicoronene	48	20	15	0	N	2	10	8	0	0	6	3	6	0	2.6427	
tetrabenzo[a_jk_tu_wx]phenanthro[8_9_10_1_2-cdefgh]pyranthrene	50	22	15	0	N	5	0	15	2	0	7	6	0	2	2.3315	
trinaphtho[2_1_8-bcd:2'_1'_8'_7'-hijk:2''_1''_8''_7''-stuv]ovalene	48	18	16	0	N	2	8	8	0	0	6	4	6	0	2.4802	-215.46
diphenaleno[2_1_9_8-hijk:2'_1'_9'_8'-stuv]ovalene	48	18	16	0	N	0	12	6	0	0	4	2	8	2	1.731	
diphenanthro[3_4_5_6-bcdef:3'_4'_5'_6'-mnopq]ovalene	48	18	16	0	N	0	12	6	0	0	4	4	4	4	1.8327	
17R	50	18	17	0	N	1	10	7	0	0	6	5	5	1	2.2761	-227.02
hexarylene	60	28	17	0	N	10	2	16	0	0	6	5	0	6	1.6672	-208.44
18R_A	52	18	18	0	N	1	10	7	0	0	7	6	5	0	2.4771	-239.68
18R_B	54	20	18	0	N	4	6	10	0	0	7	6	4	1	2.3946	-242.7
circumcoronene	54	18	19	0	N	0	12	6	0	0	7	6	6	0	3.1089	-256.55

Molecule Name	Structural Information (indication of number or					Topological Information (Number of Edge Group and Ring Types)									Results	
	Carbons	Hydrogens	Rings	5-membered Rings	Aliphatics	Armchair	Zigzag	Free Edge	Bay	Fjord	Aromatic Sextets	Empty Rings	Dbl(1)	Dbl(2)	HOMO-LUMO Gap (eV)	BE Avg (kJ/mol)
circumpentacene	56	20	19	0	N	0	14	6	0	0	4	4	6	5	1.5078	-247.32
19R_B	60	24	19	0	N	9	0	15	0	0	10	9	0	0	3.2623	-252.92
19R_A	62	26	19	0	N	4	0	18	4	0	9	6	4	0	2.3454	
20R_A	58	20	20	0	N	2	10	8	0	0	8	7	5	0	3.0706	-264.47
20R_B	60	22	20	0	N	8	0	14	0	0	10	10	0	0	2.6356	-270.25
21R	60	20	21	0	N	2	10	8	0	0	8	7	6	0	2.3402	-276.63
22R	62	20	22	0	N	1	12	7	0	0	8	7	7	0	2.2381	-288.63
23R	64	20	23	0	N	1	12	7	0	0	8	7	8	0	2.1566	-301.47
circumovalene	66	20	24	0	N	0	14	6	0	0	8	7	9	0	2.0665	-313.38
24R	72	26	24	0	N	10	0	16	0	0	12	12	0	0	3.0057	-319.42
25R_B	70	22	25	0	N	2	12	8	0	0	9	8	8	0	2.0835	-323.57
25R_A	78	30	25	0	N	12	0	18	0	0	13	12	0	0	3.0133	-330.95
26R	72	22	26	0	N	2	12	8	0	0	9	9	7	1	2.0034	-337.51
27R_A	74	22	27	0	N	2	12	8	0	0	9	8	10	0	1.8803	-350.6
27R_B	74	22	27	0	N	2	12	8	0	0	9	9	8	1	1.8802	-352.94
29R_A	78	22	29	0	N	1	14	7	0	0	10	10	9	0	1.8787	-375.17
circumcircumpyrene	80	22	30	0	N	0	16	6	0	0	10	10	10	0	1.8753	-387.11
31R_B	84	24	31	0	N	2	14	8	0	0	11	11	9	0	1.8646	-398.87
31R_A	84	24	31	0	N	6	6	12	0	0	12	13	6	0	2.7217	
32R	86	24	32	0	N	2	14	8	0	0	11	11	10	0	1.7902	-411.38
33R	88	24	33	0	N	2	14	8	0	0	11	11	11	0	1.7016	-425.87
34R	90	24	34	0	N	1	16	7	0	0	11	12	10	1	1.6327	-437.69
34B	96	30	34	0	N	12	0	18	0	0	16	18	0	0	2.6892	-440.37
35R	92	24	35	0	N	1	16	7	0	0	11	12	11	1	1.6023	-448.07
circumcircumcoronene	96	24	37	0	N	0	18	6	0	0	12	13	12	0	2.3447	-487.42
37R	98	26	37	0	N	2	16	8	0	0	12	13	11	1	1.5723	-468.44
38R	100	26	38	0	N	2	16	8	0	0	12	13	12	1	1.5826	-481.99
39R	102	26	39	0	N	1	18	7	0	0	12	13	13	1	1.5813	-494.05
40R	104	26	40	0	N	1	18	7	0	0	13	15	11	1	1.5592	-506.72
41R	106	26	41	0	N	1	18	7	0	0	13	15	12	1	1.4879	-521.28
42R	108	26	42	0	N	1	18	7	0	0	13	15	13	1	1.4022	-533.76
43R_B	110	26	43	0	N	0	20	6	0	0	13	16	12	2	1.3448	-545.33
43R_A	114	30	43	0	N	12	0	18	0	0	19	24	0	0	2.4213	-551.4
61R	150	30	61	0	N	0	24	6	0	0	19	24	18	0	1.8253	-787.66