TABLE S1. 44 symmetrically independent canonical structures of benzenoid hydrocarbons used in this work. For each structure a set of topological features χ_i, used for construction of homodesmotic reactions is given. The Fries structures are marked with an asterisks.*

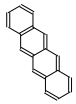
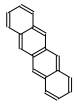
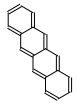
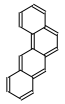
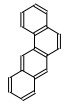
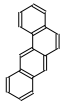
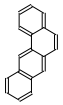
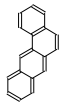
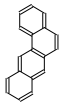
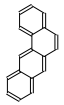
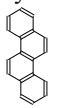
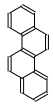
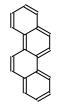
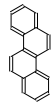
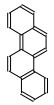
benzene	naphthalene		anthracene		phenanthrene			
								
(i)*	**(ii)***	**(iii)**	**(iv)***	**(v)**	**(vi)***	**(vii)**	**(viii)**	**(ix)**
$\chi_C = 6$ $\chi_H = 6$ $\chi_{syn} = 3$ $\chi_{anti} = 0$ $\chi_{orto} = 0$	$\chi_C = 10$ $\chi_H = 8$ $\chi_{syn} = 6$ $\chi_{anti} = 0$ $\chi_{orto} = 0$	$\chi_C = 10$ $\chi_H = 8$ $\chi_{syn} = 4$ $\chi_{anti} = 2$ $\chi_{orto} = 0$	$\chi_C = 14$ $\chi_H = 10$ $\chi_{syn} = 7$ $\chi_{anti} = 2$ $\chi_{orto} = 0$	$\chi_C = 14$ $\chi_H = 10$ $\chi_{syn} = 5$ $\chi_{anti} = 4$ $\chi_{orto} = 0$	$\chi_C = 14$ $\chi_H = 10$ $\chi_{syn} = 9$ $\chi_{anti} = 0$ $\chi_{orto} = 0$	$\chi_C = 14$ $\chi_H = 10$ $\chi_{syn} = 7$ $\chi_{anti} = 2$ $\chi_{orto} = 0$	$\chi_C = 14$ $\chi_H = 10$ $\chi_{syn} = 7$ $\chi_{anti} = 2$ $\chi_{orto} = 0$	$\chi_C = 14$ $\chi_H = 10$ $\chi_{syn} = 5$ $\chi_{anti} = 4$ $\chi_{orto} = 0$
pyrene			tetracene			benz[a]anthracene		
								
(x)*	**(xi)**	**(xii)**	**(xiii)***	**(xiv)***	**(xv)**	**(xvi)**	**(xvii)***	**(xviii)***
$\chi_C = 16$ $\chi_H = 10$ $\chi_{syn} = 9$ $\chi_{anti} = 2$ $\chi_{orto} = 0$	$\chi_C = 16$ $\chi_H = 10$ $\chi_{syn} = 8$ $\chi_{anti} = 3$ $\chi_{orto} = 0$	$\chi_C = 10$ $\chi_H = 8$ $\chi_{syn} = 5$ $\chi_{anti} = 6$ $\chi_{orto} = 0$	$\chi_C = 18$ $\chi_H = 12$ $\chi_{syn} = 8$ $\chi_{anti} = 4$ $\chi_{orto} = 0$	$\chi_C = 18$ $\chi_H = 12$ $\chi_{syn} = 8$ $\chi_{anti} = 4$ $\chi_{orto} = 0$	$\chi_C = 18$ $\chi_H = 12$ $\chi_{syn} = 6$ $\chi_{anti} = 6$ $\chi_{orto} = 0$	$\chi_C = 18$ $\chi_H = 12$ $\chi_{syn} = 6$ $\chi_{anti} = 6$ $\chi_{orto} = 0$	$\chi_C = 18$ $\chi_H = 12$ $\chi_{syn} = 10$ $\chi_{anti} = 2$ $\chi_{orto} = 0$	$\chi_C = 18$ $\chi_H = 12$ $\chi_{syn} = 10$ $\chi_{anti} = 2$ $\chi_{orto} = 0$
				chrysene				
								
(xix)*	**(xx)**	**(xxi)**	**(xxii)**	**(xxiii)***	**(xxiv)**	**(xxv)**	**(xxvi)**	**(xxvii)**
$\chi_C = 18$ $\chi_H = 12$ $\chi_{syn} = 10$ $\chi_{anti} = 2$ $\chi_{orto} = 0$	$\chi_C = 18$ $\chi_H = 12$ $\chi_{syn} = 8$ $\chi_{anti} = 4$ $\chi_{orto} = 0$	$\chi_C = 18$ $\chi_H = 12$ $\chi_{syn} = 8$ $\chi_{anti} = 4$ $\chi_{orto} = 0$	$\chi_C = 18$ $\chi_H = 12$ $\chi_{syn} = 8$ $\chi_{anti} = 4$ $\chi_{orto} = 0$	$\chi_C = 18$ $\chi_H = 12$ $\chi_{syn} = 12$ $\chi_{anti} = 0$ $\chi_{orto} = 0$	$\chi_C = 18$ $\chi_H = 12$ $\chi_{syn} = 10$ $\chi_{anti} = 2$ $\chi_{orto} = 0$	$\chi_C = 18$ $\chi_H = 12$ $\chi_{syn} = 8$ $\chi_{anti} = 4$ $\chi_{orto} = 0$	$\chi_C = 18$ $\chi_H = 12$ $\chi_{syn} = 8$ $\chi_{anti} = 4$ $\chi_{orto} = 0$	$\chi_C = 18$ $\chi_H = 12$ $\chi_{syn} = 8$ $\chi_{anti} = 4$ $\chi_{orto} = 0$

TABLE S1. continued

[4]-helicene					anthanthrene			
								
(xxviii)*	**(xxix)**	**(xxx)**	**(xxxi)**	**(xxxii)**	**(xxxiii)***	**(xxxiv)**	**(xxxv)**	**(xxxvi)**
χ_C = 18 χ_H = 12 χ_{syn} = 12 χ_{anti} = 0 χ_{orto} = 0	χ_C = 18 χ_H = 12 χ_{syn} = 10 χ_{anti} = 2 χ_{orto} = 0	χ_C = 18 χ_H = 12 χ_{syn} = 8 χ_{anti} = 4 χ_{orto} = 0	χ_C = 18 χ_H = 12 χ_{syn} = 8 χ_{anti} = 4 χ_{orto} = 0	χ_C = 18 χ_H = 12 χ_{syn} = 8 χ_{anti} = 4 χ_{orto} = 0	χ_C = 22 χ_H = 12 χ_{syn} = 12 χ_{anti} = 4 χ_{orto} = 0	χ_C = 22 χ_H = 12 χ_{syn} = 11 χ_{anti} = 5 χ_{orto} = 0	χ_C = 22 χ_H = 12 χ_{syn} = 10 χ_{anti} = 6 χ_{orto} = 0	χ_C = 22 χ_H = 12 χ_{syn} = 10 χ_{anti} = 6 χ_{orto} = 0

coronene							
							
(xxxvii)	**(xxxviii)**	**(xxxix)***	**(xl)**	**(xli)**	**(xlii)**	**(xliii)**	**(xliv)**
χ_C = 22 χ_H = 12 χ_{syn} = 9 χ_{anti} = 7 χ_{orto} = 0	χ_C = 22 χ_H = 12 χ_{syn} = 6 χ_{anti} = 10 χ_{orto} = 0	χ_C = 24 χ_H = 12 χ_{syn} = 18 χ_{anti} = 0 χ_{orto} = 0 χ_p = 0	χ_C = 24 χ_H = 12 χ_{syn} = 14 χ_{anti} = 4 χ_{orto} = 0 χ_p = 0	χ_C = 24 χ_H = 12 χ_{syn} = 12 χ_{anti} = 6 χ_{orto} = 0 χ_p = 0	χ_C = 24 χ_H = 12 χ_{syn} = 12 χ_{anti} = 6 χ_{orto} = 0 χ_p = 0	χ_C = 24 χ_H = 12 χ_{syn} = 10 χ_{anti} = 8 χ_{orto} = 0 χ_p = 0	χ_C = 24 χ_H = 12 χ_{syn} = 6 χ_{anti} = 12 χ_{orto} = 0 χ_p = 0

TABLE S2. 94 reference systems with localized π bonds used to construct homodesmotic reactions. For each system a set of topological features χ_i is given.

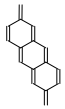
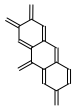
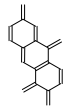
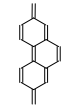
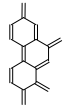
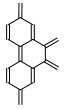
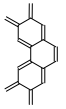
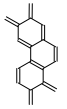
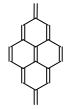
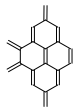
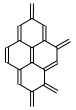
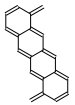
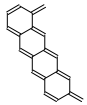
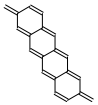
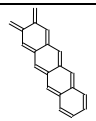
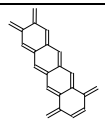
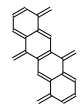
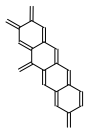
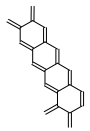
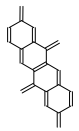
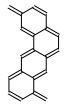
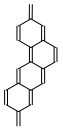
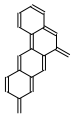
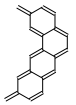
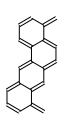
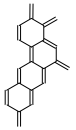
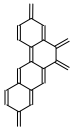
										
I	**II**	**III**	**IV**	**V**	**VI**	**VII**	**VIII**	**IX**	**X**	**XI**
$\chi_C = 8$ $\chi_H = 8$ $\chi_{syn} = 0$ $\chi_{anti} = 4$ $\chi_{orto} = 0$	$\chi_C = 8$ $\chi_H = 8$ $\chi_{syn} = 2$ $\chi_{anti} = 2$ $\chi_{orto} = 1$	$\chi_C = 10$ $\chi_H = 10$ $\chi_{syn} = 3$ $\chi_{anti} = 2$ $\chi_{orto} = 3$	$\chi_C = 12$ $\chi_H = 12$ $\chi_{syn} = 6$ $\chi_{anti} = 0$ $\chi_{orto} = 6$	$\chi_C = 12$ $\chi_H = 10$ $\chi_{syn} = 0$ $\chi_{anti} = 7$ $\chi_{orto} = 0$	$\chi_C = 12$ $\chi_H = 10$ $\chi_{syn} = 2$ $\chi_{anti} = 5$ $\chi_{orto} = 0$	$\chi_C = 12$ $\chi_H = 10$ $\chi_{syn} = 4$ $\chi_{anti} = 3$ $\chi_{orto} = 0$	$\chi_C = 12$ $\chi_H = 10$ $\chi_{syn} = 3$ $\chi_{anti} = 4$ $\chi_{orto} = 1$	$\chi_C = 14$ $\chi_H = 12$ $\chi_{syn} = 4$ $\chi_{anti} = 4$ $\chi_{orto} = 1$	$\chi_C = 14$ $\chi_H = 12$ $\chi_{syn} = 4$ $\chi_{anti} = 4$ $\chi_{orto} = 2$	$\chi_C = 14$ $\chi_H = 12$ $\chi_{syn} = 4$ $\chi_{anti} = 4$ $\chi_{orto} = 2$
										
XII	**XIII**	**XIV**	**XV**	**XIV**	**XVII**	**XVIII**	**XIX**	**XX**	**XXI**	**XXII**
$\chi_C = 16$ $\chi_H = 12$ $\chi_{syn} = 2$ $\chi_{anti} = 8$ $\chi_{orto} = 0$	$\chi_C = 16$ $\chi_H = 12$ $\chi_{syn} = 0$ $\chi_{anti} = 10$ $\chi_{orto} = 0$	$\chi_C = 16$ $\chi_H = 12$ $\chi_{syn} = 4$ $\chi_{anti} = 6$ $\chi_{orto} = 1$	$\chi_C = 18$ $\chi_H = 14$ $\chi_{syn} = 5$ $\chi_{anti} = 6$ $\chi_{orto} = 1$	$\chi_C = 18$ $\chi_H = 14$ $\chi_{syn} = 6$ $\chi_{anti} = 5$ $\chi_{orto} = 1$	$\chi_C = 18$ $\chi_H = 14$ $\chi_{syn} = 5$ $\chi_{anti} = 6$ $\chi_{orto} = 2$	$\chi_C = 18$ $\chi_H = 14$ $\chi_{syn} = 4$ $\chi_{anti} = 7$ $\chi_{orto} = 1$	$\chi_C = 18$ $\chi_H = 14$ $\chi_{syn} = 6$ $\chi_{anti} = 5$ $\chi_{orto} = 1$	$\chi_C = 18$ $\chi_H = 14$ $\chi_{syn} = 4$ $\chi_{anti} = 7$ $\chi_{orto} = 1$	$\chi_C = 16$ $\chi_H = 12$ $\chi_{syn} = 4$ $\chi_{anti} = 6$ $\chi_{orto} = 0$	$\chi_C = 16$ $\chi_H = 12$ $\chi_{syn} = 0$ $\chi_{anti} = 10$ $\chi_{orto} = 0$
										
XXIII	**XXIV**	**XXV**	**XXVI**	**XXVII**	**XXVIII**	**XXIX**	**XXX**	**XXXI**	**XXXII**	**XXXIII**
$\chi_C = 16$ $\chi_H = 12$ $\chi_{syn} = 3$ $\chi_{anti} = 7$ $\chi_{orto} = 0$	$\chi_C = 16$ $\chi_H = 12$ $\chi_{syn} = 2$ $\chi_{anti} = 8$ $\chi_{orto} = 0$	$\chi_C = 16$ $\chi_H = 12$ $\chi_{syn} = 6$ $\chi_{anti} = 4$ $\chi_{orto} = 0$	$\chi_C = 18$ $\chi_H = 14$ $\chi_{syn} = 4$ $\chi_{anti} = 7$ $\chi_{orto} = 1$	$\chi_C = 18$ $\chi_H = 14$ $\chi_{syn} = 3$ $\chi_{anti} = 8$ $\chi_{orto} = 1$	$\chi_C = 18$ $\chi_H = 14$ $\chi_{syn} = 5$ $\chi_{anti} = 6$ $\chi_{orto} = 2$	$\chi_C = 18$ $\chi_H = 14$ $\chi_{syn} = 5$ $\chi_{anti} = 6$ $\chi_{orto} = 2$	$\chi_C = 18$ $\chi_H = 14$ $\chi_{syn} = 4$ $\chi_{anti} = 7$ $\chi_{orto} = 1$	$\chi_C = 18$ $\chi_H = 12$ $\chi_{syn} = 0$ $\chi_{anti} = 12$ $\chi_{orto} = 0$	$\chi_C = 18$ $\chi_H = 12$ $\chi_{syn} = 3$ $\chi_{anti} = 9$ $\chi_{orto} = 0$	$\chi_C = 18$ $\chi_H = 12$ $\chi_{syn} = 6$ $\chi_{anti} = 6$ $\chi_{orto} = 0$

TABLE S2 continued.

										
XXXIV	**XXXV**	**XXXVI**	**XXXVII**	**XXXVIII**	**XXXIX**	**XL**	**XLI**	**XLII**	**XLIII**	**XLIV**
χ_C = 20 χ_H = 14 χ_{syn} = 3 χ_{anti} = 10 χ_{orto} = 1	χ_C = 20 χ_H = 14 χ_{syn} = 4 χ_{anti} = 9 χ_{orto} = 1	χ_C = 20 χ_H = 14 χ_{syn} = 6 χ_{anti} = 7 χ_{orto} = 1	χ_C = 20 χ_H = 14 χ_{syn} = 5 χ_{anti} = 8 χ_{orto} = 0	χ_C = 20 χ_H = 14 χ_{syn} = 7 χ_{anti} = 6 χ_{orto} = 1	χ_C = 20 χ_H = 14 χ_{syn} = 4 χ_{anti} = 9 χ_{orto} = 0	χ_C = 20 χ_H = 14 χ_{syn} = 4 χ_{anti} = 9 χ_{orto} = 0	χ_C = 20 χ_H = 14 χ_{syn} = 2 χ_{anti} = 11 χ_{orto} = 0	χ_C = 20 χ_H = 14 χ_{syn} = 0 χ_{anti} = 13 χ_{orto} = 0	χ_C = 20 χ_H = 14 χ_{syn} = 5 χ_{anti} = 8 χ_{orto} = 0	χ_C = 22 χ_H = 16 χ_{syn} = 6 χ_{anti} = 8 χ_{orto} = 1
										
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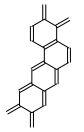
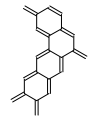
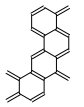
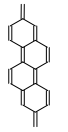
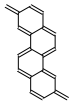
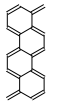
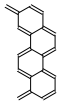
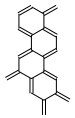
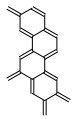
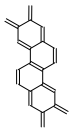
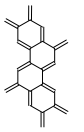
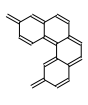
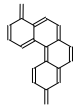
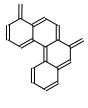
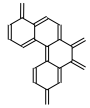
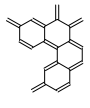
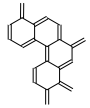
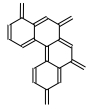
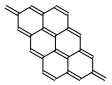
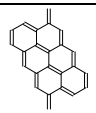
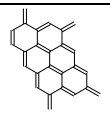
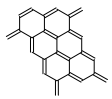
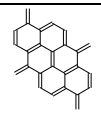
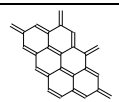
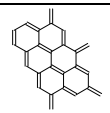
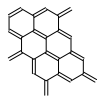
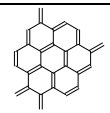
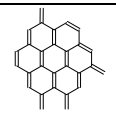
										
LVI	**LVII**	**LVIII**	**LIX**	**LX**	**LXI**	**LXII**	**LXIII**	**LXIV**	**LXV**	**LXVI**
χ_C = 22 χ_H = 16 χ_{syn} = 6 χ_{anti} = 8 χ_{orto} = 2	χ_C = 22 χ_H = 16 χ_{syn} = 5 χ_{anti} = 9 χ_{orto} = 1	χ_C = 22 χ_H = 16 χ_{syn} = 8 χ_{anti} = 6 χ_{orto} = 1	χ_C = 20 χ_H = 14 χ_{syn} = 0 χ_{anti} = 13 χ_{orto} = 0	χ_C = 20 χ_H = 14 χ_{syn} = 4 χ_{anti} = 9 χ_{orto} = 0	χ_C = 20 χ_H = 14 χ_{syn} = 8 χ_{anti} = 5 χ_{orto} = 0	χ_C = 20 χ_H = 14 χ_{syn} = 6 χ_{anti} = 7 χ_{orto} = 0	χ_C = 22 χ_H = 16 χ_{syn} = 8 χ_{anti} = 6 χ_{orto} = 1	χ_C = 22 χ_H = 16 χ_{syn} = 6 χ_{anti} = 8 χ_{orto} = 1	χ_C = 22 χ_H = 16 χ_{syn} = 6 χ_{anti} = 8 χ_{orto} = 2	χ_C = 24 χ_H = 18 χ_{syn} = 8 χ_{anti} = 7 χ_{orto} = 2

TABLE S2 continued.

										
LXVII	**LXVIII**	**LXIX**	**LXX**	**LXXI**	**LXXII**	**LXXIII**	**LXXIV**	**LXXV**	**LXXVI**	**LXXVII**
χ_C = 20 χ_H = 14 χ_{syn} = 2 χ_{anti} = 11 χ_{orto} = 0	χ_C = 20 χ_H = 14 χ_{syn} = 4 χ_{anti} = 9 χ_{orto} = 0	χ_C = 20 χ_H = 14 χ_{syn} = 7 χ_{anti} = 6 χ_{orto} = 0	χ_C = 22 χ_H = 16 χ_{syn} = 6 χ_{anti} = 8 χ_{orto} = 2	χ_C = 22 χ_H = 16 χ_{syn} = 7 χ_{anti} = 7 χ_{orto} = 1	χ_C = 22 χ_H = 16 χ_{syn} = 5 χ_{anti} = 9 χ_{orto} = 1	χ_C = 22 χ_H = 16 χ_{syn} = 8 χ_{anti} = 6 χ_{orto} = 1	χ_C = 22 χ_H = 16 χ_{syn} = 4 χ_{anti} = 10 χ_{orto} = 0	χ_C = 22 χ_H = 16 χ_{syn} = 6 χ_{anti} = 8 χ_{orto} = 0	χ_C = 22 χ_H = 16 χ_{syn} = 4 χ_{anti} = 10 χ_{orto} = 1	χ_C = 24 χ_H = 14 χ_{syn} = 0 χ_{anti} = 17 χ_{orto} = 0

										
LXXVIII	**LXXIX**	**LXXX**	**LXXXI**	**LXXXII**	**LXXXIII**	**LXXXIV**	**LXXXV**	**LXXXVI**	**LXXXVII**	**LXXXVIII**
χ_C = 24 χ_H = 14 χ_{syn} = 3 χ_{anti} = 14 χ_{orto} = 0	χ_C = 24 χ_H = 14 χ_{syn} = 8 χ_{anti} = 9 χ_{orto} = 0	χ_C = 24 χ_H = 14 χ_{syn} = 6 χ_{anti} = 11 χ_{orto} = 0	χ_C = 26 χ_H = 16 χ_{syn} = 6 χ_{anti} = 12 χ_{orto} = 0	χ_C = 26 χ_H = 16 χ_{syn} = 6 χ_{anti} = 12 χ_{orto} = 0	χ_C = 26 χ_H = 16 χ_{syn} = 10 χ_{anti} = 8 χ_{orto} = 0	χ_C = 26 χ_H = 16 χ_{syn} = 4 χ_{anti} = 14 χ_{orto} = 0	χ_C = 26 χ_H = 16 χ_{syn} = 8 χ_{anti} = 10 χ_{orto} = 0	χ_C = 26 χ_H = 16 χ_{syn} = 7 χ_{anti} = 11 χ_{orto} = 0	χ_C = 28 χ_H = 16 χ_{syn} = 10 χ_{anti} = 10 χ_{orto} = 1 χ_p = 0	χ_C = 28 χ_H = 16 χ_{syn} = 3 χ_{anti} = 17 χ_{orto} = 0 χ_p = 1

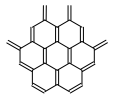
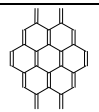
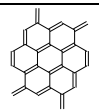
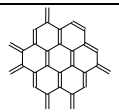
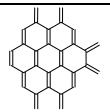
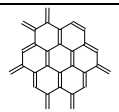
					
LXXXIX	**XC**	**XCI**	**XCII**	**XCIII**	**XCIV**
χ_C = 28 χ_H = 16 χ_{syn} = 6 χ_{anti} = 14 χ_{orto} = 0 χ_p = 1	χ_C = 28 χ_H = 16 χ_{syn} = 0 χ_{anti} = 20 χ_{orto} = 0 χ_p = 2	χ_C = 28 χ_H = 16 χ_{syn} = 6 χ_{anti} = 14 χ_{orto} = 0 χ_p = 0	χ_C = 30 χ_H = 18 χ_{syn} = 6 χ_{anti} = 15 χ_{orto} = 1 χ_p = 1	χ_C = 30 χ_H = 18 χ_{syn} = 3 χ_{anti} = 18 χ_{orto} = 1 χ_p = 2	χ_C = 30 χ_H = 18 χ_{syn} = 7 χ_{anti} = 14 χ_{orto} = 1 χ_p = 1

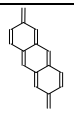
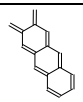
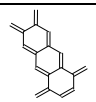
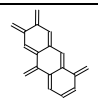
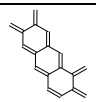
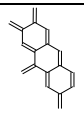
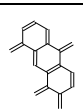
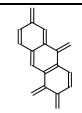
TABLE S3. Coefficients c_i and *ASE* values for 331 homodesmotic reactions of 8 different π-electron systems

benzene reaction	 **I**	 **II**	 **III**	 **IV**	 **(i)**	***ASE*** kcal/mole
1	-1.167	3.000	-0.667	-0.167	1	29.1

naphthalene reaction	 **V**	 **VI**	 **VII**	 **VIII**	 **IX**	 **X**	 **XI**	 **(ii)**	***ASE*** kcal/mole
2	-1.909	1.727	–	2.182	0.182	-1.182	–	1	37.7
3	-1.909	1.727	–	2.182	0.182	–	-1.182	1	40.1
4	-2.000	2.000	–	2.000	–	-0.500	-0.500	1	38.9
5	-0.833	0.667	2.167	–	-2.000	1.000	–	1	40.7
6	-0.833	0.667	2.167	–	-2.000	–	1.000	1	38.7
7	-0.828	–	1.517	1.310	-0.690	-0.310	–	1	39.2
8	-0.828	–	1.517	1.310	-0.690	–	-0.310	1	39.8
9	-1.000	–	1.000	2.000	–	-0.500	-0.500	1	39.3
10	–	-1.571	2.429	1.143	-0.857	-0.143	–	1	39.7
11	–	-1.571	2.429	1.143	-0.857	–	-0.143	1	40.0
12	–	-2.000	2.000	2.000	–	-0.500	-0.500	1	39.7
13	-0.917	0.333	1.583	1.000	-1.000	–	–	1	39.5
14	-1.000	–	1.000	2.000	–	-1.000	–	1	38.2
15	-1.000	–	1.000	2.000	–	–	-1.000	1	40.3
16	-3.000	5.000	–	–	-2.000	0.500	0.500	1	38.9
								mean value	39.4
								s.d.	0.8

naphthalene reaction	 **V**	 **VI**	 **VII**	 **VIII**	 **IX**	 **X**	 **XI**	 **(iii)**	***ASE*** kcal/mole
17	-1.091	1.273	–	1.818	-0.182	-0.818	–	1	32.2
18	-1.091	1.273	–	1.818	-0.182	–	-0.818	1	33.9
19	-1.000	1.000	–	2.000	–	-0.500	-0.500	1	33.1
20	-0.333	0.667	1.667	–	-2.000	1.000	–	1	34.7
21	-0.333	0.667	1.667	–	-2.000	–	1.000	1	32.7
22	-0.310	–	1.069	1.241	-0.759	-0.241	–	1	33.2
23	-0.310	–	1.069	1.241	-0.759	–	-0.241	1	33.7
24	-0.500	–	0.500	2.000	–	-0.500	-0.500	1	33.3
25	–	-0.571	1.429	1.143	-0.857	-0.143	–	1	33.5
26	–	-0.571	1.429	1.143	-0.857	–	-0.143	1	33.8
27	–	-1.000	1.000	2.000	–	-0.500	-0.500	1	33.5
28	-0.417	0.333	1.083	1.000	-1.000	–	–	1	33.5
29	-0.500	–	0.500	2.000	–	-1.000	–	1	32.2
30	-0.500	–	0.500	2.000	–	–	-1.000	1	34.3
31	-2.000	4.000	–	–	-2.000	0.500	0.500	1	33.1
								mean value	33.4
								s.d.	0.7

TABLE S3. continued

anthracene											
reaction	**XII**	**XIII**	**XIV**	**XV**	**XVI**	**XVII**	**XVII**	**XIX**	**XX**	**(iv)**	***ASE*** kcal/mole
32	4.000	-3.000	1.000	-2.000	1.000	–	–	–	–	1	45.3
33	4.000	-3.000	1.000	-2.000	0.000	–	–	1.000	–	1	46.0
34	1.250	-1.625	2.375	0.375	–	-1.375	–	–	–	1	41.9
35	3.100	-2.100	1.000	0.800	–	–	-1.800	–	–	1	40.9
36	3.100	-2.100	1.000	0.800	–	–	–	–	-1.800	1	39.0
37	0.913	-1.348	2.435	–	0.435	-1.435	–	–	–	1	42.5
38	0.913	-1.348	2.435	–	–	-1.435	–	0.435	–	1	42.8
39	2.250	-1.250	1.000	–	1.250	–	-2.250	–	–	1	42.5
40	2.250	-1.250	1.000	–	–	–	-2.250	1.250	–	1	43.3
41	2.250	-1.250	1.000	–	1.250	–	–	–	-2.250	1	40.1
42	2.250	-1.250	1.000	–	–	–	–	1.250	-2.250	1	41.0
43	4.500	-3.500	1.000	–	-0.500	–	–	-0.500	–	1	39.7
44	1.727	-1.909	2.182	–	–	-1.182	0.182	–	–	1	41.9
45	1.727	-1.909	2.182	–	–	-1.182	–	–	0.182	1	42.1
46	3.500	-2.500	1.000	–	–	–	-0.500	–	-0.500	1	40.6
										mean value	42.0
										s.d.	1.9

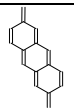
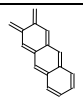
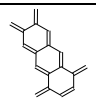
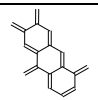
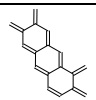
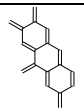
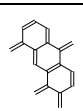
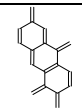
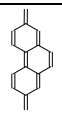
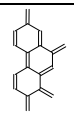
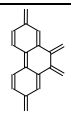
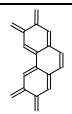
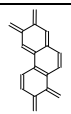
anthracene											
reaction	**XII**	**XIII**	**XIV**	**XV**	**XVI**	**XVII**	**XVII**	**XIX**	**XX**	**(v)**	***ASE*** kcal/mole
47	2.700	-1.700	1.000	-1.600	0.600	–	–	–	–	1	37.1
48	2.700	-1.700	1.000	-1.600	–	–	–	0.600	–	1	37.5
49	1.000	-1.000	2.000	–	–	-1.000	–	–	–	1	36.6
50	2.300	-1.300	1.000	0.400	–	–	-1.400	–	–	1	35.9
51	2.300	-1.300	1.000	0.400	–	–	–	–	-1.400	1	34.4
52	0.783	-0.870	2.087	–	0.087	-1.087	–	–	–	1	36.8
53	0.783	-0.870	2.087	–	–	-1.087	–	0.087	–	1	36.8
54	1.750	-0.750	1.000	–	0.750	–	-1.750	–	–	1	36.8
55	1.750	-0.750	1.000	–	–	–	-1.750	0.750	–	1	37.3
56	1.750	-0.750	1.000	–	0.750	–	–	–	-1.750	1	34.9
57	1.750	-0.750	1.000	–	–	–	–	0.750	-1.750	1	35.5
58	3.500	-2.500	1.000	–	-0.500	–	–	-0.500	–	1	34.5
59	1.273	-1.091	1.818	–	–	-0.818	-0.182	–	–	1	36.5
60	1.273	-1.091	1.818	–	–	-0.818	–	–	-0.182	1	36.3
61	2.500	-1.500	1.000	–	–	–	-0.500	–	-0.500	1	35.4
										mean value	36.1
										s.d.	1.0

TABLE S3. continued

phenanthrene												
reaction	**XXI**	**XXII**	**XXIII**	**XXIV**	**XXV**	**XXVI**	**XXVII**	**XXVIII**	**XXIX**	**XXX**	**(vi)**	***ASE*** kcal/mole
62	1.692	-0.769	1.077	–	–	–	-2.000	1.000	–	–	1	53.0
63	2.077	-1.308	1.231	–	–	–	–	–	1.000	-2.000	1	49.4
64	2.077	-1.308	1.231	–	–	–	–	1.000	–	-2.000	1	48.5
65	2.667	-1.333	–	0.667	–	-2.000	–	1.000	–	–	1	48.0
66	2.667	-1.333	–	0.667	–	-2.000	–	–	1.000	–	1	48.9
67	1.692	-0.769	1.077	–	–	–	-2.000	–	1.000	–	1	53.8
68	2.167	-0.833	-	0.667	–	–	-2.000	1.000	–	–	1	51.0
69	2.167	-0.833	–	0.667	–	–	-2.000	–	1.000	–	1	51.8
70	2.667	-1.333	–	0.667	–	–	–	1.000	–	-2.000	1	46.5
71	0.786	0.071	–	–	1.143	–	-2.000	1.000	–	–	1	53.1
72	0.786	0.071	–	–	1.143	–	-2.000	–	1.000	–	1	53.9
73	2.647	-0.647	–	–	–	–	-1.412	1.000	–	-0.588	1	50.7
74	2.647	-0.647	–	–	–	–	-1.412	–	1.000	-0.588	1	51.5
75	2.667	–	0.667	-1.333	–	–	-2.000	1.000	–	–	1	54.7
76	2.667	–	0.667	-1.333	–	–	-2.000	–	1.000	–	1	55.5
											mean value	51.4
											s.d.	2.7

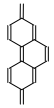
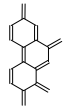
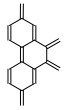
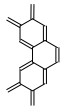
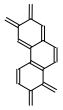
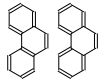
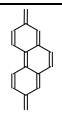
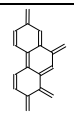
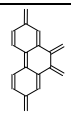
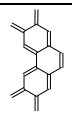
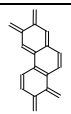
phenanthrene												
reaction	**XXI**	**XXII**	**XXIII**	**XXIV**	**XXV**	**XXVI**	**XXVII**	**XXVIII**	**XXIX**	**XXX**	**(vii, viii)**	***ASE*** kcal/mole
77	1.308	-0.231	0.923	–	–	–	-2.000	1.000	–	–	1	48.3
78	1.692	-0.769	1.077	–	–	–	–	–	1.000	-2.000	1	44.7
79	1.692	-0.769	1.077	–	–	–	–	1.000	–	-2.000	1	43.9
80	2.167	-0.833	–	0.667	–	-2.000	–	1.000	–	–	1	43.5
81	2.167	-0.833	–	0.667	–	-2.000	–	–	1.000	–	1	44.3
82	1.308	-0.231	0.923	–	–	–	-2.000	–	1.000	–	1	49.1
83	1.667	-0.333	–	0.667	–	–	-2.000	1.000	–	–	1	46.5
84	1.667	-0.333	–	0.667	–	–	-2.000	–	1.000	–	1	47.3
85	2.167	-0.833	–	0.667	–	–	–	1.000	–	-2.000	1	41.9
86	0.714	0.429	–	–	0.857	–	-2.000	1.000	–	–	1	48.3
87	0.714	0.429	–	–	0.857	–	-2.000	–	1.000	–	1	49.1
88	2.680	-0.680	–	–	–	–	0.720	1.000	–	-2.720	1	41.3
89	2.680	-0.680	–	–	–	–	0.720	–	1.000	-2.720	1	42.1
90	1.667	–	0.667	-0.333	–	–	-2.000	1.000	–	–	1	48.6
91	1.667	–	0.667	-0.333	–	–	-2.000	1.000	–	–	1	48.6
											mean value	45.9
											s.d.	2.9

TABLE S3. continued

phenanthrene												
reaction	**XXI**	**XXII**	**XXIII**	**XXIV**	**XXV**	**XXVI**	**XXVII**	**XXVIII**	**XXIX**	**XXX**	**(ix)**	***ASE*** kcal/mole
92	0.923	0.308	0.769	–	–	–	-2.000	1.000	–	–	1	43.7
93	1.308	-0.231	0.923	–	–	–	–	–	1.000	-2.000	1	40.1
94	1.308	-0.231	0.923	–	–	–	–	1.000	–	-2.000	1	39.2
95	1.667	-0.333	–	0.667	–	-2.000	–	1.000	–	–	1	39.0
96	1.667	-0.333	–	0.667	–	-2.000	–	–	1.000	–	1	39.8
97	0.923	0.308	0.769	–	–	–	-2.000	–	1.000	–	1	44.5
98	1.167	0.167	–	0.667	–	–	-2.000	1.000	–	–	1	42.0
99	1.167	0.167	–	0.667	–	–	-2.000	–	1.000	–	1	42.8
100	1.667	-0.333	–	0.667	–	–	–	1.000	–	-2.000	1	37.4
101	0.643	0.786	–	–	0.571	–	-2.000	1.000	–	–	1	43.6
102	0.643	0.786	–	–	0.571	–	-2.000	–	1.000	–	1	44.4
103	1.706	0.294	–	–	–	–	-1.176	1.000	–	-0.824	1	41.1
104	1.706	0.294	–	–	–	–	-1.176	–	1.000	-0.824	1	42.0
105	0.667	–	0.667	0.667	–	–	-2.000	1.000	–	–	1	42.5
106	0.667	–	0.667	0.667	–	–	-2.000	–	1.000	–	1	43.4
											mean value	41.7
											s.d.	2.2

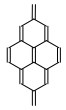
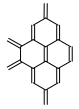
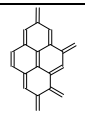
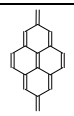
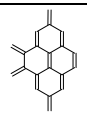
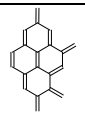
pyrene												
reaction	**XXXI**	**XXXII**	**XXXIII**	**XXXIV**	**XXXV**	**XXXVI**	**XXXVII**	**XXXVIII**	**XXXIX**	**(x)**		***ASE*** kcal/mole
107	-0.550	0.667	1.883	–	–	–	-0.297	–	-0.703	1		48.6
108	-2.300	4.300	–	-1.100	1.100	–	-1.000	–	–	1		50.0
109	-2.000	4.000	–	-1.000	1.000	–	–	–	-1.000	1		48.8
110	-0.833	2.833	–	-1.833	–	1.833	-1.000	–	–	1		50.3
111	-0.667	2.667	–	-1.667	–	1.667	–	–	-1.000	1		49.1
112	-0.320	2.320	–	-1.760	–	–	-1.000	1.760	–	1		52.5
113	-2.150	4.150	–	–	–	–	0.550	–	-1.550	1		46.5
114	-0.200	2.200	–	-1.600	–	–	–	1.600	-1.000	1		51.1
115	-1.538	3.538	–	–	-1.692	1.692	-1.000	–	–	1		47.1
116	-1.308	3.308	–	–	-1.538	1.538	–	–	-1.000	1		46.2
117	-0.833	2.833	–	–	-1.833	–	-1.000	1.833	–	1		49.4
118	-0.667	2.667	–	–	-1.667	–	–	1.667	-1.000	1		48.3
119	-2.300	4.300	–	–	–	-1.100	-1.000	1.100	–	1		49.5
120	-2.000	4.000	–	–	–	-1.000	–	1.000	-1.000	1		48.4
121	-0.667	0.667	2.000	–	–	–	-1.000	–	–	1		49.3
										mean value		49.0
										s.d.		1.67

TABLE S3. continued

pyrene											
reaction	**XXXI**	**XXXII**	**XXXIII**	**XXXIV**	**XXXV**	**XXXVI**	**XXXVII**	**XXXVIII**	**XXXIX**	**(xi)**	***ASE*** kcal/mole
122	-0.721	1.000	1.721	–	–	–	-0.324	–	-0.676	1	48.5
123	-2.000	4.000	–	-1.000	1.000	–	-1.000	–	–	1	47.9
124	-1.700	3.700	–	-0.900	0.900	–	–	–	-1.000	1	46.7
125	-0.667	2.667	–	-1.667	–	1.667	-1.000	–	–	1	48.2
126	-0.500	2.500	–	-1.500	–	1.500	–	–	-1.000	1	47.0
127	-0.200	2.200	–	-1.600	–	–	-1.000	1.600	–	1	50.2
128	-1.850	3.850	–	–	–	–	0.450	–	-1.450	1	44.7
129	-0.080	2.080	–	-1.440	–	–	–	1.440	-1.000	1	48.8
130	-1.308	3.308	–	–	-1.538	1.538	-1.000	–	–	1	45.3
131	-1.077	3.077	–	–	-1.385	1.385	–	–	-1.000	1	44.3
132	-0.667	2.667	–	–	-1.667	–	-1.000	1.667	–	1	47.4
133	-0.500	2.500	–	–	-1.500	–	–	1.500	-1.000	1	46.2
134	-2.000	4.000	–	–	–	-1.000	-1.000	1.000	–	1	47.4
135	-1.700	3.700	–	–	–	-0.900	–	0.900	-1.000	1	46.3
136	-0.500	0.667	1.833	–	–	–	-1.000	–	–	1	47.3
										mean value	47.1
										s.d.	1.6

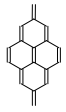
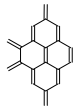
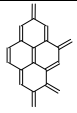
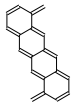
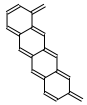
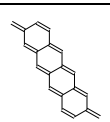
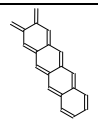
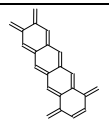
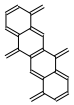
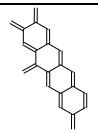
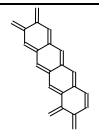
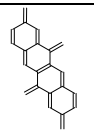
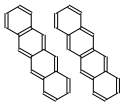
pyrene											
reaction	**XXXI**	**XXXII**	**XXXIII**	**XXXIV**	**XXXV**	**XXXVI**	**XXXVII**	**XXXVIII**	**XXXIX**	**(xii)**	***ASE*** kcal/mole
137	0.099	0.667	1.234	–	–	–	-0.405	–	-0.595	1	40.5
138	-1.100	3.100	–	-0.700	0.700	–	-1.000	–	–	1	41.6
139	-0.800	2.800	–	-0.600	0.600	–	–	–	-1.000	1	40.4
140	-0.167	2.167	–	-1.167	–	1.167	-1.000	–	–	1	41.8
141	0.000	2.000	–	-1.000	–	1.000	–	–	-1.000	1	40.6
142	0.160	1.840	–	-1.120	–	–	-1.000	1.120	–	1	43.2
143	-0.950	2.950	–	–	–	–	0.150	–	-1.150	1	39.2
144	0.280	1.720	–	-0.960	–	–	–	0.960	-1.000	1	41.8
145	-0.615	2.615	–	–	-1.077	1.077	-1.000	–	–	1	39.7
146	-0.385	2.385	–	–	-0.923	0.923	–	–	-1.000	1	38.8
147	-0.167	2.167	–	–	-1.167	–	-1.000	1.167	–	1	41.2
148	–	2.000	–	–	-1.000	–	–	1.000	-1.000	1	40.1
149	-1.100	3.100	–	–	–	-0.700	-1.000	0.700	–	1	41.3
150	-0.800	2.800	–	–	–	-0.600	–	0.600	-1.000	1	40.1
151	0.000	0.667	1.333	–	–	–	-1.000	–	–	1	41.2
										mean value	40.8
										s.d.	1.1

TABLE S3. continued

tetracene											
reaction	**XL**	**XLI**	**XLII**	**XLIII**	**XLIV**	**XLV**	**XLVI**	**XLVII**	**XLVIII**	**(xiii, xiv)**	***ASE*** kcal/mole
152	3.167	0.667	-1.833	–	-2.000	–	–	1.000	–	1	42.5
153	2.667	0.667	-1.333	–	–	–	–	–	-1.000	1	41.1
154	2.167	0.667	-0.833	–	–	–	-2.000	1.000	–	1	40.5
155	1.286	-2.429	–	3.143	–	-1.000	–	–	–	1	35.5
156	1.143	-1.714	–	2.571	-2.000	–	–	1.000	–	1	40.2
157	1.000	-1.000	–	2.000	–	–	–	–	-1.000	1	39.3
158	1.286	-2.429	–	3.143	–	-1.000	–	–	–	1	35.5
159	0.857	-0.286	–	1.429	–	–	-2.000	1.000	–	1	39.2
160	1.381	–	-1.476	2.095	–	-1.000	–	–	–	1	36.6
161	1.238	–	-1.048	1.810	-2.000	–	–	1.000	–	1	41.0
162	1.095	–	-0.619	1.524	–	–	–	–	-1.000	1	39.8
163	0.952	–	-0.190	1.238	–	–	-2.000	1.000	–	1	39.4
164	–	0.368	-1.421	3.053	–	-1.000	–	–	–	1	35.8
165	–	0.421	-1.053	2.632	-2.000	–	–	1.000	–	1	40.3
166	–	0.474	-0.684	2.211	–	–	–	–	-1.000	1	39.3
										mean value	39.1
										s.d.	2.2

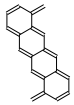
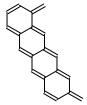
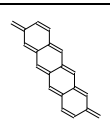
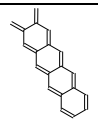
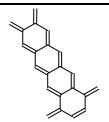
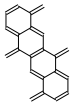
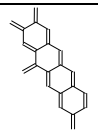
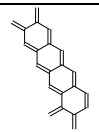
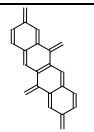
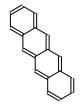
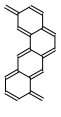
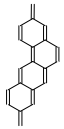
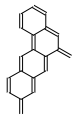
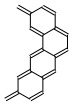
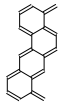
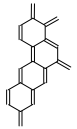
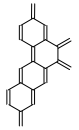
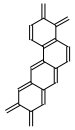
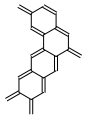
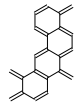
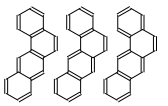
tetracene											
reaction	**XL**	**XLI**	**XLII**	**XLIII**	**XLIV**	**XLV**	**XLVI**	**XLVII**	**XLVIII**	**(xv)**	***ASE*** kcal/mole
167	2.667	0.667	-1.333	–	-2.000	–	–	1.000	–	1	37.9
168	2.167	0.667	-0.833	–	–	–	–	–	-1.000	1	36.5
169	1.667	0.667	-0.333	–	–	–	-2.000	1.000	–	1	35.9
170	1.143	-1.714	–	2.571	–	-1.000	–	–	–	1	31.4
171	1.000	-1.000	–	2.000	-2.000	–	–	1.000	–	1	36.1
172	0.857	-0.286	–	1.429	–	–	–	–	-1.000	1	35.3
173	1.143	-1.714	–	2.571	–	-1.000	–	–	–	1	31.4
174	0.714	0.429	–	0.857	–	–	-2.000	1.000	–	1	35.2
175	1.238	–	-1.048	1.810	–	-1.000	–	–	–	1	32.2
176	1.095	–	-0.619	1.524	-2.000	–	–	1.000	–	1	36.6
177	0.952	–	-0.190	1.238	–	–	–	–	-1.000	1	35.5
178	0.810	–	0.238	0.952	–	–	-2.000	1.000	–	1	35.1
179	–	0.421	-1.053	2.632	–	-1.000	–	–	–	1	31.6
180	–	0.474	-0.684	2.211	-2.000	–	–	1.000	–	1	36.1
181	–	0.526	-0.316	1.789	–	–	–	–	-1.000	1	35.1
										mean value	34.8
										s.d.	2.1

TABLE S3. continued

benz[a]anthracene												
reaction	**XLIX**	**L**	**LI**	**LII**	**LIII**	**LIV**	**LV**	**LVI**	**LVII**	**LVIII**	**(xvii-xix)**	***ASE*** kcal/mole
182	0.600	-	-	-	1.400	-0.800	-1.200	1.000	-	-	1	54.3
183	-	-	0.400	-	1.600	-0.800	-1.200	1.000	-	-	1	55.5
184	0.500	-	-	-	1.500	-	-1.500	1.000	-0.500	-	1	53.9
185	-	-	-	0.294	1.706	-0.824	-1.176	1.000	-	-	1	54.7
186	-	-	-	-	2.000	-0.667	-0.667	1.000	-0.667	-	1	52.7
187	-	0.189	-	-	1.811	-0.865	-1.135	1.000	-	-	1	55.1
188	-	-	0.308	-	1.692	-	-1.462	1.000	-0.538	-	1	54.7
189	-	-	-	0.200	1.800	-	-1.400	1.000	-0.600	-	1	54.0
190	-	-	-	-	2.000	-0.810	-0.952	1.000	-	-0.238	1	54.0
191	0.571	-	0.286	-	1.143	-	-2.000	1.000	-	-	1	56.0
192	0.655	-	-	-	1.345	-	-1.862	1.000	-	-0.138	1	55.1
193	-	0.100	-	-	1.900	-	-1.300	1.000	-0.700	-	1	53.8
194	0.667	-	-	0.167	1.167	-	-2.000	1.000	-	-	1	55.5
195	-	-	-	-	2.000	-	-1.158	1.000	-0.737	-0.105	1	53.2
196	0.786	0.071	-	-	1.143	-	-2.000	1.000	-	-	1	55.5
											mean value	54.5
											s.d.	0.9

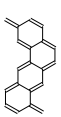
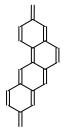
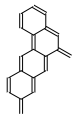
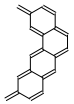
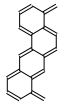
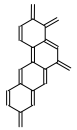
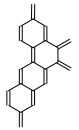
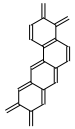
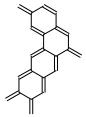
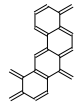
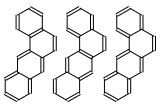
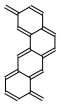
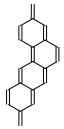
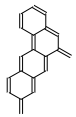
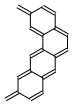
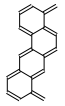
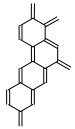
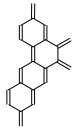
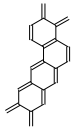
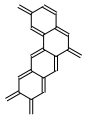
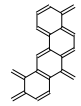
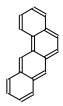
benz[a]anthracene												
reaction	**XLIX**	**L**	**LI**	**LII**	**LIII**	**LIV**	**LV**	**LVI**	**LVII**	**LVIII**	**(xx-xxii)**	***ASE*** kcal/mole
197	1.400	-	-	-	0.600	-1.200	-0.800	1.000	-	-	1	48.3
198	-	-	1.000	-	1.000	-1.000	-1.000	1.000	-	-	1	51.4
199	1.000	-	-	-	1.000	-	-1.000	1.000	-1.000	-	1	47.1
200	-	-	-	0.765	1.235	-0.941	-1.059	1.000	-	-	1	49.8
201	-	-	-	-	2.000	-0.667	0.333	1.000	-1.667	-	1	44.6
202	-	0.514	-	-	1.486	-0.919	-1.081	1.000	-	-	1	51.0
203	-	-	0.769	-	1.231	-	-1.154	1.000	-0.846	-	1	49.7
204	-	-	-	0.600	1.400	-	-1.200	1.000	-0.800	-	1	48.5
205	-	-	-	-	2.000	-0.667	-0.667	1.000	-	-0.667	1	48.2
206	0.714	-	0.857	-	0.429	-	-2.000	1.000	-	-	1	52.1
207	0.793	-	-	-	1.207	-	-1.517	1.000	-	-0.483	1	49.2
208	-	0.400	-	-	1.600	-	-1.200	1.000	-0.800	-	1	49.4
209	0.667	-	-	0.667	0.667	-	-2.000	1.000	-	-	1	50.7
210	-	-	-	-	2.000	-	-0.789	1.000	-0.684	-0.526	1	47.4
211	0.714	0.429	-	-	0.857	-	-2.000	1.000	-	-	1	51.6
											mean value	49.3
											s.d.	2.0

TABLE S3. continued

benz[a]anthracene												
reaction	**XLIX**	**L**	**LI**	**LII**	**LIII**	**LIV**	**LV**	**LVI**	**LVII**	**LVIII**	**(xvi)**	***ASE*** kcal/mole
212	2.200	-	-	-	-0.200	-1.600	-0.400	1.000	-	-	1	42.4
213	-	-	1.600	-	0.400	-1.200	-0.800	1.000	-	-	1	47.4
214	1.500	-	-	-	0.500	-	-0.500	1.000	-1.500	-	1	40.3
215	-	-	-	1.235	0.765	-1.059	-0.941	1.000	-	-	1	44.9
216	-	-	-	-	2.000	-0.667	1.333	1.000	-2.667	-	1	36.5
217	-	0.838	-	-	1.162	-0.973	-1.027	1.000	-	-	1	46.8
218	-	-	1.231	-	0.769	-	-0.846	1.000	-1.154	-	1	44.7
219	-	-	-	1.000	1.000	-	-1.000	1.000	-1.000	-	1	43.1
220	-	-	-	-	2.000	-0.524	-0.381	1.000	-	-1.095	1	42.4
221	0.857	-	1.429	-	-0.286	-	-2.000	1.000	-	-	1	48.3
222	0.931	-	-	-	1.069	-	-1.172	1.000	-	-0.828	1	43.3
223	-	0.700	-	-	1.300	-	-1.100	1.000	-0.900	-	1	45.0
224	0.667	-	-	1.167	0.167	-	-2.000	1.000	-	-	1	46.0
225	-	-	-	-	2.000	-	-0.421	1.000	-0.632	-0.947	1	41.5
226	0.643	0.786	-	-	0.571	-	-2.000	1.000	-	-	1	47.7
											mean value	44.0
											s.d.	3.2

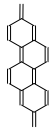
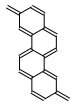
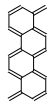
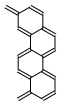
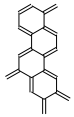
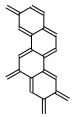
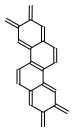
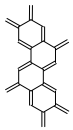
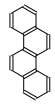
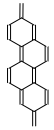
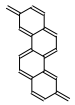
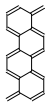
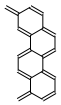
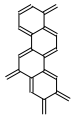
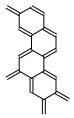
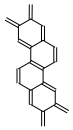
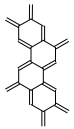
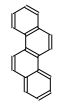
chrysene										***ASE***
reaction	**LIX**	**LX**	**LXI**	**LXII**	**LXIII**	**LXIV**	**LXV**	**LXVI**	**(xxiii)**	kcal/mole
227	-0.923	-	1.231	0.692	-	-	1.000	-1.000	1	56.7
228	-0.917	0.333	1.583	-	-	-	1.000	-1.000	1	56.6
229	-0.750	-	1.625	-	0.250	-	1.000	-1.125	1	58.0
230	-0.705	-	1.795	-	-	-0.182	1.000	-0.909	1	57.0
231	-1.210	-	-	1.839	0.742	-	1.000	-1.371	1	58.2
232	-1.571	0.714	-	1.857	-	-	1.000	-1.000	1	54.6
233	-0.500	-	1.500	1.000	-	-2.000	1.000	-	1	54.5
234	-1.340	-	-	2.320	-	0.040	1.000	-1.020	1	55.6
235	-0.412	-	2.412	-	-0.647	-1.353	1.000	-	1	53.9
236	-	-1.083	2.500	-	-	-0.833	1.000	-0.583	1	58.3
237	-0.583	0.667	1.917	-	-	-2.000	1.000	-	1	53.9
238	-	-1.500	2.250	-	0.500	-	1.000	-1.250	1	61.5
239	-	-1.667	2.333	0.333	-	-	1.000	-1.000	1	60.0
240	-	-0.833	2.167	0.667	-	-2.000	1.000	-	1	56.2
241	-1.038	-	1.885	1.154	-2.000	-	1.000	-	1	50.4
									mean value	56.4
									s.d.	2.7

TABLE S3. continued

chrysene										
reaction	**LIX**	**LX**	**LXI**	**LXII**	**LXIII**	**LXIV**	**LXV**	**LXVI**	**(xxiv)**	***ASE*** kcal/mole
242	-0.654	-	1.038	0.615	-	-	1.000	-1.000	1	53.0
243	-0.667	0.333	1.333	-	-	-	1.000	-1.000	1	52.8
244	-0.500	-	1.417	-	0.167	-	1.000	-1.083	1	54.0
245	-0.455	-	1.545	-	-	-0.182	1.000	-0.909	1	53.3
246	-0.903	-	-	1.613	0.581	-	1.000	-1.290	1	54.1
247	-1.214	0.643	-	1.571	-	-	1.000	-1.000	1	51.2
248	-0.231	-	1.308	0.923	-	-2.000	1.000	-	1	50.7
249	-1.000	-	-	2.000	-	-	1.000	-1.000	1	52.1
250	-0.176	-	2.176	-	-0.706	-1.294	1.000	-	1	50.0
251	-	-0.667	2.000	-	-	-0.667	1.000	-0.667	1	54.0
252	-0.333	0.667	1.667	-	-	-2.000	1.000	-	1	50.2
253	-	-1.000	1.833	-	0.333	-	1.000	-1.167	1	56.3
254	-	-1.167	1.833	0.333	-	-	1.000	-1.000	1	55.4
255	-	-0.333	1.667	0.667	-	-2.000	1.000	-	1	51.5
256	-0.769	-	1.692	1.077	-2.000	-	1.000	-	1	46.7
									mean value	52.4
									s.d.	2.4

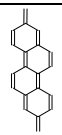
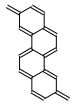
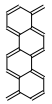
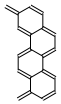
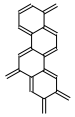
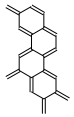
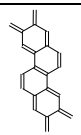
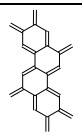
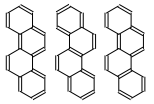
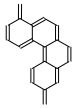
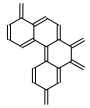
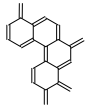
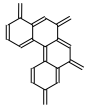
chrysene										
reaction	**LIX**	**LX**	**LXI**	**LXII**	**LXIII**	**LXIV**	**LXV**	**LXVI**	**(xxv-xxvii)**	***ASE*** kcal/mole
257	-0.385	-	0.846	0.538	-	-	1.000	-1.000	1	49.3
258	-0.417	0.333	1.083	-	-	-	1.000	-1.000	1	49.1
259	-0.250	-	1.208	-	0.083	-	1.000	-1.042	1	49.9
260	-0.205	-	1.295	-	-	-0.182	1.000	-0.909	1	49.5
261	-0.597	-	-	1.387	0.419	-	1.000	-1.210	1	50.0
262	-0.857	0.571	-	1.286	-	-	1.000	-1.000	1	47.8
263	0.038	-	1.115	0.846	-	-2.000	1.000	-	1	47.0
264	-0.660	-	-	1.680	-	-0.040	1.000	-0.980	1	48.5
265	0.059	-	1.941	-	-0.765	-1.235	1.000	-	1	46.1
266	-	-0.250	1.500	-	-	-0.500	1.000	-0.750	1	49.6
267	-0.083	0.667	1.417	-	-	-2.000	1.000	-	1	46.4
268	-	-0.500	1.417	-	0.167	-	1.000	-1.083	1	51.1
269	-	-0.667	1.333	0.333	-	-	1.000	-1.000	1	50.7
270	-	0.167	1.167	0.667	-	-2.000	1.000	-	1	46.9
271	-0.500	-	1.500	1.000	-2.000	-	1.000	-	1	43.0
									mean value	48.3
									s.d.	2.1

TABLE S3. continued

[4]-helicene												
reaction	**LXVII**	**LXVIII**	**LXIX**	**LXX**	**LXXI**	**LXXII**	**LXXIII**	**LXXIV**	**LXXV**	**LXXVI**	**(xxviii)**	***ASE*** kcal/mole
272	-	0.400	1.600	-	-	-	0.800	-1.000	-	-0.800	1	51.0
273	0.146	-	1.854	-	-	-	0.683	-1.000	-	-0.683	1	51.3
274	-	-	2.000	-	-	-	0.600	-0.800	-0.200	-0.600	1	51.3
275	-	-	2.000	0.111	-	-	0.444	-0.889	-	-0.667	1	52.0
276	-	-	2.000	-	-	-0.154	0.538	-1.000	-	-0.385	1	52.4
277	-	-	2.000	-	0.692	-	-	-0.962	-0.038	-0.692	1	49.7
278	-	0.167	1.833	-	-	-0.833	0.833	-1.000	-	-	1	54.9
279	-	0.167	1.833	-	0.833	-	-	-1.000	-	-0.833	1	49.1
280	-	-	2.000	0.132	0.579	-	-	-0.868	-	-0.842	1	50.4
281	-0.266	-	2.266	0.335	-	-	-	-0.665	-	-0.671	1	53.4
282	-0.029	-	2.029	-	0.618	-	-	-1.000	-	-0.618	1	50.1
283	-	-	2.000	-0.056	-	-0.556	0.667	-1.056	-	-	1	54.0
284	-0.029	-	2.029	-	-	-0.618	0.618	-1.000	-	-	1	54.4
285	-0.029	-	2.029	-	0.618	-	-	-1.000	-	-0.618	1	50.1
286	-	-	2.000	-	-	-0.692	0.692	-0.962	-0.038	-	1	54.6
											mean value	51.9
											s.d.	1.9

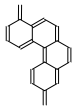
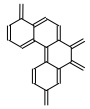
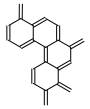
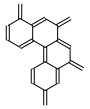
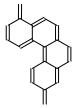
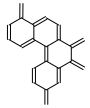
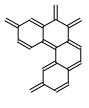
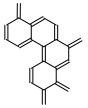
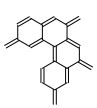
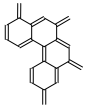
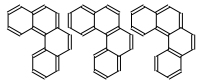
[4]-helicene												
reaction	**LXVII**	**LXVIII**	**LXIX**	**LXX**	**LXXI**	**LXXII**	**LXXIII**	**LXXIV**	**LXXV**	**LXXVI**	**(xxix)**	***ASE*** kcal/mole
287	-	0.640	1.360	-	-	-	0.480	-1.000	-	-0.480	1	47.5
288	0.390	-	1.610	-	-	-	0.488	-1.000	-	-0.488	1	47.4
289	-	-	2.000	-	-	-	0.200	-0.600	-0.400	-0.200	1	47.9
290	-	-	2.000	0.222	-	-	-0.111	-0.778	-	-0.333	1	49.2
291	-	-	2.000	-	-	-	-	-1.000	-	-	1	48.7
292	-	-	2.000	-	0.231	-	-	-0.654	-0.346	-0.231	1	47.4
293	-	0.500	1.500	-	-	-0.500	0.500	-1.000	-	-	1	49.9
294	-	0.500	1.500	-	0.500	-	-	-1.000	-	-0.500	1	46.4
295	-	-	2.000	0.237	-0.158	-	-	-0.763	-	-0.316	1	49.7
296	0.114	-	1.886	0.285	-	-	-	-0.715	-	-0.570	1	49.0
297	0.265	-	1.735	-	0.441	-	-	-1.000	-	-0.441	1	46.6
298	-	-	2.000	0.167	-	-0.333	-	-0.833	-	-	1	50.5
299	0.265	-	1.735	-	-	-0.441	0.441	-1.000	-	-	1	49.7
300	0.265	-	1.735	-	0.441	-	-	-1.000	-	-0.441	1	46.6
301	-	-	2.000	-	-	-0.231	0.231	-0.654	-0.346	-	1	49.0
											mean value	48.4
											s.d.	1.3

TABLE S3. continued

[4]-helicene												
reaction	**LXVII**	**LXVIII**	**LXIX**	**LXX**	**LXXI**	**LXXII**	**LXXIII**	**LXXIV**	**LXXV**	**LXXVI**	**(xxx-xxxii)**	***ASE*** kcal/mole
302	-	0.880	1.120	-	-	-	0.160	-1.000	-	-0.160	1	44.1
303	0.634	-	1.366	-	-	-	0.293	-1.000	-	-0.293	1	43.6
304	-	-	2.000	-	-	-	-0.200	-0.400	-0.600	0.200	1	44.5
305	-	-	2.000	0.333	-	-	-0.667	-0.667	-	-	1	46.4
306	-	-	2.000	-	-	0.154	-0.538	-1.000	-	0.385	1	45.0
307	-	-	2.000	-	-0.231	-	-	-0.346	-0.654	0.231	1	45.0
308	-	0.833	1.167	-	-	-0.167	0.167	-1.000	-	-	1	44.9
309	-	0.833	1.167	-	0.167	-	-	-1.000	-	-0.167	1	43.7
310	-	-	2.000	0.342	-0.895	-	-	-0.658	-	0.211	1	49.0
311	0.494	-	1.506	0.234	-	-	-	-0.766	-	-0.468	1	44.6
312	0.559	-	1.441	-	0.265	-	-	-1.000	-	-0.265	1	43.1
313	-	-	2.000	0.389	-	-0.111	-0.667	-0.611	-	-	1	47.0
314	0.559	-	1.441	-	-	-0.265	0.265	-1.000	-	-	1	44.9
315	0.559	-	1.441	-	0.265	-	-	-1.000	-	-0.265	1	43.1
316	-	-	2.000	-	-	0.231	-0.231	-0.346	-0.654	-	1	43.4
											mean value	44.8
											s.d.	1.6

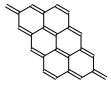
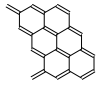
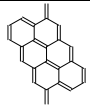
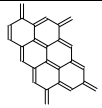
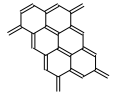
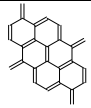
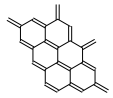
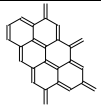
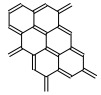
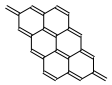
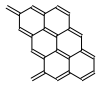
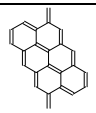
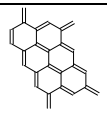
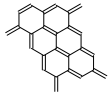
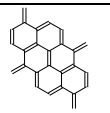
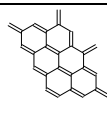
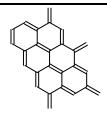
anthanthrene												
reaction	**LXXVII**	**LXXVIII**	**LXXIX**	**LXXX**	**LXXXI**	**LXXXII**	**LXXXIII**	**LXXXIV**	**LXXXV**	**LXXXVI**	**(xxxiii)**	***ASE*** kcal/mole
317	-0.980	0.367	2.612	–	–	–	-1.000	–	–	–	1	50.9
318	-0.306	0.490	1.816	–	–	–	–	-1.000	–	–	1	47.4
319	-0.755	0.408	2.347	–	–	–	–	–	-1.000	–	1	45.5
320	-0.643	0.429	2.214	–	–	–	–	–	–	-1.000	1	44.9
321	-1.333	0.667	–	2.667	-1.000	–	–	–	–	–	1	45.4
322	-2.000	0.667	–	3.333	–	–	-1.000	–	–	–	1	48.7
323	-1.000	0.667	–	2.333	–	–	–	-1.000	–	–	1	45.9
324	-1.667	0.667	–	3.000	–	–	–	–	-1.000	–	1	43.5
325	-1.500	0.667	–	2.833	–	–	–	–	–	-1.000	1	43.0
326	-0.500	–	1.500	1.000	-1.000	–	–	–	–	–	1	46.2
327	-0.500	–	1.500	1.000	–	-1.000	–	–	–	–	1	46.8
328	-1.038	–	1.885	1.154	–	–	-1.000	–	–	–	1	49.9
329	-0.231	–	1.308	0.923	–	–	–	-1.000	–	–	1	46.5
330	-0.769	–	1.692	1.077	–	–	–	–	-1.000	–	1	44.5
331	-0.635	–	1.596	1.038	–	–	–	–	–	-1.000	1	43.9
											mean value	46.2
											s.d.	2.3

TABLE S3. continued

anthanthrene												
reaction	**LXXVII**	**LXXVIII**	**LXXIX**	**LXXX**	**LXXXI**	**LXXXII**	**LXXXIII**	**LXXXIV**	**LXXXV**	**LXXXVI**	**(xxxiv)**	***ASE*** kcal/mole
332	-0.867	0.388	2.480	–	–	–	-1.000	–	–	–	1	49.8
333	-0.194	0.510	1.684	–	–	–	–	-1.000	–	–	1	46.3
334	-0.643	0.429	2.214	–	–	–	–	–	-1.000	–	1	44.3
335	-0.531	0.449	2.082	–	–	–	–	–	–	-1.000	1	43.8
336	-1.167	0.667	–	2.500	-1.000	–	–	–	–	–	1	44.3
337	-1.833	0.667	–	3.167	–	–	-1.000	–	–	–	1	47.7
338	-0.833	0.667	–	2.167	–	–	–	-1.000	–	–	1	44.8
339	-1.500	0.667	–	2.833	–	–	–	–	-1.000	–	1	42.4
340	-1.333	0.667	–	2.667	–	–	–	–	–	-1.000	1	42.0
341	-0.365	–	1.404	0.962	-1.000	–	–	–	–	–	1	45.1
342	-0.365	–	1.404	0.962	–	-1.000	–	–	–	–	1	45.7
343	-0.904	–	1.788	1.115	–	–	-1.000	–	–	–	1	48.8
344	-0.096	–	1.212	0.885	–	–	–	-1.000	–	–	1	45.4
345	-0.635	–	1.596	1.038	–	–	–	–	-1.000	–	1	43.4
346	-0.500	–	1.500	1.000	–	–	–	–	–	-1.000	1	42.8
											mean value	45.1
											s.d.	2.3

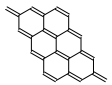
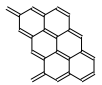
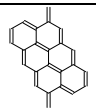
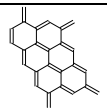
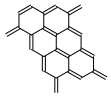
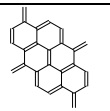
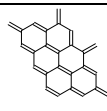
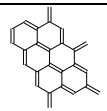
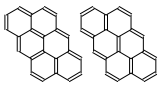
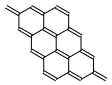
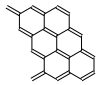
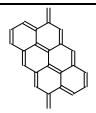
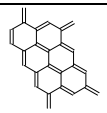
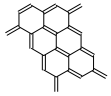
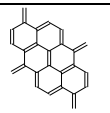
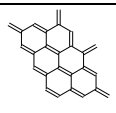
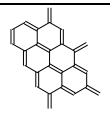
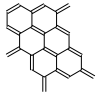
anthanthrene												
reaction	**LXXVII**	**LXXVIII**	**LXXIX**	**LXXX**	**LXXXI**	**LXXXII**	**LXXXIII**	**LXXXIV**	**LXXXV**	**LXXXVI**	**(xxxv,xxxvi)**	***ASE*** kcal/mole
347	-0.755	0.408	2.347	–	–	–	-1.000	–	–	–	1	48.7
348	-0.082	0.531	1.551	–	–	–	–	-1.000	–	–	1	45.2
349	-0.531	0.449	2.082	–	–	–	–	–	-1.000	–	1	43.2
350	-0.418	0.469	1.949	–	–	–	–	–	–	-1.000	1	42.6
351	-1.000	0.667	–	2.333	-1.000	–	–	–	–	–	1	43.3
352	-1.667	0.667	–	3.000	–	–	-1.000	–	–	–	1	46.6
353	-0.667	0.667	–	2.000	–	–	–	-1.000	–	–	1	43.8
354	-1.333	0.667	–	2.667	–	–	–	–	-1.000	–	1	41.4
355	-1.167	0.667	–	2.500	–	–	–	–	–	-1.000	1	40.9
356	-0.231	–	1.308	0.923	-1.000	–	–	–	–	–	1	44.0
357	-0.231	–	1.308	0.923	–	-1.000	–	–	–	–	1	44.6
358	-0.769	–	1.692	1.077	–	–	-1.000	–	–	–	1	47.7
359	0.038	–	1.115	0.846	–	–	–	-1.000	–	–	1	44.3
360	-0.500	–	1.500	1.000	–	–	–	–	-1.000	–	1	42.2
361	-0.365	–	1.404	0.962	–	–	–	–	–	-1.000	1	41.7
											mean value	44.0
											s.d.	2.3

TABLE S3. continued

anthanthrene												
reaction	**LXXVII**	**LXXVIII**	**LXXIX**	**LXXX**	**LXXXI**	**LXXXII**	**LXXXIII**	**LXXXIV**	**LXXXV**	**LXXXVI**	**(xxxvii)**	***ASE*** kcal/mole
362	-0.643	0.429	2.214	–	–	–	-1.000	–	–	–	1	47.5
363	0.031	0.551	1.418	–	–	–	–	-1.000	–	–	1	44.0
364	-0.418	0.469	1.949	–	–	–	–	–	-1.000	–	1	42.1
365	-0.306	0.490	1.816	–	–	–	–	–	–	-1.000	1	41.5
366	-0.833	0.667	–	2.167	-1.000	–	–	–	–	–	1	42.3
367	-1.500	0.667	–	2.833	–	–	-1.000	–	–	–	1	45.6
368	-0.500	0.667	–	1.833	–	–	–	-1.000	–	–	1	42.8
369	-1.167	0.667	–	2.500	–	–	–	–	-1.000	–	1	40.4
370	-1.000	0.667	–	2.333	–	–	–	–	–	-1.000	1	39.9
371	-0.096	–	1.212	0.885	-1.000	–	–	–	–	–	1	42.8
372	-0.096	–	1.212	0.885	–	-1.000	–	–	–	–	1	43.5
373	-0.635	–	1.596	1.038	–	–	-1.000	–	–	–	1	46.5
374	0.173	–	1.019	0.808	–	–	–	-1.000	–	–	1	43.1
375	-0.365	–	1.404	0.962	–	–	–	–	-1.000	–	1	41.1
376	-0.231	–	1.308	0.923	–	–	–	–	–	-1.000	1	40.6
											mean value	42.9
											s.d.	2.2

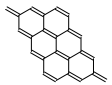
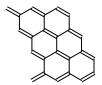
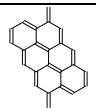
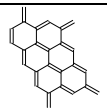
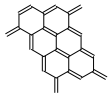
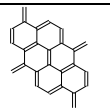
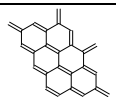
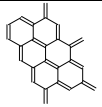
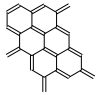
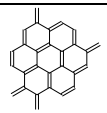
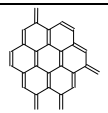
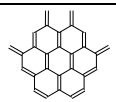
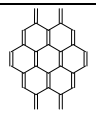
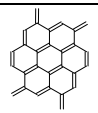
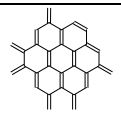
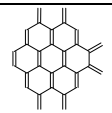
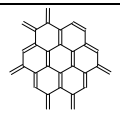
anthanthrene												
reaction	**LXXVII**	**LXXVIII**	**LXXIX**	**LXXX**	**LXXXI**	**LXXXII**	**LXXXIII**	**LXXXIV**	**LXXXV**	**LXXXVI**	**(xxxviii)**	***ASE*** kcal/mole
377	-0.306	0.490	1.816	–	–	–	-1.000	–	–	–	1	44.1
378	0.367	0.612	1.020	–	–	–	–	-1.000	–	–	1	40.6
379	-0.082	0.531	1.551	–	–	–	–	–	-1.000	–	1	38.6
380	0.031	0.551	1.418	–	–	–	–	–	–	-1.000	1	38.1
381	0.444	-0.111	–	1.667	-1.000	–	–	–	–	–	1	36.0
382	-1.000	0.667	–	2.333	–	–	-1.000	–	–	–	1	42.5
383	0.000	0.667	–	1.333	–	–	–	-1.000	–	–	1	39.7
384	-0.667	0.667	–	2.000	–	–	–	–	-1.000	–	1	37.3
385	-0.500	0.667	–	1.833	–	–	–	–	–	-1.000	1	36.8
386	0.308	–	0.923	0.769	-1.000	–	–	–	–	–	1	39.5
387	0.308	–	0.923	0.769	–	-1.000	–	–	–	–	1	40.1
388	-0.231	–	1.308	0.923	–	–	-1.000	–	–	–	1	43.1
389	0.577	–	0.731	0.692	–	–	–	-1.000	–	–	1	39.7
390	0.038	–	1.115	0.846	–	–	–	–	-1.000	–	1	37.7
391	0.173	–	1.020	0.806	–	–	–	–	–	-1.000	1	37.2
											mean value	39.4
											s.d.	2.4

TABLE S3. continued

coronene										
reaction	**LXXXVII**	**LXXXVIII**	**LXXXIX**	**XC**	**XCI**	**XCII**	**XCIII**	**XCIV**	**(xxxix)**	***ASE*** kcal/mole
392	2.000	-0.778	3.333	-0.278	-1.278	-2.000	–	–	1	59.1
393	2.000	-0.778	3.333	0.722	-2.278	–	-2.000	–	1	58.8
394	2.000	-1.000	4.000	-0.500	-1.500	–	–	-2.000	1	54.1
395	2.000	-2.750	3.333	0.417	–	-2.583	0.583	–	1	60.1
396	2.000	-3.300	3.300	1.000	–	-2.100	–	0.100	1	60.6
397	2.000	-3.937	4.031	0.906	–	–	0.094	-2.094	1	54.0
398	2.000	-0.750	3.333	–	-1.583	-1.417	-0.583	–	1	58.4
399	2.000	-1.400	3.400	–	-1.000	-1.800	–	-0.200	1	58.9
400	2.000	-0.636	3.659	–	-2.023	–	-1.023	-0.977	1	57.5
401	2.000	–	3.333	-0.367	-1.967	-1.400	-0.600	–	1	58.6
402	2.000	–	3.410	-0.705	-1.705	-1.769	–	-0.231	1	58.1
403	2.000	–	3.583	-0.167	-2.417	–	-1.250	-0.750	1	56.6
404	2.000	-2.500	3.500	–	–	-2.500	1.000	-0.500	1	58.8
405	2.000	–	3.438	-2.438	–	-5.125	3.438	-0.313	1	58.3
406	2.000	–	3.179	–	-2.179	-1.286	-1.179	0.464	1	59.7
									mean value	58.1
									s.d.	1.9

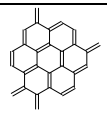
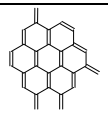
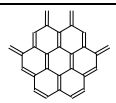
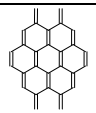
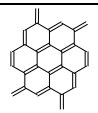
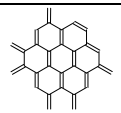
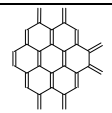
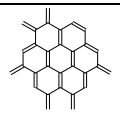
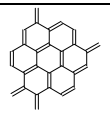
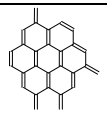
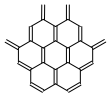
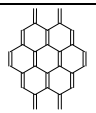
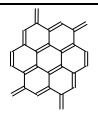
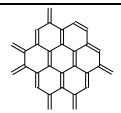
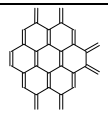
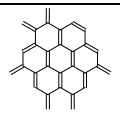
coronene										
reaction	**LXXXVII**	**LXXXVIII**	**LXXXIX**	**XC**	**XCI**	**XCII**	**XCIII**	**XCIV**	**(xl)**	***ASE*** kcal/mole
407	2.000	-0.333	2.000	0.167	-0.833	-2.000	–	–	1	55.6
408	2.000	-0.333	2.000	1.167	-1.833	–	-2.000	–	1	55.4
409	2.000	-0.556	2.667	-0.056	-1.056	–	–	-2.000	1	50.6
410	2.000	-1.750	2.000	0.750	–	-2.250	0.250	–	1	56.3
411	2.000	-2.100	2.100	1.000	–	-1.700	–	-0.300	1	55.7
412	2.000	-2.687	2.656	1.031	–	–	-0.031	-1.969	1	51.8
413	2.000	0.250	2.000	–	-1.250	-1.750	-0.250	–	1	55.3
414	2.000	-0.200	2.200	–	-1.000	-1.400	–	-0.600	1	54.0
415	2.000	0.091	2.477	–	-1.568	–	-0.568	-1.432	1	51.7
416	2.000	–	2.000	0.300	-1.300	-1.400	-0.600	–	1	55.4
417	2.000	–	2.179	-0.090	-1.090	-1.462	–	-0.538	1	54.0
418	2.000	–	2.333	0.333	-1.667	–	-1.000	-1.000	1	52.8
419	2.000	-1.300	2.300	–	–	-2.100	1.000	-0.900	1	53.9
420	2.000	–	2.188	-1.188	–	-3.625	2.188	-0.563	1	54.2
421	2.000	–	2.179	–	-1.179	-1.286	-0.179	-0.536	1	54.0
									mean value	54.0
									s.d.	1.7

TABLE S3. continued

coronene											
reaction	**LXXXVII**	**LXXXVIII**	**LXXXIX**	**XC**	**XCI**	**XCII**	**XCIII**	**XCIV**	**(xli,**	**xlii)**	***ASE*** kcal/mole
422	2.000	-0.111	1.333	0.389	-0.611	-2.000	–	–	1		53.9
423	2.000	-0.111	1.333	1.389	-1.611	–	-2.000	–	1		53.6
424	2.000	-0.333	2.000	0.167	-0.833	–	–	-2.000	1		48.9
425	2.000	-1.250	1.333	0.917	–	-2.083	0.083	–	1		54.4
426	2.000	-1.500	1.500	1.000	–	-1.500	–	-0.500	1		53.3
427	2.000	-2.062	1.969	1.094	–	–	-0.094	-1.906	1		50.0
428	2.000	0.750	1.333	–	-1.083	-1.917	-0.083	–	1		53.4
429	2.000	0.400	1.600	–	-1.000	-1.200	–	-0.800	1		51.6
430	2.000	0.455	1.886	–	-1.341	–	-0.341	-1.659	1		49.3
431	2.000	–	1.333	0.633	-0.967	-1.400	-0.600	–	1		53.7
432	2.000	–	1.564	0.218	-0.782	-1.308	–	-0.692	1		52.0
433	2.000	–	1.708	0.583	-1.292	–	-0.875	-1.125	1		50.8
434	2.000	-0.700	1.700	–	–	-1.900	1.000	-1.100	1		51.5
435	2.000	–	1.563	-0.563	–	-3.333	1.333	–	1		54.3
436	2.000	–	1.679	–	-0.679	-1.286	0.321	-1.036	1		51.2
										mean value	52.1
										s.d.	1.8

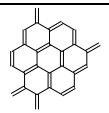
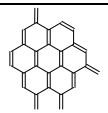
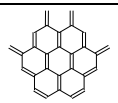
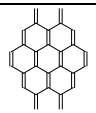
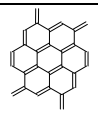
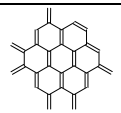
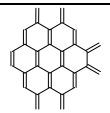
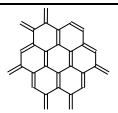
coronene										
reaction	**LXXXVII**	**LXXXVIII**	**LXXXIX**	**XC**	**XCI**	**XCII**	**XCIII**	**XCIV**	**(xliii)**	***ASE*** kcal/mole
437	2.000	0.111	0.667	0.611	-0.389	-2.000	–	–	1	52.1
438	2.000	0.111	0.667	1.611	-1.389	–	-2.000	–	1	51.9
439	2.000	-0.111	1.333	0.389	-0.611	–	–	-2.000	1	47.1
440	2.000	-0.750	0.667	1.083	–	-1.917	-0.083	–	1	52.5
441	2.000	-0.900	0.900	1.000	–	-1.300	–	-0.700	1	50.8
442	2.000	-1.437	1.281	1.156	–	–	-0.156	-1.844	1	48.2
443	2.000	1.250	0.667	–	-0.917	-2.083	0.083	–	1	51.5
444	2.000	1.000	1.000	–	-1.000	-1.000	–	-1.000	1	49.1
445	2.000	0.818	1.295	–	-1.114	–	-0.114	-1.886	1	46.9
446	2.000	–	0.667	0.967	-0.633	-1.400	-0.600	–	1	52.1
447	2.000	–	0.949	0.526	-0.474	-1.154	–	-0.846	1	50.0
448	2.000	–	1.083	0.833	-0.917	–	-0.750	-1.250	1	48.9
449	2.000	-0.100	1.100	–	–	-1.700	1.000	-1.300	1	49.0
450	2.000	–	0.938	0.062	–	-2.125	0.938	-0.813	1	50.2
451	2.000	–	1.179	–	-0.179	-1.286	0.821	-1.536	1	48.3
									mean value	49.9
									s.d.	1.9

TABLE S3. continued

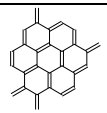
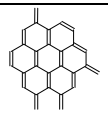
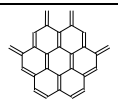
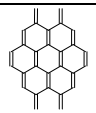
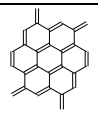
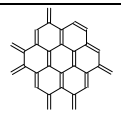
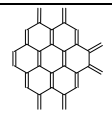
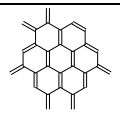
coronene										
reaction	**LXXXVII**	**LXXXVIII**	**LXXXIX**	**XC**	**XCI**	**XCII**	**XCIII**	**XCIV**	**(xliv)**	***ASE*** kcal/mole
452	2.000	0.556	-0.667	1.056	0.056	-2.000	–	–	1	48.6
453	2.000	0.556	-0.667	2.056	-0.944	–	-2.000	–	1	48.4
454	2.000	0.333	0.000	0.833	-0.167	–	–	-2.000	1	43.6
455	2.000	0.250	-0.667	1.417	–	-1.583	-0.417	–	1	48.7
456	2.000	0.300	-0.300	1.000	–	-0.900	–	-1.100	1	46.0
457	2.000	-0.187	-0.094	1.281	–	–	-0.281	-1.719	1	44.6
458	2.000	2.250	-0.667	–	-0.583	-2.417	0.417	–	1	47.8
459	2.000	2.200	-0.200	–	-1.000	-0.600	–	-1.400	1	43.6
460	2.000	1.545	0.114	–	-0.659	–	0.341	-2.341	1	42.2
461	2.000	–	-0.667	1.633	0.033	-1.400	-0.600	–	1	48.9
462	2.000	–	-0.282	1.141	0.141	-0.846	–	-1.154	1	46.0
463	2.000	–	-0.167	1.333	-0.167	–	-0.500	-1.500	1	45.0
464	2.000	1.100	-0.100	–	–	-1.300	1.000	-1.700	1	44.1
465	2.000	–	-0.312	1.312	–	-0.625	-0.312	-1.063	1	46.2
466	2.000	–	0.179	–	0.821	-1.286	1.821	-2.536	1	42.7
									mean value	45.8
									s.d.	2.3

TABLE S4. Additivity of energies of reference compounds

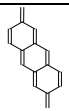
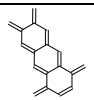
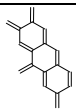
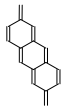
reaction																**ΔE** [kcal/mole]
467	-0.083		+	-0.333		+	-0.583		+	1.000		+	1.000		→		-1.2
468	-0.083		+	-0.333		+	-0.583		+	1.000		+	1.000		→		0.8
469	0.091		+	-0.273		+	0.182		+	0.182		+	0.818		→		1.9
470	-0.069		+	-0.207		+	0.276		+	0.276		+	0.724		→		1.7
471	-0.143		+	-0.143		+	0.286		+	0.286		+	0.714		→		1.7
472				-0.600		+	0.600		+	0.800		+	0.200		→		-0.004
473	0.087		+	0.348		+	-0.435		+	0.565		+	0.435		→		0.3
474				0.200		+	-0.200		+	0.400		+	0.600		→		-1.2
475				-0.600		+	0.600		+	0.800		+	0.200		→		-1.1
476	0.217		+	-0.130		+	-0.087		+	0.913		+	0.087		→		-0.8

TABLE S4. continued

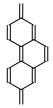
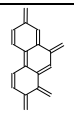
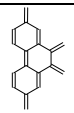
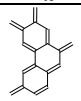
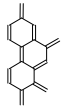
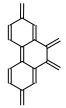
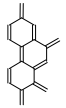
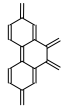
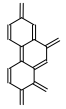
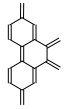
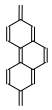
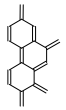
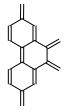
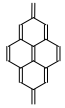
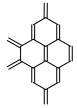
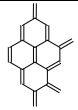
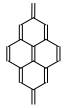
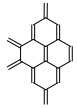
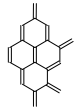
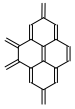
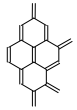
reaction														R_X	**ΔE** [kcal/mole]
477	0.118		+	-0.118		+	0.529		+	0.471		→		-1.5
478	0.250		+	-0.250		+	0.750		+	0.250		→		-1.4
479	0.200		+	-0.200		+	0.600		+	0.400		→		-1.1
480	-0.200		+	0.200		+	0.600		+	0.400		→		-1.2
481	-0.081		+	0.081		+	0.514		+	0.486		→		-1.4
482	-0.405		+	0.405		+	0.432		+	0.568		→		0.4
483	-0.273		+	0.182		+	0.182		+	0.818		→		-1.0
484	0.286		+	0.071		+	-0.357		+	1.000		→		-1.3
485	-0.538		+	1.538		+	-0.692		+	0.692		→		-1.0
486	1.000		+	1.071		+	-0.214		+	-0.857		→		-0.5

TABLE S4. continued

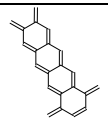
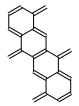
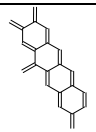
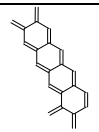
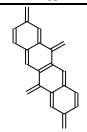
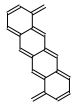
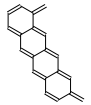
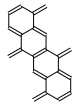
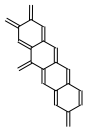
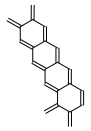
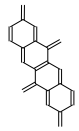
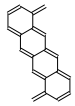
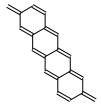
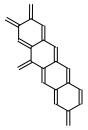
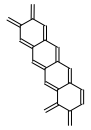
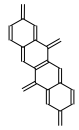
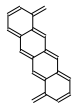
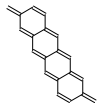
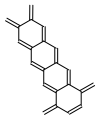
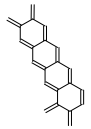
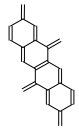
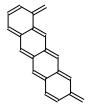
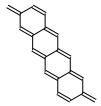
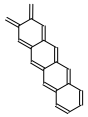
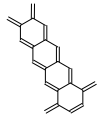
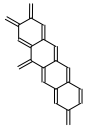
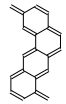
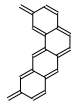
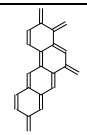
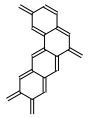
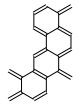
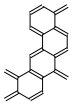
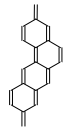
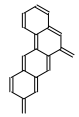
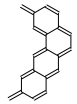
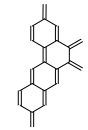
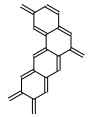
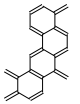
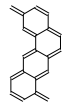
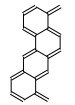
reaction																	R_X	**ΔE** [kcal/mole]
487				0.250		+	0.250		+	1.250		+	-0.750		→		0.9
488	-0.375		+	0.375		+	0.458		+	1.083		+	-0.542		→		1.7
489				0.500		+	-0.500		+	2.000		+	-1.000		→		0.6
490				-0.500		+	0.500		+	2.000		+	-1.000		→		-1.4
491				0.053		+	0.368		+	-0.421		+	1.000		→		-1.8
492	0.219		+	-0.219		+	-0.031		+	0.188		+	0.844		→		-0.1
493	-1.000		+	0.800		+	0.200		+	-0.100		+	1.100		→		-0.1
494	-0.219		+	0.219		+	-0.031		+	0.188		+	0.844		→		0.3
495	-0.266		+	0.266		+	0.041		+	0.215		+	0.747		→		-0.1
496	-0.233		+	0.233		+	-0.029		+	0.282		+	0.748		→		-0.2

TABLE S4. continued

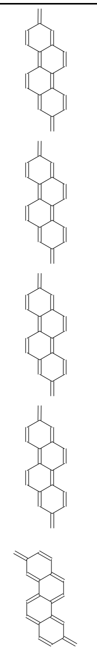
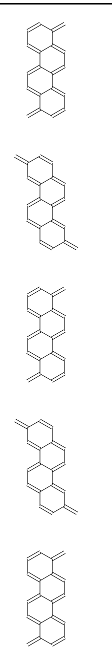
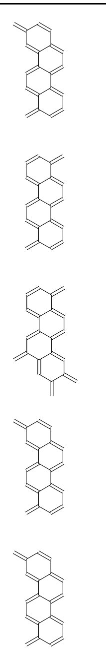
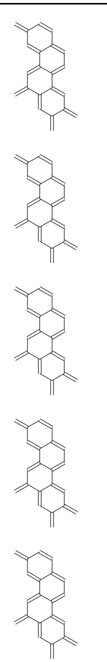
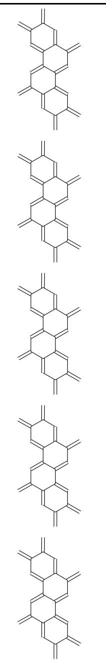
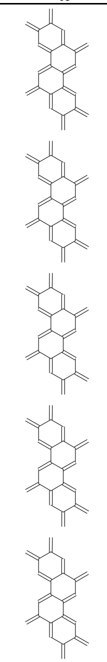
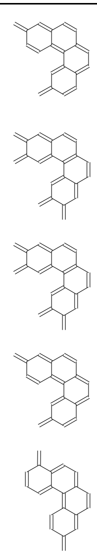
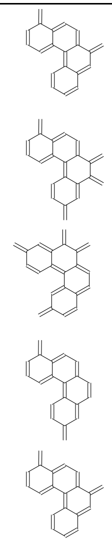
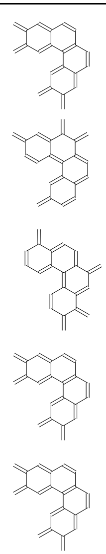
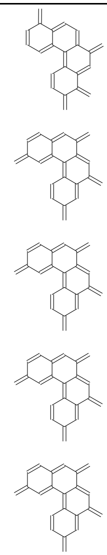
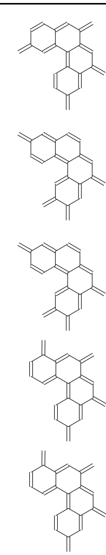
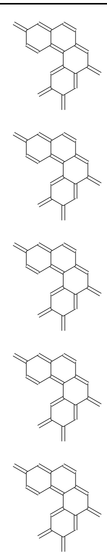
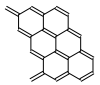
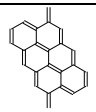
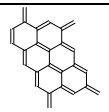
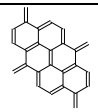
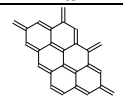
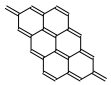
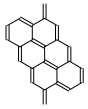
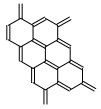
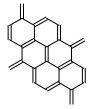
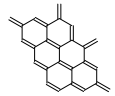
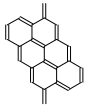
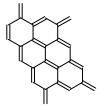
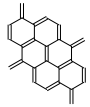
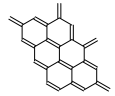
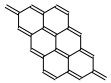
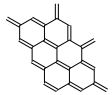
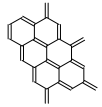
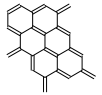
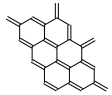
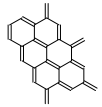
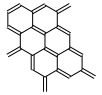
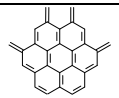
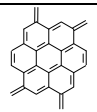
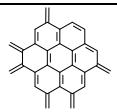
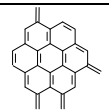
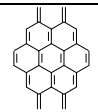
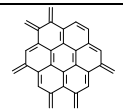
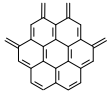
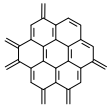
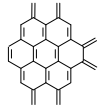
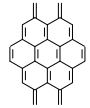
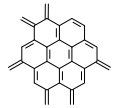
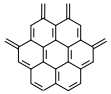
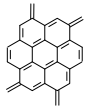
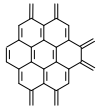
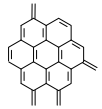
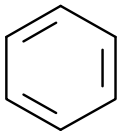
reaction																		ΔE [kcal/mole]
																	R_X	
497	-0.079		+	-0.050		+	-0.058		+	0.374		+	0.813		→			0.4
498	-0.062		+	-0.062		+	-0.062		+	0.375		+	0.812		→			0.5
499	-0.073		+	-0.203		+	0.260		+	0.293		+	0.724		→			1.1
500	-0.040		+	-0.067		+	-0.080		+	0.373		+	0.813		→			0.6
501	-0.143		+	0.028		+	-0.057		+	0.343		+	0.828		→			0.7
502	0.270		+	-0.270		+	0.441		+	0117		+	0.441		→			0.1
503	0.250		+	-0.250		+	0.250		+	0.250		+	0.500		→			0.2
504	0.261		+	0.261		+	-0.196		+	0.261		+	0.413		→			-0.5
505	0.875		+	-0.375		+	0.500		+	0.625		+	-0.125		→			0.3
506	0.346		+	-0.346		+	0.500		+	0.481		+	0.019		→			0.5

TABLE S4. continued

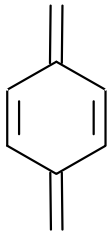
reaction																		R_X	**ΔE** [kcal/mole]
507				0.488		+	-0.488		+	0.890		+	0.110		→		0.1
508				0.400		+	-0.400		+	0.700		+	0.300		→		-0.9
509				-0.400		+	0.400		+	1.300		+	-0.300		→		1.1
510				-0.115		+	0.115		+	0.423		+	0.577		→		-1.5
511				-0.120		+	0.120		+	0.340		+	0.660		→		-1.4
512	0.333		+	0.111		+	1.000		+	-0.111		+	-0.111		→		1.6
513				0.333		+	0.667		+	0.333		+	-0.333		→		1.2
514	0.333		+	0.389		+	0.333		+	-0.111		+	-0.611		→		0.6
515	0.333		+	0.167		+	0.833		+	0.167		+	-0.500		→		1.6
516				0.333		+	0.033		+	0.600		+	0.400		→		1.8

Symmetry, number of imaginary frequencies, absolute electronic energy at B3LYP/6-311G (in Hartree), absolute electronic energy corrected for zero point energy (in Hartree) and Cartesian coordinates at B3LYP/6-311G** for the molecules studied.**



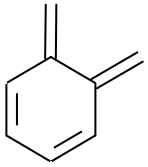
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
D6h	0	-232,3085482	-232,2083672

C	0.000000	1.393581	0.000000
C	1.206877	0.696791	0.000000
C	1.206877	-0.696791	0.000000
C	0.000000	-1.393581	0.000000
C	-1.206877	-0.696791	0.000000
C	-1.206877	0.696791	0.000000
H	0.000000	2.477909	0.000000
H	2.145932	1.238955	0.000000
H	2.145932	-1.238955	0.000000
H	0.000000	-2.477909	0.000000
H	-2.145932	-1.238955	0.000000
H	-2.145932	1.238955	0.000000



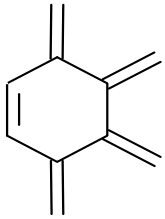
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
D2h	0	-309,6962699	-309,5644649

C	0.000000	0.000000	1.445621
C	0.000000	1.238775	0.672974
C	0.000000	1.238775	-0.672974
C	0.000000	0.000000	-1.445621
C	0.000000	-1.238775	-0.672974
C	0.000000	-1.238775	0.672974
C	0.000000	0.000000	2.796557
C	0.000000	0.000000	-2.796557
H	0.000000	2.175354	1.221122
H	0.000000	2.175354	-1.221122
H	0.000000	-2.175354	-1.221122
H	0.000000	-2.175354	1.221122
H	0.000000	0.924621	3.361771
H	0.000000	-0.924621	3.361771
H	0.000000	0.924621	-3.361771
H	0.000000	-0.924621	-3.361771



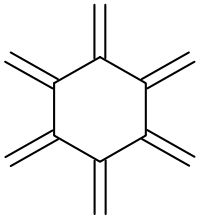
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2	0	-309,6849615	-309,5533425

C	-0.179832	1.402975	0.673657
C	-0.009501	0.747250	-0.620664
C	0.009501	-0.747250	-0.620664
C	0.179832	-1.402975	0.673657
C	0.111693	-0.716768	1.832287
C	-0.111693	0.716768	1.832287
C	0.179832	1.489825	-1.731146
C	-0.179832	-1.489825	-1.731146
H	-0.311889	2.479745	0.675084
H	0.311889	-2.479745	0.675084
H	0.204372	-1.233445	2.781034
H	-0.204372	1.233445	2.781034
H	0.405594	1.048410	-2.693438
H	0.130060	2.571581	-1.687488
H	-0.130060	-2.571581	-1.687488
H	-0.405594	-1.048410	-2.693438



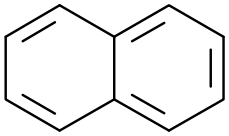
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2	0	-387,0969603	-386,9327134

C	0.088300	1.463731	-0.488090
C	0.024623	0.672631	-1.713959
C	-0.024623	-0.672631	-1.713959
C	-0.088300	-1.463731	-0.488090
C	-0.278004	-0.691358	0.772370
C	0.278004	0.691358	0.772370
H	0.031253	1.214876	-2.654103
H	-0.031253	-1.214876	-2.654103
C	-0.024623	2.803361	-0.518248
C	0.961689	1.172953	1.818229
C	-0.961689	-1.172953	1.818229
C	0.024623	-2.803361	-0.518248
H	-0.029119	3.399393	0.385493
H	-0.133821	3.330573	-1.459188
H	1.128892	0.570839	2.702930
H	1.396387	2.165091	1.803048
H	-1.128892	-0.570839	2.702930
H	-1.396387	-2.165091	1.803048
H	0.029119	-3.399393	0.385493
H	0.133821	-3.330573	-1.459188



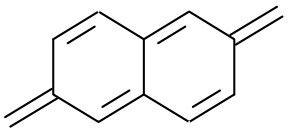
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
D2	0	-464,5025919	-464,3062069

C	-0.291636	1.222705	0.686282
C	0.000000	0.000000	1.487766
C	0.291636	-1.222705	0.686282
C	-0.291636	-1.222705	-0.686282
C	0.000000	0.000000	-1.487766
C	0.291636	1.222705	-0.686282
C	0.000000	0.000000	2.829692
C	0.000000	0.000000	-2.829692
C	1.055066	-2.234251	1.121093
C	-1.055066	-2.234251	-1.121093
C	1.055066	2.234251	-1.121093
C	-1.055066	2.234251	1.121093
H	0.151778	-0.910279	3.396032
H	-0.151778	0.910279	3.396032
H	-0.151778	-0.910279	-3.396032
H	0.151778	0.910279	-3.396032
H	-1.521397	-2.218337	-2.098939
H	-1.251504	-3.093678	-0.491809
H	1.251504	-3.093678	0.491809
H	1.521397	-2.218337	2.098939
H	1.251504	3.093678	-0.491809
H	1.521397	2.218337	-2.098939
H	-1.251504	3.093678	0.491809
H	-1.521397	2.218337	2.098939



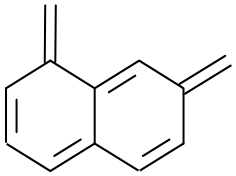
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
Cs	0	-385,9849295	-385,8379705

C	2.428778	0.707222	0.000000
C	1.243063	1.400045	0.000000
C	0.000000	0.715518	0.000000
C	0.000002	-0.715533	0.000000
C	1.243094	-1.400023	0.000000
C	2.428783	-0.707170	0.000000
C	-1.243107	1.400037	0.000000
C	-2.428775	0.707179	0.000000
C	-2.428765	-0.707222	0.000000
C	-1.243083	-1.400060	0.000000
H	-3.371458	1.242617	0.000000
H	-3.371457	-1.242640	0.000000
H	3.371437	1.242696	0.000000
H	1.241468	2.485125	0.000000
H	1.241500	-2.485107	0.000000
H	3.371457	-1.242622	0.000000
H	-1.241464	2.485115	0.000000
H	-1.241418	-2.485140	0.000000



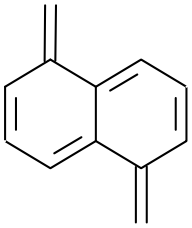
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2h	0	-463,3591259	-463,1809119

C	2.455681	0.671076	0.000000
C	1.309037	1.379017	0.000000
C	0.010931	0.731915	0.000000
C	-0.010931	-0.731915	0.000000
C	1.157272	-1.433465	0.000000
C	2.455681	-0.788051	0.000000
C	-1.157272	1.433465	0.000000
C	-2.455681	0.788051	0.000000
C	-2.455681	-0.671076	0.000000
C	-1.309037	-1.379017	0.000000
C	-3.610042	1.499290	0.000000
C	3.610042	-1.499290	0.000000
H	3.414763	1.178081	0.000000
H	1.333813	2.464062	0.000000
H	1.129953	-2.518936	0.000000
H	-1.129953	2.518936	0.000000
H	-3.414763	-1.178081	0.000000
H	-1.333813	-2.464062	0.000000
H	-4.575505	1.007802	0.000000
H	-3.605862	2.582756	0.000000
H	4.575505	-1.007802	0.000000
H	3.605862	-2.582756	0.000000



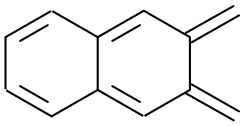
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-463,3495623	-463,1716553

C	-2.649696	-1.080546	-0.062930
C	-1.396136	-1.773195	0.000922
C	-0.208197	-1.095490	0.030594
C	-0.189376	0.370185	0.001170
C	-1.494903	1.088842	0.008031
C	-2.697510	0.272090	-0.066501
C	1.013183	1.008279	-0.044054
C	2.286206	0.316476	-0.022845
C	2.236625	-1.135368	0.045328
C	1.058647	-1.791087	0.066839
C	3.462575	0.994044	-0.064474
H	3.174159	-1.680320	0.072199
H	1.052727	2.090229	-0.102049
H	1.034661	-2.875445	0.106603
H	4.412979	0.474414	-0.046814
H	3.489579	2.075882	-0.115656
H	-1.390742	-2.857924	0.013831
C	-1.618744	2.433617	0.104453
H	-3.650140	0.789020	-0.102680
H	-3.566938	-1.657487	-0.103007
H	-2.599220	2.893893	0.092727
H	-0.773101	3.100654	0.205646



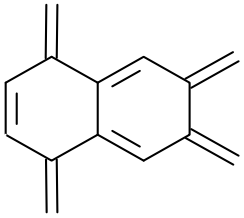
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2	0	-463,3396538	-463,1617778

C	-2.458517	0.591430	-0.290435
C	-1.238404	1.340908	-0.198207
C	-0.029663	0.730942	-0.004744
C	0.029663	-0.730942	-0.004744
C	-1.238404	-1.490903	0.108734
C	-2.465439	-0.754171	-0.144896
C	1.238404	1.490903	0.108734
C	2.465439	0.754171	-0.144896
C	2.458517	-0.591430	-0.290435
C	1.238404	-1.340908	-0.198207
C	-1.294703	-2.794043	0.476148
C	1.294703	2.794043	0.476148
H	-3.385748	1.126021	-0.464621
H	-1.283831	2.416700	-0.319826
H	-3.395477	-1.311391	-0.173404
H	3.395477	1.311391	-0.173404
H	3.385748	-1.126021	-0.464621
H	1.283831	-2.416700	-0.319826
H	-2.242900	-3.317533	0.503653
H	-0.417339	-3.352907	0.774603
H	2.242900	3.317533	0.503653
H	0.417339	3.352907	0.774603



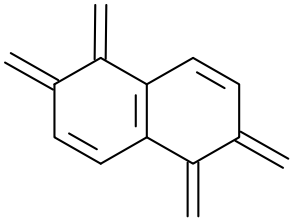
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2	0	-463,3451592	-463,1673382

C	-0.028876	1.412439	-0.559179
C	0.077788	0.743259	-1.839346
C	-0.077788	-0.743259	-1.839346
C	0.028876	-1.412439	-0.559179
C	0.036197	-0.735622	0.626367
C	-0.036197	0.735622	0.626367
C	0.372641	1.452339	-2.954139
C	-0.372641	-1.452339	-2.954139
H	-0.033990	2.497907	-0.556388
H	0.033990	-2.497907	-0.556388
C	0.077788	-1.413383	1.903299
C	-0.077788	1.413383	1.903299
H	0.570976	0.977300	-3.906094
H	0.442039	2.533189	-2.919409
H	-0.442039	-2.533189	-2.919409
H	-0.570976	-0.977300	-3.906094
C	-0.040945	0.721369	3.066700
C	0.040945	-0.721369	3.066700
H	0.134184	-2.496891	1.904238
H	-0.134184	2.496891	1.904238
H	-0.070579	1.245234	4.015438
H	0.070579	-1.245234	4.015438



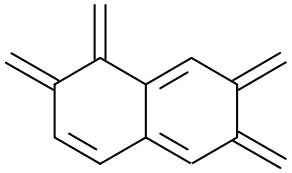
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-540,74988	-540,539835

C	-2.823845	-0.670143	0.044107
C	-1.606982	-1.469386	0.105625
C	-0.315219	-0.739660	0.007518
C	0.869325	-1.395336	-0.080349
C	2.156315	-0.728431	-0.148874
C	2.156314	0.728461	0.148716
C	0.869314	1.395359	0.080241
C	-0.315245	0.739679	-0.007381
C	-1.607058	1.469345	-0.105515
C	-2.823871	0.669906	-0.045436
C	3.261791	-1.416439	-0.507862
C	3.261803	1.416490	0.507621
C	-1.710547	-2.802799	0.278331
C	-1.710753	2.802918	-0.276906
H	-0.855286	-3.457669	0.375627
H	-2.685832	-3.270644	0.339128
H	-3.765780	-1.207322	0.084822
H	-3.765827	1.206984	-0.086957
H	-0.855575	3.458106	-0.372766
H	-2.686090	3.270619	-0.337960
H	0.886158	2.476408	0.148640
H	4.220756	0.935371	0.650999
H	3.216297	2.484650	0.684910
H	4.220729	-0.935308	-0.651292
H	3.216287	-2.484599	-0.685152
H	0.886118	-2.476371	-0.149013



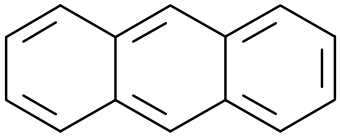
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-540,749056	-540,538522

C	2.588591	0.374387	-0.021691
C	1.721737	-0.833247	0.087058
C	0.267046	-0.630013	-0.071609
C	-0.609045	-1.759274	-0.335663
C	-1.950796	-1.645932	-0.288355
C	-2.588591	-0.374387	0.021691
C	-1.721737	0.833247	-0.087058
C	-0.267046	0.630013	0.071609
C	0.609045	1.759274	0.335663
C	1.950796	1.645932	0.288355
C	3.876708	0.322120	-0.413804
C	2.244916	-2.030880	0.415136
C	-2.244916	2.030880	-0.415136
C	-3.876708	-0.322120	0.413804
H	1.637167	-2.920375	0.512983
H	3.299258	-2.137567	0.635701
H	4.488427	1.216903	-0.427990
H	4.339404	-0.597900	-0.747483
H	2.584659	2.513875	0.433770
H	0.161514	2.719325	0.559406
H	-3.299258	2.137567	-0.635701
H	-1.637167	2.920375	-0.512983
H	-4.339404	0.597900	0.747483
H	-4.488427	-1.216903	0.427990
H	-2.584659	-2.513875	-0.433770
H	-0.161514	-2.719325	-0.559406



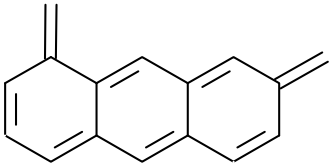
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-540,752129	-540,541772

C	2.694222	-0.108856	-0.162403
C	1.629819	0.848027	0.258520
C	0.225430	0.407739	0.075085
C	-0.801435	1.274614	-0.092222
C	-2.188032	0.849734	-0.219030
C	-2.479452	-0.585510	0.067978
C	-1.337130	-1.481686	0.078720
C	-0.052783	-1.038949	0.072778
C	1.072052	-1.951980	0.032651
C	2.342331	-1.523746	-0.108559
C	1.932695	2.004192	0.870518
C	3.914724	0.283487	-0.570928
C	-3.127786	1.729625	-0.624159
C	-3.716816	-1.052546	0.340871
H	1.161945	2.666243	1.245010
H	2.959687	2.298702	1.045283
H	4.178170	1.328149	-0.676004
H	4.673443	-0.445589	-0.831491
H	3.149642	-2.240935	-0.214965
H	0.855783	-3.015296	0.053991
H	-1.534593	-2.548274	0.122671
H	-4.578317	-0.401917	0.416799
H	-3.882859	-2.109159	0.515309
H	-4.153975	1.438333	-0.807374
H	-2.874482	2.768966	-0.797283
H	-0.601467	2.335902	-0.190877



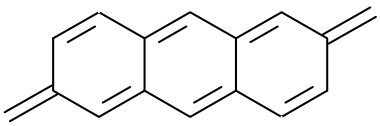
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
D2h	0	-539,6551832	-539,4618432

C	0.000000	3.654546	0.712190
C	0.000000	2.476478	1.404833
C	0.000000	1.221792	0.721491
C	0.000000	1.221792	-0.721491
C	0.000000	2.476478	-1.404833
C	0.000000	3.654546	-0.712190
C	0.000000	0.000000	1.401613
C	0.000000	-1.221792	0.721491
C	0.000000	-1.221792	-0.721491
C	0.000000	0.000000	-1.401613
C	0.000000	-2.476478	1.404833
C	0.000000	-3.654546	0.712190
C	0.000000	-3.654546	-0.712190
C	0.000000	-2.476478	-1.404833
H	0.000000	-4.599234	1.244199
H	0.000000	-4.599234	-1.244199
H	0.000000	4.599234	1.244199
H	0.000000	2.475539	2.489871
H	0.000000	2.475539	-2.489871
H	0.000000	4.599234	-1.244199
H	0.000000	0.000000	2.487469
H	0.000000	0.000000	-2.487469
H	0.000000	-2.475539	2.489871
H	0.000000	-2.475539	-2.489871



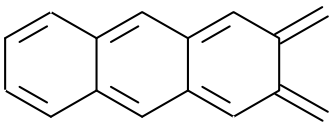
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-617,0152041	-616,7910711

C	2.708288	1.123277	0.000195
C	1.385561	0.440322	0.000034
C	1.359964	-1.024871	0.000239
C	2.537448	-1.737118	-0.000249
C	3.803650	-1.079530	-0.001039
C	0.196740	1.110949	-0.000465
C	-1.079977	0.451735	-0.000236
C	-1.095742	-1.005656	0.000460
C	0.089218	-1.686214	0.000634
C	-2.261571	1.148980	-0.000630
C	-3.548792	0.493911	-0.000319
C	-3.536963	-0.964988	0.000439
C	-2.383861	-1.664798	0.000800
C	3.887852	0.274780	-0.000930
C	2.868177	2.469656	0.001675
C	-4.714141	1.194744	-0.000700
H	2.501398	-2.821147	-0.000196
H	4.707335	-1.678903	-0.001649
H	0.182506	2.195153	-0.001112
H	0.083536	-2.772189	0.000974
H	-2.241183	2.234452	-0.001161
H	-4.491954	-1.479661	0.000699
H	-2.400040	-2.750045	0.001341
H	4.855270	0.764524	-0.001351
H	2.040671	3.166231	0.003195
H	3.861992	2.900227	0.001535
H	-4.720907	2.278069	-0.001263
H	-5.673722	0.692212	-0.000450



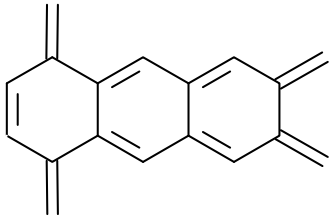
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2h	0	-617,0237091	-616,7992701

C	3.646310	0.835024	0.000000
C	2.463572	1.482092	0.000000
C	1.203271	0.768252	0.000000
C	1.253330	-0.694206	0.000000
C	2.463572	-1.334389	0.000000
C	3.721887	-0.621961	0.000000
C	-0.003421	1.406658	0.000000
C	-1.253330	0.694206	0.000000
C	-1.203271	-0.768252	0.000000
C	0.003421	-1.406658	0.000000
C	4.915326	-1.270352	0.000000
H	4.577578	1.391307	0.000000
H	2.431552	2.566936	0.000000
H	2.493162	-2.419656	0.000000
H	-0.035298	2.492158	0.000000
C	-2.463572	-1.482092	0.000000
H	0.035298	-2.492158	0.000000
H	5.852262	-0.726563	0.000000
C	-3.646310	-0.835024	0.000000
C	-3.721887	0.621961	0.000000
C	-2.463572	1.334389	0.000000
H	-2.431552	-2.566936	0.000000
H	-2.493162	2.419656	0.000000
C	-4.915326	1.270352	0.000000
H	-4.970118	2.352368	0.000000
H	-4.577578	-1.391307	0.000000
H	-5.852262	0.726563	0.000000
H	4.970118	-2.352368	0.000000



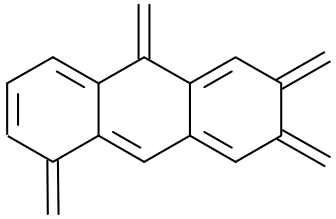
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2	0	-617,0076599	-616,7838059

C	-1.413663	0.046223	-1.788021
C	-0.737404	0.123045	-3.061382
C	0.737404	-0.123045	-3.061382
C	1.413663	-0.046223	-1.788021
C	0.737404	-0.001248	-0.595175
C	-0.737404	0.001248	-0.595175
C	-1.420604	0.476227	-4.177992
C	1.420604	-0.476227	-4.177992
H	-2.497432	0.103790	-1.785273
H	2.497432	-0.103790	-1.785273
C	1.413064	0.004899	0.666841
C	-1.413064	-0.004899	0.666841
H	-0.925427	0.663561	-5.121822
H	-2.495940	0.607020	-4.150241
H	2.495940	-0.607020	-4.150241
H	0.925427	-0.663561	-5.121822
C	-0.733867	-0.003464	1.859844
C	0.733867	0.003464	1.859844
H	2.498694	0.004088	0.668624
H	-2.498694	-0.004088	0.668624
C	-1.413037	-0.006044	3.132119
C	1.413037	0.006044	3.132119
C	-0.720410	-0.003053	4.298676
C	0.720410	0.003053	4.298676
H	-2.498020	-0.010469	3.132783
H	2.498020	0.010469	3.132783
H	-1.246763	-0.005160	5.246470
H	1.246763	0.005160	5.246470



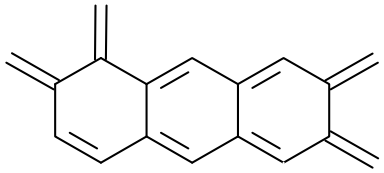
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-694,410598	-694,154393

C	-2.766532	-1.464650	0.080240
C	-3.968304	-0.680754	-0.178594
C	-3.968280	0.660474	-0.243256
C	-2.766634	1.465879	-0.060919
C	-1.473185	0.737106	-0.011163
C	-1.473222	-0.734417	0.058749
C	-0.282905	-1.398314	0.061230
C	-0.282629	1.398354	-0.064956
C	0.989307	0.732678	-0.029938
C	0.989125	-0.732836	0.027575
C	2.174152	-1.413909	0.005554
C	3.452921	-0.744189	-0.098813
C	3.454284	0.742161	0.067195
C	2.175042	1.412842	-0.026262
C	-2.887382	-2.782740	0.338773
C	-2.888137	2.802844	0.067892
C	4.567288	-1.451942	-0.400372
C	4.572008	1.449043	0.358013
H	-2.048425	-3.416899	0.591745
H	-3.861441	-3.256562	0.316532
H	-4.900699	-1.226902	-0.277019
H	-4.900696	1.194509	-0.393905
H	-2.049641	3.459237	0.257598
H	-3.862465	3.271600	-0.000669
H	-0.266463	2.478455	-0.149286
H	2.171640	2.498216	-0.022677
H	5.525649	0.972759	0.544605
H	4.537902	2.529298	0.435733
H	5.519230	-0.976316	-0.597019
H	4.531733	-2.532213	-0.477227
H	2.169622	-2.499258	-0.001666
H	-0.267458	-2.481701	0.067551



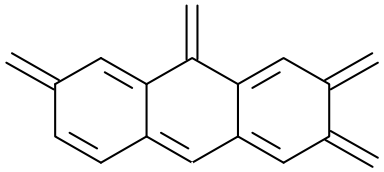
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-694,404485	-694,148097

C	2.687441	1.600922	-0.350662
C	3.946557	0.971169	-0.656146
C	4.120184	-0.357761	-0.485192
C	3.041074	-1.202965	0.007554
C	1.693788	-0.584280	0.077397
C	1.603720	0.874327	0.038892
C	0.311042	1.499636	0.408651
C	-0.911392	0.702187	0.156581
C	-0.770260	-0.761136	0.089694
C	0.549657	-1.329561	0.092895
C	-2.132060	1.256062	-0.033922
C	-3.338117	0.470715	-0.250856
C	-3.226778	-1.003056	-0.043319
C	-1.883982	-1.544178	0.001567
C	0.265060	2.694349	1.024577
C	3.300616	-2.468154	0.411746
C	-4.469079	1.077602	-0.667902
C	-4.296139	-1.812551	0.128152
H	-0.671224	3.126568	1.354268
H	1.166441	3.250219	1.248708
H	2.603189	2.675585	-0.460770
H	4.767103	1.589536	-1.002734
H	5.083715	-0.821291	-0.666358
H	2.551869	-3.095920	0.877236
H	4.292548	-2.889282	0.299001
H	0.616688	-2.409718	0.021739
H	-1.776290	-2.624306	-0.001205
H	-5.308810	-1.433751	0.173990
H	-4.166003	-2.881759	0.246900
H	-5.365370	0.525344	-0.918765
H	-4.508370	2.154437	-0.783004
H	-2.233484	2.334378	-0.087244



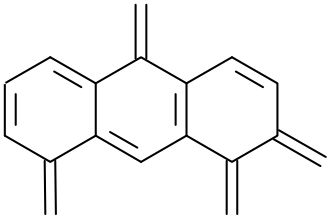
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-694,412261	-694,155917

C	2.755546	-0.906622	0.262050
C	3.881891	-0.045707	-0.203065
C	3.646523	1.392955	-0.167027
C	2.416493	1.922339	-0.009932
C	1.225258	1.101831	0.067886
C	1.385936	-0.357641	0.110794
C	0.281585	-1.147362	0.032958
C	-1.054997	-0.610342	-0.014645
C	-1.216278	0.851310	0.031594
C	-0.023347	1.652105	0.052412
C	-2.470220	1.393151	0.059262
C	-3.670180	0.583233	0.070930
C	-3.501967	-0.876782	-0.204324
C	-2.157251	-1.408823	-0.117652
C	2.985954	-2.074135	0.885284
C	5.056124	-0.541460	-0.635255
C	-4.524945	-1.678492	-0.581297
C	-4.864335	1.140834	0.380386
H	2.179294	-2.670378	1.292694
H	3.992062	-2.443341	1.037243
H	5.232293	-1.605233	-0.730503
H	5.863785	0.120589	-0.925756
H	4.505170	2.041815	-0.304745
H	2.284650	2.999564	-0.007164
H	-0.131292	2.732297	0.035184
H	-2.587065	2.469387	0.137807
H	-5.763945	0.551480	0.500955
H	-4.950505	2.209000	0.540765
H	-5.522208	-1.298292	-0.760320
H	-4.366743	-2.738776	-0.739341
H	-2.034604	-2.484380	-0.197164
H	0.388360	-2.226081	-0.001815



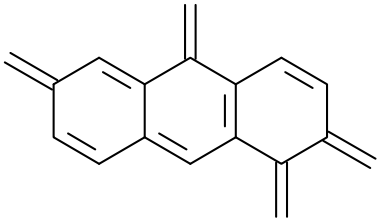
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-694,414652	-694,158047

C	2.790361	0.958298	-0.115833
C	3.994943	0.165188	-0.293263
C	3.843907	-1.278064	-0.172267
C	2.636695	-1.840305	0.038111
C	1.430822	-1.046171	0.148281
C	1.573439	0.408427	0.129720
C	0.363406	1.220342	0.421239
C	-0.950274	0.591619	0.144194
C	-1.028185	-0.879348	0.168292
C	0.195750	-1.628277	0.220046
C	-2.245050	-1.492478	0.102336
C	-3.489487	-0.762086	-0.022420
C	-3.371975	0.691730	-0.338844
C	-2.068476	1.304857	-0.127038
C	5.195932	0.739390	-0.547800
C	-4.386634	1.425023	-0.842244
C	-4.672991	-1.386666	0.170655
H	5.300847	1.814040	-0.637586
H	6.091444	0.141914	-0.669880
H	4.730584	-1.895109	-0.271001
H	2.537605	-2.919019	0.105154
H	0.122378	-2.711674	0.232846
H	-2.300237	-2.574497	0.169400
H	-5.616830	-0.857496	0.155937
H	-4.709700	-2.451214	0.369695
H	-5.348082	0.992739	-1.087568
H	-4.261069	2.483908	-1.035638
H	-2.007654	2.381075	-0.245677
C	0.452850	2.426357	1.008663
H	-0.430319	2.986668	1.287516
H	1.409129	2.865831	1.261162
H	2.891702	2.035814	-0.185325



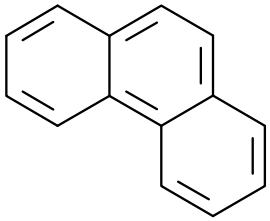
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-694,403616	-694,147006

C	-2.782413	1.439114	-0.419033
C	-3.971143	0.640095	-0.534117
C	-3.962389	-0.675320	-0.216365
C	-2.748273	-1.334505	0.239563
C	-1.495951	-0.550143	0.138452
C	-1.590534	0.892286	-0.035906
C	-0.363855	1.696190	0.164222
C	0.923484	1.005515	-0.017134
C	0.955512	-0.375814	-0.036512
C	-0.258591	-1.129548	0.103630
C	2.246458	-1.071053	-0.247510
C	3.485015	-0.289516	0.026689
C	3.365846	1.154054	-0.110908
C	2.158865	1.755529	-0.140972
C	4.646294	-0.859590	0.404285
H	-4.873093	-1.262776	-0.257278
H	-0.184650	-2.208445	0.143851
H	5.540157	-0.260963	0.537828
H	4.726017	-1.919873	0.608005
H	2.104169	2.832360	-0.237692
C	-0.439553	2.981940	0.576561
H	0.438998	3.592511	0.732580
H	-1.392379	3.438799	0.809543
H	-2.836274	2.492271	-0.668549
C	-2.807528	-2.583707	0.761102
C	2.317288	-2.312659	-0.762559
H	-4.888753	1.115907	-0.861863
H	-1.947949	-3.070736	1.203134
H	-3.741762	-3.132263	0.771344
H	3.272242	-2.760131	-1.006964
H	1.435316	-2.895876	-0.992292
H	4.276766	1.742008	-0.142569



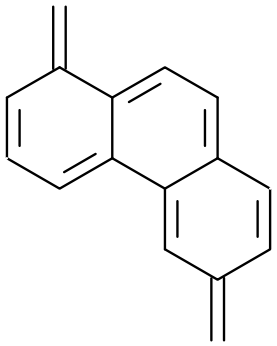
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-694,413074	-694,156372

C	-2.812529	0.856390	0.191621
C	-3.927787	-0.070765	0.147163
C	-3.611176	-1.454531	-0.173869
C	-2.335417	-1.855777	-0.353447
C	-1.226980	-0.935094	-0.244635
C	-1.527180	0.477597	-0.045699
C	-0.396292	1.437017	-0.124357
C	0.961732	0.894755	0.064901
C	1.177229	-0.467439	-0.031266
C	0.073779	-1.356492	-0.260785
C	2.545305	-1.004570	0.153827
C	3.674688	-0.045990	-0.004941
C	3.361029	1.349568	0.261600
C	2.084140	1.782393	0.302369
C	4.909012	-0.421142	-0.394467
H	-4.429240	-2.162887	-0.248098
H	0.276578	-2.408847	-0.419268
H	5.718120	0.298714	-0.442311
H	5.133117	-1.437479	-0.692612
H	1.884924	2.828708	0.495553
C	-0.603893	2.730696	-0.454737
H	0.205376	3.442865	-0.536015
H	-1.592217	3.098506	-0.696841
H	-3.038003	1.890788	0.427042
C	2.769030	-2.271431	0.550536
H	3.769378	-2.614625	0.781639
H	1.966982	-2.983012	0.694818
H	4.184080	2.045795	0.380937
C	-5.199920	0.336173	0.389289
H	-2.110313	-2.896642	-0.563082
H	-5.426835	1.368266	0.628243
H	-6.030566	-0.358291	0.351384



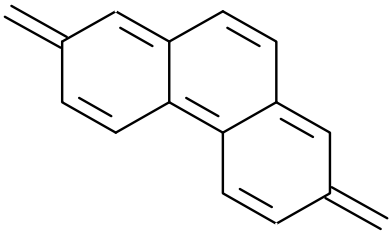
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2v	0	-539,6631988	-539,4695116

C	0.000000	3.555072	-0.296433
C	0.000000	2.833106	0.876895
C	0.000000	2.877382	-1.526851
C	0.000000	1.420782	0.864836
C	0.000000	0.727973	-0.379768
C	0.000000	1.497845	-1.563996
C	0.000000	0.678152	2.090997
C	0.000000	-0.678152	2.090997
C	0.000000	-1.420782	0.864836
C	0.000000	-0.727973	-0.379768
C	0.000000	-3.555072	-0.296433
C	0.000000	-2.833106	0.876895
H	0.000000	-3.344193	1.834022
C	0.000000	-2.877382	-1.526851
C	0.000000	-1.497845	-1.563996
H	0.000000	3.344193	1.834022
H	0.000000	3.439831	-2.453660
H	0.000000	1.228750	3.025822
H	0.000000	-3.439831	-2.453660
H	0.000000	4.638765	-0.272468
H	0.000000	1.005650	-2.527805
H	0.000000	-1.228750	3.025822
H	0.000000	-1.005650	-2.527805
H	0.000000	-4.638765	-0.272468



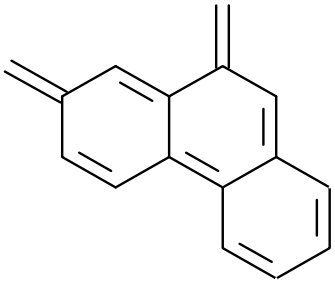
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-617,0072437	-616,7831577

C	-3.052636	0.159027	0.141873
C	-1.626997	0.534330	0.013519
C	-0.623824	-0.518085	-0.066742
C	-1.040929	-1.815153	-0.254036
C	-2.424833	-2.165263	-0.290490
C	-3.388927	-1.230573	-0.102721
C	-1.220827	1.846023	-0.100474
C	0.141354	2.208627	-0.192014
C	1.145431	1.268747	-0.138633
C	0.802957	-0.141933	-0.018198
C	1.814459	-1.050160	0.151711
C	3.212638	-0.687519	0.143056
C	3.520845	0.719883	-0.045530
C	2.537954	1.637696	-0.171088
C	4.193370	-1.618373	0.308410
H	-2.695965	-3.201300	-0.460521
H	0.401530	3.257296	-0.291118
H	2.779689	2.688858	-0.291728
H	-1.964593	2.632397	-0.147270
H	4.563278	1.018653	-0.070558
H	1.584263	-2.096625	0.315658
C	-4.028506	1.028934	0.512790
H	5.240162	-1.340156	0.302126
H	3.958718	-2.666338	0.450418
H	-0.312845	-2.600780	-0.412847
H	-4.437215	-1.508007	-0.096979
H	-5.061640	0.706372	0.556375
H	-3.824557	2.052374	0.797848



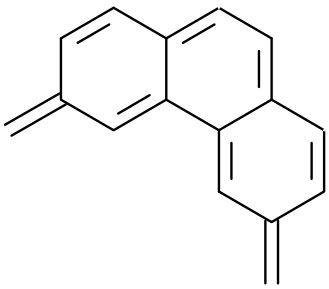
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2v	0	-617,0219773	-616,7975503

C	0.000000	0.673435	2.155956
C	0.000000	-0.673435	2.155956
C	0.000000	-1.428950	0.920995
C	0.000000	-0.696484	-0.340904
C	0.000000	0.696484	-0.340904
C	0.000000	1.428950	0.920995
C	0.000000	-2.797396	0.932904
C	0.000000	-3.589742	-0.273477
C	0.000000	-2.845343	-1.521802
C	0.000000	-1.494176	-1.547515
C	0.000000	1.494176	-1.547515
C	0.000000	2.845343	-1.521802
C	0.000000	3.589742	-0.273477
C	0.000000	2.797396	0.932904
H	0.000000	1.226633	3.089324
H	0.000000	-1.226633	3.089324
H	0.000000	-3.317955	1.885631
C	0.000000	-4.949349	-0.249151
H	0.000000	-3.406737	-2.450147
H	0.000000	-0.995713	-2.507898
H	0.000000	0.995713	-2.507898
H	0.000000	3.406737	-2.450147
C	0.000000	4.949349	-0.249151
H	0.000000	3.317955	1.885631
H	0.000000	-5.497248	0.685472
H	0.000000	-5.528820	-1.164421
H	0.000000	5.528820	-1.164421
H	0.000000	5.497248	0.685472



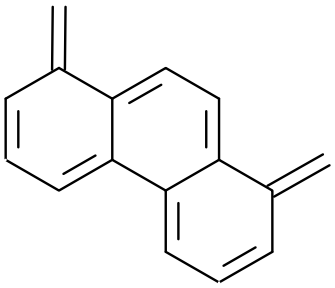
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-617,0095647	-616,7853977

C	-0.313949	1.957130	0.059225
C	1.115740	1.903112	-0.088882
C	1.818830	0.726487	-0.078470
C	1.123595	-0.554012	0.058698
C	-0.276775	-0.579070	0.101994
C	-1.040662	0.660169	0.019876
C	3.259730	0.729499	-0.174110
C	3.972894	-0.422073	-0.125620
C	3.296022	-1.678585	0.022762
C	1.939065	-1.737003	0.108884
C	-1.030855	-1.805085	0.170836
C	-2.381235	-1.836814	0.089535
C	-3.152990	-0.625159	-0.092712
C	-2.399610	0.604866	-0.120278
C	-0.919589	3.153925	0.277738
H	1.655016	2.842673	-0.152237
H	3.758104	1.687128	-0.281319
H	1.467559	-2.704545	0.214779
H	-0.499898	-2.740739	0.283963
H	-2.909963	-2.782258	0.146228
C	-4.508545	-0.639574	-0.229461
H	-2.959948	1.520948	-0.268366
H	-5.067049	-1.567361	-0.204425
H	-5.071103	0.275991	-0.365998
H	5.054491	-0.404001	-0.195809
H	-0.340862	4.069459	0.263901
H	-1.974983	3.247743	0.494572
H	3.878632	-2.591905	0.064617



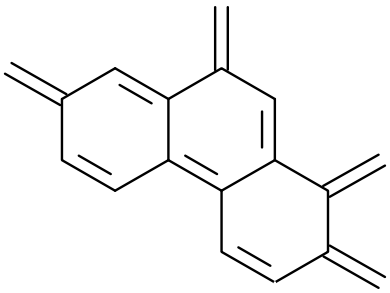
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2v	0	-617,0170026	-616,7928426

C	0.000000	0.706405	2.426100
C	0.000000	-0.706405	2.426100
C	0.000000	-1.430022	1.254554
C	0.000000	-0.741532	-0.032688
C	0.000000	0.741532	-0.032688
C	0.000000	1.430022	1.254554
C	0.000000	-2.871046	1.261354
C	0.000000	-3.593155	0.120055
C	0.000000	-2.939614	-1.176677
C	0.000000	-1.494124	-1.174623
C	0.000000	1.494124	-1.174623
C	0.000000	2.939614	-1.176677
C	0.000000	3.593155	0.120055
C	0.000000	2.871046	1.261354
H	0.000000	-1.235179	3.373695
H	0.000000	-3.369535	2.225717
C	0.000000	3.649197	-2.338729
C	0.000000	-3.649197	-2.338729
H	0.000000	1.235179	3.373695
H	0.000000	-4.677559	0.150226
H	0.000000	-1.013254	-2.146163
H	0.000000	3.369535	2.225717
H	0.000000	3.154726	-3.302783
H	0.000000	4.732565	-2.336762
H	0.000000	-4.732565	-2.336762
H	0.000000	-3.154726	-3.302783
H	0.000000	1.013254	-2.146163
H	0.000000	4.677559	0.150226



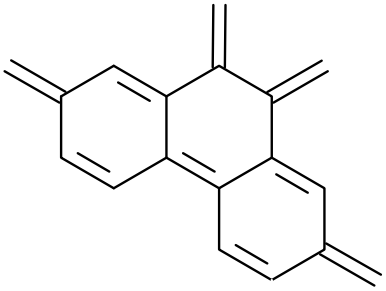
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-616,9983916	-616,7744836

C	2.920541	-0.611615	0.114501
C	1.442155	-0.617074	0.051429
C	0.732742	0.645756	-0.058048
C	1.452331	1.791121	-0.326564
C	2.875283	1.780521	-0.403137
C	3.582330	0.641056	-0.190260
C	0.704427	-1.780625	0.032951
C	-0.704362	-1.780617	-0.033560
C	-1.442135	-0.617080	-0.051499
C	-0.732706	0.645759	0.057992
C	-1.452235	1.791194	0.326323
C	-2.875193	1.780729	0.402646
C	-3.582276	0.641274	0.189893
C	-2.920563	-0.611611	-0.114206
H	-3.392258	2.706902	0.628124
H	3.392367	2.706591	-0.628993
H	-1.212380	-2.737508	-0.042246
C	-3.662911	-1.694248	-0.469276
H	1.212514	-2.737487	0.041169
H	-4.666228	0.648847	0.217943
H	-0.933574	2.721707	0.520667
C	3.662641	-1.694098	0.470668
H	0.933718	2.721647	-0.520974
H	4.666278	0.648534	-0.218570
H	4.744394	-1.639965	0.468947
H	3.222502	-2.630732	0.785556
H	-4.744651	-1.639885	-0.467338
H	-3.223107	-2.631290	-0.783404



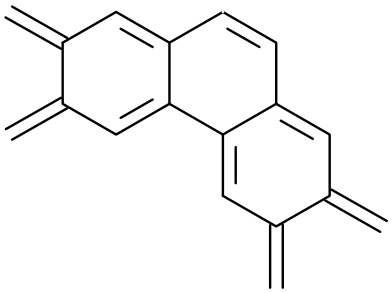
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-694,4136054	-694,1568854

C	-3.466428	-0.671425	-0.129161
C	-2.750115	0.545835	0.339720
C	-2.662081	-1.880130	-0.193726
C	-1.289575	0.607499	0.075421
C	-0.541353	-0.648674	-0.019170
C	-1.312920	-1.868939	-0.102155
C	-0.648014	1.792746	-0.077341
C	0.783030	1.892883	-0.275962
C	1.567549	0.647583	-0.088602
C	0.848175	-0.624636	-0.054902
C	3.725796	-0.535494	0.151434
C	2.923582	0.662994	0.051111
H	3.448006	1.611028	0.092054
C	3.001810	-1.790832	0.082722
C	1.655019	-1.824503	-0.014256
H	-3.182524	-2.819665	-0.347655
H	-1.219151	2.713556	-0.107160
H	3.569221	-2.714403	0.126228
H	-0.790538	-2.813507	-0.170518
H	1.164037	-2.788038	-0.035440
C	5.076380	-0.485881	0.295594
C	1.324274	3.074088	-0.653620
C	-3.374157	1.489526	1.062198
C	-4.768686	-0.679308	-0.472155
H	5.668778	-1.390246	0.364383
H	5.604450	0.458733	0.345969
H	0.702586	3.956081	-0.750244
H	2.373468	3.189273	-0.890762
H	-4.429301	1.415364	1.293398
H	-2.839602	2.337323	1.471898
H	-5.258702	-1.599841	-0.768004
H	-5.364441	0.224369	-0.487048



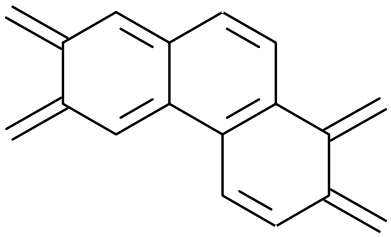
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2	0	-694,419779	-694,1628444

C	-0.007611	3.588762	-0.673706
C	0.097656	2.803609	0.538003
C	-0.065480	2.835432	-1.912366
C	0.132905	1.442900	0.538721
C	0.016460	0.698474	-0.710161
C	-0.048853	1.483718	-1.921925
C	0.310739	0.673609	1.793086
C	-0.310739	-0.673609	1.793086
C	-0.132905	-1.442900	0.538721
C	-0.016460	-0.698474	-0.710161
C	0.007611	-3.588762	-0.673706
C	-0.097656	-2.803609	0.538003
H	-0.144592	-3.338405	1.480089
C	0.065480	-2.835432	-1.912366
C	0.048853	-1.483718	-1.921925
H	0.144592	3.338405	1.480089
H	-0.138480	3.385550	-2.844518
H	0.138480	-3.385550	-2.844518
H	-0.118100	0.975215	-2.874091
H	0.118100	-0.975215	-2.874091
C	-0.048853	4.945991	-0.653101
C	0.048853	-4.945991	-0.653101
C	1.026202	1.121468	2.833818
C	-1.026202	-1.121468	2.833818
H	-0.125311	5.520760	-1.568223
H	-0.006444	5.498208	0.278032
H	0.125311	-5.520760	-1.568223
H	0.006444	-5.498208	0.278032
H	-1.165327	-0.511485	3.717786
H	-1.515365	-2.087711	2.816719
H	1.515365	2.087711	2.816719
H	1.165327	0.511485	3.717786



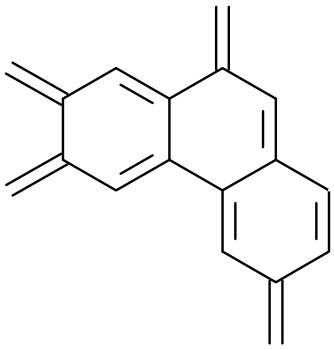
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2	0	-694,409345	-694,1531311

C	0.004007	3.630490	0.062323
C	-0.023253	2.808536	1.255889
C	0.304616	2.920781	-1.214343
C	-0.004007	1.448848	1.225914
C	0.047023	0.737229	-0.066146
C	0.217781	1.471061	-1.196807
C	-0.014774	0.674736	2.446605
C	0.014774	-0.674736	2.446605
C	0.004007	-1.448848	1.225914
C	-0.047023	-0.737229	-0.066146
C	-0.004007	-3.630490	0.062323
C	0.023253	-2.808536	1.255889
H	0.097241	-3.316388	2.212496
C	-0.304616	-2.920781	-1.214343
C	-0.217781	-1.471061	-1.196807
H	-0.097241	3.316388	2.212496
H	-0.027450	1.219605	3.384884
H	0.352265	0.976637	-2.151738
H	0.027450	-1.219605	3.384884
H	-0.352265	-0.976637	-2.151738
C	0.266044	-4.952034	0.137016
C	-0.688333	-3.555200	-2.343875
C	0.688333	3.555200	-2.343875
C	-0.266044	4.952034	0.137016
H	0.326219	-5.583318	-0.739851
H	0.453566	-5.423652	1.094410
H	-0.874591	-2.998655	-3.254811
H	-0.841109	-4.625739	-2.384852
H	0.874591	2.998655	-3.254811
H	0.841109	4.625739	-2.384852
H	-0.326219	5.583318	-0.739851
H	-0.453566	5.423652	1.094410



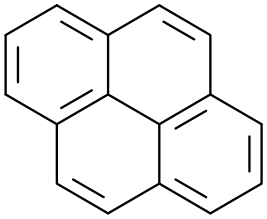
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-694,4082596	-694,1518447

C	-3.533523	-0.806517	-0.069958
C	-2.989535	0.566119	0.123297
C	-2.608204	-1.895956	0.202502
C	-1.527807	0.734223	-0.016885
C	-0.695173	-0.362705	0.098382
C	-1.281777	-1.681186	0.293374
C	-0.966715	2.050962	-0.227936
C	0.366806	2.257835	-0.282611
C	1.299779	1.168398	-0.137518
C	0.759514	-0.193561	0.027951
C	3.609353	0.317043	0.041093
C	2.647268	1.381650	-0.139507
H	3.024036	2.396490	-0.218711
C	3.075530	-1.072859	-0.040490
C	1.639479	-1.237684	0.072518
H	-3.010043	-2.900462	0.280688
H	-1.641414	2.885383	-0.369428
H	-0.629644	-2.523273	0.481359
H	0.764197	3.253744	-0.446848
H	1.283662	-2.258211	0.124013
C	4.901297	0.600955	0.326358
C	3.861113	-2.149760	-0.274664
C	-4.786765	-1.049201	-0.500670
C	-3.794290	1.576643	0.506264
H	5.621840	-0.168436	0.571481
H	5.251753	1.626268	0.339841
H	3.440868	-3.148408	-0.294237
H	4.921362	-2.059120	-0.472033
H	-5.160149	-2.064152	-0.576106
H	-5.453690	-0.253171	-0.806480
H	-4.844249	1.406311	0.707074
H	-3.426610	2.580642	0.670384



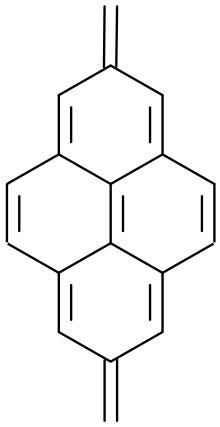
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-694,4118931	-694,1556143

C	3.952023	0.106175	0.047014
C	3.177111	1.204191	-0.027408
C	3.362343	-1.223030	0.118242
C	1.728461	1.127323	-0.044848
C	1.109041	-0.198162	-0.011304
C	1.912763	-1.292070	0.086852
C	0.973794	2.259030	-0.082791
C	-0.471682	2.277290	-0.095004
C	-1.166538	0.967269	-0.003850
C	-0.369184	-0.276950	-0.059129
C	-3.237202	-0.374258	0.198312
C	-2.512503	0.881373	0.139531
H	-3.101939	1.781925	0.261820
C	-2.468090	-1.590402	-0.175460
C	-1.023460	-1.463489	-0.163841
H	3.625419	2.191543	-0.071013
H	1.476737	3.220611	-0.116302
H	5.033342	0.190256	0.062565
H	1.482425	-2.284089	0.154212
H	-0.465932	-2.383157	-0.290598
C	-1.111207	3.463032	-0.217861
C	4.125329	-2.339300	0.210275
C	-4.522130	-0.401420	0.613020
C	-3.046878	-2.752665	-0.549338
H	-0.544610	4.384521	-0.274748
H	-2.186991	3.553467	-0.278520
H	5.206987	-2.281941	0.231317
H	3.680479	-3.325721	0.265425
H	-4.119461	-2.858146	-0.649056
H	-2.443578	-3.622039	-0.783100
H	-5.065982	-1.327474	0.747709
H	-5.048846	0.516629	0.845820



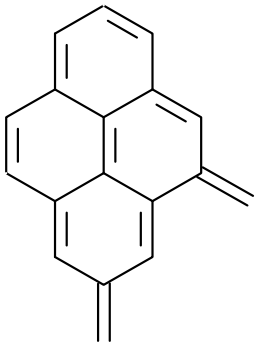
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
D2h	0	-615,9104804	-615,7040734

C	0.000000	0.000000	0.712776
C	0.000000	0.000000	-0.712776
C	0.000000	0.000000	3.518140
C	0.000000	0.000000	-3.518140
C	0.000000	1.208541	2.829020
C	0.000000	1.208541	-2.829020
C	0.000000	-1.208541	-2.829020
C	0.000000	-1.208541	2.829020
C	0.000000	1.234412	1.427117
C	0.000000	-1.234412	1.427117
C	0.000000	1.234412	-1.427117
C	0.000000	-1.234412	-1.427117
C	0.000000	2.460668	-0.679214
C	0.000000	2.460668	0.679214
C	0.000000	-2.460668	0.679214
C	0.000000	-2.460668	-0.679214
H	0.000000	-3.397424	-1.226767
H	0.000000	3.397424	1.226767
H	0.000000	3.397424	-1.226767
H	0.000000	-3.397424	1.226767
H	0.000000	2.146053	3.374890
H	0.000000	-2.146053	3.374890
H	0.000000	2.146053	-3.374890
H	0.000000	-2.146053	-3.374890
H	0.000000	0.000000	4.602331
H	0.000000	0.000000	-4.602331



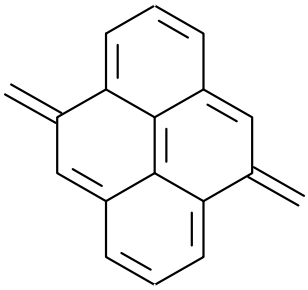
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
D2h	0	-693,2622674	-693,0253944

C	0.000000	2.483186	0.674591
C	0.000000	1.248985	1.433885
C	0.000000	0.000000	0.690248
C	0.000000	0.000000	-0.690248
C	0.000000	1.248985	-1.433885
C	0.000000	2.483186	-0.674591
C	0.000000	-1.248985	1.433885
C	0.000000	-2.483186	0.674591
C	0.000000	-2.483186	-0.674591
C	0.000000	-1.248985	-1.433885
C	0.000000	1.232361	-2.800131
C	0.000000	0.000000	-3.559071
C	0.000000	-1.232361	-2.800131
C	0.000000	1.232361	2.800131
C	0.000000	0.000000	3.559071
C	0.000000	-1.232361	2.800131
H	0.000000	3.418417	1.224755
H	0.000000	-3.418417	-1.224755
H	0.000000	-3.418417	1.224755
H	0.000000	3.418417	-1.224755
H	0.000000	-2.169698	-3.347482
H	0.000000	2.169698	-3.347482
H	0.000000	-2.169698	3.347482
H	0.000000	2.169698	3.347482
C	0.000000	0.000000	-4.921859
C	0.000000	0.000000	4.921859
H	0.000000	0.924955	5.485777
H	0.000000	-0.924955	5.485777
H	0.000000	0.924955	-5.485777
H	0.000000	-0.924955	-5.485777



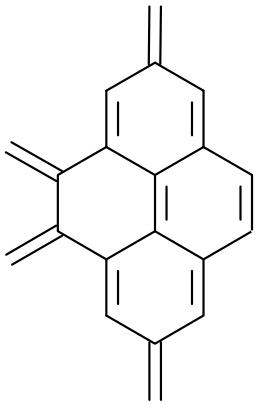
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-693,2527757	-693,0161947

C	3.150645	1.228292	-0.077967
C	1.714995	1.169831	-0.040237
C	1.076948	-0.141178	0.006219
C	1.911247	-1.323977	0.021049
C	3.282949	-1.191087	-0.011430
C	3.900745	0.089887	-0.062989
C	-0.306161	-0.246457	0.024401
C	-0.935891	-1.552422	0.040038
C	-0.082237	-2.718947	0.075193
C	1.264437	-2.611511	0.065999
C	0.942318	2.304019	-0.034298
C	-0.496001	2.277251	0.035336
C	-1.151799	0.939301	0.004140
C	-2.505794	0.783404	-0.055188
C	-3.156713	-0.507305	-0.050737
C	-2.302188	-1.662803	0.012039
H	1.889336	-3.498198	0.086999
C	-1.174293	3.449908	0.151815
H	1.426768	3.274801	-0.052165
H	-0.557124	-3.694027	0.102136
H	-3.150709	1.652470	-0.112887
H	-2.760934	-2.646219	0.026587
H	3.624905	2.202972	-0.115397
H	3.902958	-2.081076	0.000117
C	-4.518527	-0.611260	-0.104313
H	4.982861	0.152322	-0.089694
H	-0.638337	4.390990	0.154476
H	-2.249075	3.504428	0.257409
H	-5.148688	0.268209	-0.152072
H	-5.010033	-1.576349	-0.099936



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2	0	-693,2422996	-693,0059616

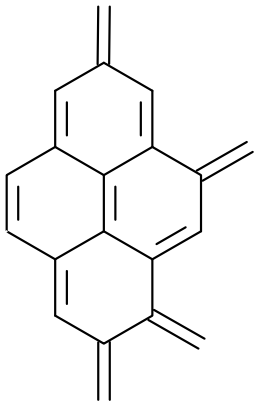
C	-1.450965	2.177755	0.113175
C	0.002742	1.902268	-0.001226
C	0.454875	0.531056	0.007585
C	-0.454875	-0.531056	0.007585
C	-1.881630	-0.251431	-0.042751
C	-2.331942	1.049075	0.005016
C	1.881630	0.251431	-0.042751
C	2.331942	-1.049075	0.005016
C	1.450965	-2.177755	0.113175
C	-0.002742	-1.902268	-0.001226
C	-2.794354	-1.354028	-0.135795
C	-2.331942	-2.634061	-0.193185
C	-0.938678	-2.905675	-0.137976
C	0.938678	2.905675	-0.137976
C	2.331942	2.634061	-0.193185
C	2.794354	1.354028	-0.135795
C	-1.971348	3.416339	0.346171
C	1.971348	-3.416339	0.346171
H	3.400450	-1.237621	0.001274
H	-3.400450	1.237621	0.001274
H	-0.613997	-3.936156	-0.213500
H	-3.857641	-1.143600	-0.172571
H	3.857641	1.143600	-0.172571
H	0.613997	3.936156	-0.213500
H	-3.025176	-3.462484	-0.285857
H	3.025176	3.462484	-0.285857
H	-3.044076	3.557545	0.391733
H	-1.357579	4.290938	0.512847
H	3.044076	-3.557545	0.391733
H	1.357579	-4.290938	0.512847



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2	0	-770,6603282	-770,3909442

C	0.265694	0.694284	2.121131
C	0.066145	1.452799	0.862691
C	-0.000414	0.692596	-0.376093
C	0.000414	-0.692596	-0.376093
C	-0.066145	-1.452799	0.862691
C	-0.265694	-0.694284	2.121131
C	-0.047822	1.430304	-1.629112
C	-0.028247	0.673328	-2.863833
C	0.028247	-0.673328	-2.863833
C	0.047822	-1.430304	-1.629112
C	0.028247	-2.808271	0.835958
C	0.138375	-3.560592	-0.399585
C	0.117547	-2.795132	-1.623960
C	-0.028247	2.808271	0.835958
C	-0.138375	3.560592	-0.399585
C	-0.117547	2.795132	-1.623960
H	0.053523	-1.224767	-3.797842
H	-0.053523	1.224767	-3.797842
H	0.167760	-3.331864	-2.566100
H	0.023630	-3.366760	1.765363
H	-0.167760	3.331864	-2.566100
H	-0.023630	3.366760	1.765363
C	0.244826	-4.916985	-0.400830
C	-0.244826	4.916985	-0.400830
H	-0.258184	5.483187	0.522591
H	-0.320063	5.476287	-1.325547
H	0.258184	-5.483187	0.522591
H	0.320063	-5.476287	-1.325547
C	-0.934957	-1.190283	3.170874
H	-1.357687	-2.187485	3.159250
H	-1.103700	-0.593729	4.058844
C	0.934957	1.190283	3.170874
H	1.357687	2.187485	3.159250

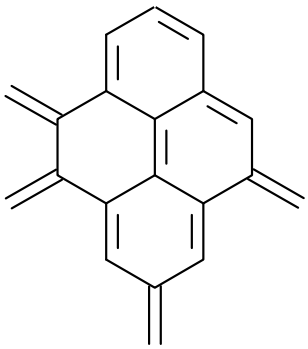
H	1.103700	0.593729	4.058844



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-770,654172	-770,38502

C	-3.449874	-0.451921	-0.126837
C	-2.787447	0.813339	0.300046
C	-1.325664	0.911665	0.066204
C	-0.549320	-0.325130	0.007528
C	-1.253583	-1.596242	-0.036297
C	-2.617261	-1.633530	-0.135106
C	-0.693510	2.102506	-0.082139
C	0.829158	-0.283650	-0.028619
C	1.544191	0.985380	-0.072909
C	0.743102	2.223565	-0.248081
C	2.901161	0.991320	0.042736
H	3.438965	1.932186	0.069823
C	3.691563	-0.219314	0.131347
C	2.968140	-1.468328	0.082119
C	1.605633	-1.514066	0.009308
C	0.884881	-2.770372	-0.017476
C	-0.462426	-2.808580	-0.050050
H	-0.987483	-3.757421	-0.081744
H	1.463621	-3.688022	-0.012751
H	-1.272739	3.017668	-0.126829
H	-3.110804	-2.592541	-0.259180
H	3.534936	-2.393258	0.118824
C	5.047660	-0.174364	0.247449
C	1.274337	3.421577	-0.584783
C	-3.462370	1.765291	0.963491
C	-4.751817	-0.515876	-0.479957
H	5.579347	0.768628	0.283663
H	5.638132	-1.080491	0.307112
H	0.641227	4.295561	-0.678790
H	2.327940	3.560202	-0.787434
H	-2.969079	2.651126	1.343300
H	-4.518948	1.663347	1.176015

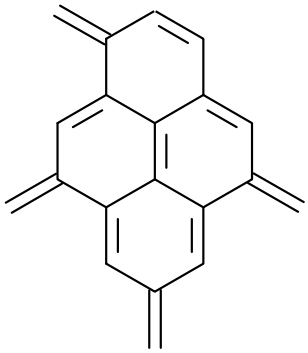
H	-5.375712	0.366386	-0.537633
H	-5.208718	-1.462995	-0.742209



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-770,648859	-770,379778

C	-3.120419	-0.791072	-0.247079
C	-2.763629	0.606417	-0.203430
C	-1.482934	1.040666	-0.013977
C	-0.405446	0.064818	0.043355
C	-0.754901	-1.340803	0.111711
C	-2.047241	-1.737483	-0.042520
C	-1.142994	2.484373	0.100516
C	0.926912	0.470660	0.012368
C	1.252947	1.894475	0.002684
C	0.252249	2.831134	0.037592
C	2.640197	2.283480	-0.009550
H	2.876262	3.341873	-0.000254
C	3.623759	1.348600	-0.021543
C	3.305425	-0.045314	-0.052752
C	2.009411	-0.488128	-0.064156
C	1.666455	-1.923798	-0.178864
C	0.339515	-2.307938	0.366491
H	-3.563050	1.324933	-0.342194
H	-2.292948	-2.793243	-0.034061
H	0.513290	3.883712	0.070877
H	4.665453	1.648659	-0.013935
H	4.116110	-0.763705	-0.063911
C	2.455456	-2.819132	-0.791480
C	0.165480	-3.422902	1.089168
C	-4.405845	-1.192095	-0.459884
C	-2.066350	3.458257	0.314915
H	3.406340	-2.539970	-1.227972
H	2.147357	-3.851385	-0.900081
H	0.994358	-4.087009	1.300443
H	-0.796585	-3.680485	1.514818
H	-5.202951	-0.473790	-0.607516

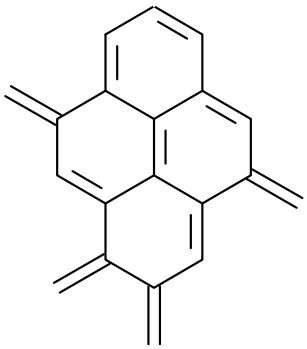
H	-4.671407	-2.241795	-0.486306
H	-1.763688	4.497056	0.363227
H	-3.116823	3.249862	0.465474



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-770,649245	-770,380324

C	-2.268323	-1.677022	-0.141765
C	-0.956947	-1.382105	0.076033
C	-0.516799	0.005804	0.070137
C	-1.532603	1.052142	0.031249
C	-2.833874	0.713568	-0.183136
C	-3.276533	-0.656174	-0.306206
C	-1.096784	2.463853	0.186134
C	0.323073	2.714115	0.085142
C	1.246041	1.717257	0.008303
C	0.829128	0.318004	0.024568
C	1.839164	-0.739259	-0.021656
C	3.269391	-0.367131	-0.197007
C	3.597128	1.051518	-0.143545
C	2.662332	2.014866	-0.053818
C	0.067952	-2.429904	0.295170
C	1.448638	-2.032546	0.130699
C	-1.942986	3.486357	0.453744
C	-4.578281	-0.968585	-0.557953
H	2.188751	-2.821157	0.187713
H	0.656350	3.746466	0.117567
C	-0.226331	-3.696536	0.673909
H	-3.584482	1.488139	-0.289534
H	-2.586706	-2.710637	-0.215238
H	2.955635	3.059494	-0.037518
C	4.254173	-1.259547	-0.429704
H	4.646812	1.317875	-0.207370
H	-1.569299	4.500199	0.531997
H	-3.002389	3.343583	0.619349
H	-5.329837	-0.197662	-0.676621
H	-4.903820	-1.997976	-0.645123

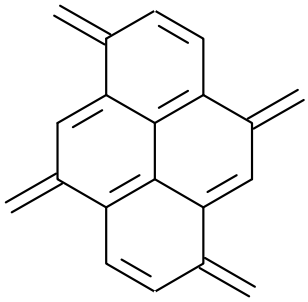
H	-1.234788	-4.020493	0.894288
H	0.560235	-4.432389	0.790214
H	5.279070	-0.925611	-0.538401
H	4.079113	-2.321893	-0.533120



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-770,643436	-770,374625

C	3.089339	-0.098772	-0.366272
C	2.396406	1.168511	-0.284462
C	1.073341	1.284514	0.037556
C	0.242851	0.092775	0.085578
C	0.882655	-1.215050	0.093626
C	2.361154	-1.270828	0.190287
C	0.426386	2.606719	0.214796
C	-1.138743	0.195154	0.018906
C	-1.766856	1.515814	-0.039190
C	-1.001853	2.652409	0.048680
C	-3.197660	1.589354	-0.155881
H	-3.661423	2.569028	-0.193512
C	-3.948059	0.458333	-0.221321
C	-3.335705	-0.828257	-0.174003
C	-1.977783	-0.987847	-0.045160
C	-1.326621	-2.318936	-0.000952
C	0.121824	-2.337039	0.025951
H	2.964248	2.059816	-0.527903
H	-1.488468	3.622052	0.062026
H	-5.026203	0.521569	-0.316279
H	-3.976571	-1.697518	-0.253528
C	-1.996565	-3.497743	0.027614
C	4.323617	-0.186717	-0.905911
C	1.119221	3.717008	0.579867
H	-3.075789	-3.565925	0.042381
H	-1.452416	-4.433942	0.048170
H	4.838571	0.698492	-1.260830
H	4.832338	-1.135185	-1.019733
H	0.623113	4.677227	0.654990
H	2.170207	3.683291	0.834651

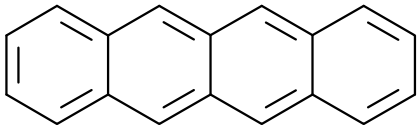
C	3.003359	-2.263756	0.824183
H	2.466837	-3.080226	1.291190
H	4.081642	-2.264276	0.922291
H	0.602064	-3.308283	-0.007266



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-770,650871	-770,381816

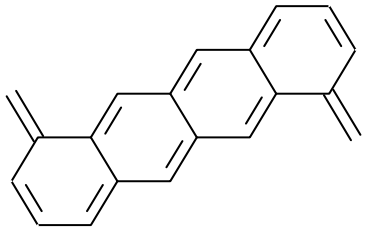
C	3.156694	0.320739	0.205036
C	1.751723	0.772109	0.046234
C	0.687965	-0.230678	-0.005168
C	1.000489	-1.575030	-0.096512
C	2.392002	-1.979643	-0.127480
C	3.401344	-1.097394	0.005133
C	-0.687971	0.230670	-0.005159
C	-1.751726	-0.772116	0.046019
C	-1.428097	-2.083991	-0.089910
C	-0.070721	-2.572359	-0.189267
C	1.428030	2.084016	-0.089253
C	0.070662	2.572407	-0.188528
C	-1.000537	1.575025	-0.096321
C	-2.392063	1.979571	-0.127656
C	-3.401403	1.097289	0.004829
C	-3.156658	-0.320760	0.205080
C	0.138999	-3.905274	-0.354718
C	-0.139060	3.905405	-0.353313
H	2.214710	2.827874	-0.141275
H	-2.214820	-2.827783	-0.142258
H	-2.626725	3.029310	-0.241589
C	-4.174027	-1.133932	0.566519
C	4.174290	1.133921	0.565829
H	2.626640	-3.029416	-0.241152
H	-4.430794	1.438841	0.012200
H	4.430717	-1.438995	0.012789
H	-0.702580	-4.584683	-0.413125
H	1.120724	-4.348649	-0.436793
H	0.702512	4.584858	-0.411306
H	-1.120787	4.348815	-0.435174
H	5.184231	0.748370	0.638081
H	4.032053	2.177038	0.815600
H	-5.184011	-0.748517	0.638918

H	-4.031490	-2.176905	0.816726



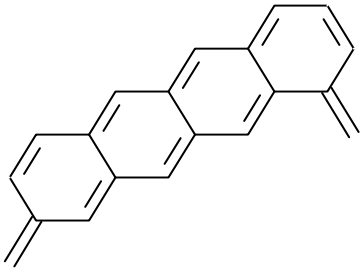
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
D2h	0	-693,322943	-693,08334

C	0.000000	4.880979	0.714549
C	0.000000	3.706412	1.407154
C	0.000000	2.446518	0.724891
C	0.000000	2.446518	-0.724891
C	0.000000	3.706412	-1.407154
C	0.000000	4.880979	-0.714549
C	0.000000	1.233713	1.404464
C	0.000000	0.000000	0.725072
C	0.000000	0.000000	-0.725072
C	0.000000	1.233713	-1.404464
C	0.000000	-1.233713	1.404464
C	0.000000	-2.446518	0.724891
C	0.000000	-2.446518	-0.724891
C	0.000000	-1.233713	-1.404464
C	0.000000	-3.706412	1.407154
C	0.000000	-4.880979	0.714549
C	0.000000	-4.880979	-0.714549
C	0.000000	-3.706412	-1.407154
H	0.000000	-5.826549	1.244940
H	0.000000	-5.826549	-1.244940
H	0.000000	5.826549	1.244940
H	0.000000	3.705918	2.492157
H	0.000000	3.705918	-2.492157
H	0.000000	5.826549	-1.244940
H	0.000000	1.234053	2.490190
H	0.000000	1.234053	-2.490190
H	0.000000	-1.234053	2.490190
H	0.000000	-1.234053	-2.490190
H	0.000000	-3.705918	2.492157
H	0.000000	-3.705918	-2.492157



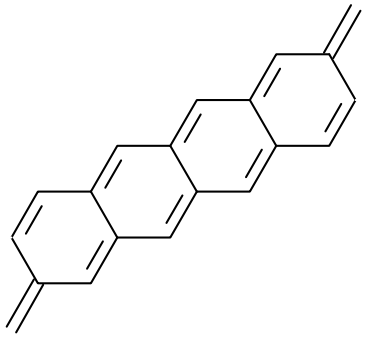
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2h	0	-770,673839	-770,403825

C	4.901839	0.716017	0.000000
C	3.656540	1.397646	0.000000
C	2.457753	0.705021	0.000000
C	2.457753	-0.759419	0.000000
C	3.765638	-1.467638	0.000000
C	4.958823	-0.644099	0.000000
C	1.209853	1.388794	0.000000
C	0.002010	0.725255	0.000000
C	-0.002010	-0.725255	0.000000
C	1.254773	-1.409640	0.000000
C	3.897465	-2.819235	0.000000
H	5.819065	1.294513	0.000000
H	3.640209	2.481947	0.000000
H	5.917016	-1.151461	0.000000
C	-1.254773	1.409640	0.000000
C	-1.209853	-1.388794	0.000000
H	1.220820	-2.493250	0.000000
H	4.882025	-3.270322	0.000000
H	3.055913	-3.498515	0.000000
C	-2.457753	0.759419	0.000000
C	-2.457753	-0.705021	0.000000
H	1.222467	2.474475	0.000000
H	-1.222467	-2.474475	0.000000
C	-3.765638	1.467638	0.000000
C	-3.656540	-1.397646	0.000000
C	-4.958823	0.644099	0.000000
C	-4.901839	-0.716017	0.000000
C	-3.897465	2.819235	0.000000
H	-1.220820	2.493250	0.000000
H	-3.640209	-2.481947	0.000000
H	-5.917016	1.151461	0.000000
H	-5.819065	-1.294513	0.000000
H	-4.882025	3.270322	0.000000
H	-3.055913	3.498515	0.000000



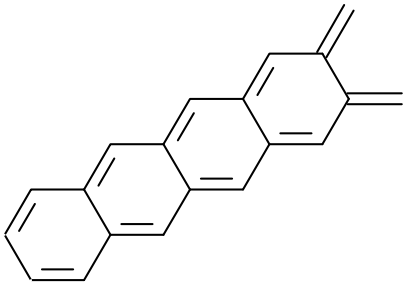
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
Cs	0	-770,681321	-770,411006

C	4.798091	-0.627640	0.000000
C	3.713954	0.323694	0.000000
C	2.393249	-0.057605	0.000000
C	2.048937	-1.479725	0.000000
C	3.138121	-2.433181	0.000000
C	4.427730	-2.039054	0.000000
C	1.320510	0.890059	0.000000
C	0.000000	0.505835	0.000000
C	-0.337379	-0.911381	0.000000
C	0.736277	-1.861823	0.000000
H	3.962158	1.380541	0.000000
H	5.226619	-2.772868	0.000000
C	-1.072900	1.457059	0.000000
C	-1.661401	-1.279131	0.000000
H	0.485860	-2.918522	0.000000
C	-2.390949	1.098856	0.000000
C	-2.724586	-0.327993	0.000000
H	1.569419	1.946929	0.000000
H	-1.922417	-2.333113	0.000000
C	-3.504186	2.085976	0.000000
C	-4.045781	-0.728549	0.000000
C	-4.855011	1.554905	0.000000
C	-5.107345	0.219342	0.000000
C	-3.326159	3.431029	0.000000
H	-0.792816	2.504486	0.000000
H	-4.277574	-1.788032	0.000000
H	-5.672410	2.267299	0.000000
H	-6.131245	-0.137704	0.000000
H	-4.182477	4.094165	0.000000
H	-2.352177	3.901234	0.000000
H	2.887582	-3.489195	0.000000
C	6.101464	-0.237733	0.000000
H	6.906247	-0.962748	0.000000
H	6.377415	0.809903	0.000000



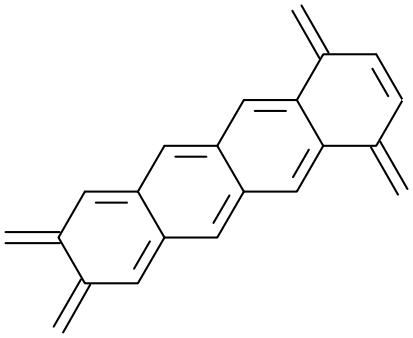
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2h	0	-770,689149	-770,4185

C	4.901331	0.706677	0.000000
C	3.740530	1.392768	0.000000
C	2.457693	0.721680	0.000000
C	2.457693	-0.741646	0.000000
C	3.649396	-1.422248	0.000000
C	4.928381	-0.752102	0.000000
C	1.272278	1.400715	0.000000
C	0.001883	0.731338	0.000000
C	-0.001883	-0.731338	0.000000
C	1.189967	-1.411256	0.000000
C	6.101128	-1.439562	0.000000
H	5.850435	1.231916	0.000000
H	3.744808	2.478077	0.000000
H	3.642630	-2.507829	0.000000
H	1.277385	2.486658	0.000000
C	-1.272278	-1.400715	0.000000
H	1.184940	-2.497066	0.000000
H	7.055205	-0.926616	0.000000
C	-2.457693	-0.721680	0.000000
C	-2.457693	0.741646	0.000000
C	-1.189967	1.411256	0.000000
H	-1.277385	-2.486658	0.000000
H	-1.184940	2.497066	0.000000
C	-3.649396	1.422248	0.000000
H	-3.642630	2.507829	0.000000
C	-3.740530	-1.392768	0.000000
C	-4.928381	0.752102	0.000000
C	-4.901331	-0.706677	0.000000
C	-6.101128	1.439562	0.000000
H	6.120338	-2.522755	0.000000
H	-3.744808	-2.478077	0.000000
H	-5.850435	-1.231916	0.000000
H	-7.055205	0.926616	0.000000
H	-6.120338	2.522755	0.000000



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2	0	-770,67133	-770,401461

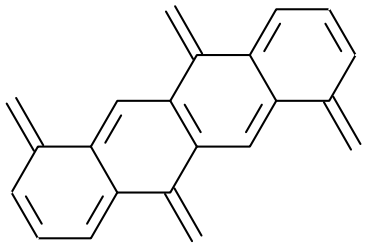
C	0.053158	1.414431	-3.015784
C	0.130287	0.736248	-4.285371
C	-0.130287	-0.736248	-4.285371
C	-0.053158	-1.414431	-3.015784
C	-0.003593	-0.738315	-1.818980
C	0.003593	0.738315	-1.818980
C	0.499709	1.411831	-5.402798
C	-0.499709	-1.411831	-5.402798
H	0.119167	2.497648	-3.013160
H	-0.119167	-2.497648	-3.013160
C	-0.000116	-1.414086	-0.563529
C	0.000116	1.414086	-0.563529
H	0.693311	0.909414	-6.341495
H	0.638252	2.486295	-5.379307
H	-0.638252	-2.486295	-5.379307
H	-0.693311	-0.909414	-6.341495
C	-0.000775	0.734961	0.638367
C	0.000775	-0.734961	0.638367
H	-0.005815	-2.499528	-0.562014
H	0.005815	2.499528	-0.562014
C	-0.000420	1.410908	1.893989
C	0.000420	-1.410908	1.893989
C	-0.000116	0.731908	3.091338
C	0.000116	-0.731908	3.091338
H	-0.000335	2.496568	1.895510
H	0.000335	-2.496568	1.895510
C	0.000143	1.411846	4.360845
C	-0.000143	-1.411846	4.360845
C	0.000116	0.719230	5.529064
C	-0.000116	-0.719230	5.529064
H	0.000414	2.496838	4.361211
H	-0.000414	-2.496838	4.361211
H	0.000291	1.246388	6.476410
H	-0.000291	-1.246388	6.476410



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-848,073344	-847,77115

C	4.724356	-0.742710	-0.102732
C	3.451445	-1.414844	0.005660
C	2.257989	-0.737566	0.025760
C	2.258079	0.737123	-0.033311
C	3.451888	1.413958	-0.020143
C	4.725219	0.741348	0.079979
C	0.997593	-1.412626	0.062456
C	-0.195363	-0.729882	0.039049
C	-0.195313	0.730526	-0.028266
C	0.997729	1.412576	-0.064388
H	3.448634	-2.500025	-0.006428
C	-1.462632	-1.395867	0.064805
C	-1.462582	1.396205	-0.061106
H	0.995081	2.497142	-0.109723
C	-2.656345	-0.732540	0.054313
C	-2.656259	0.734618	-0.011020
H	0.994768	-2.497331	0.104314
H	-1.446343	2.476307	-0.144657
C	-3.948356	-1.465163	0.068713
C	-3.948150	1.465926	-0.058313
C	-5.152276	-0.679160	-0.172078
C	-5.152213	0.662322	-0.230371
C	-4.066957	-2.788180	0.302946
H	-1.446157	-2.479112	0.077407
H	-6.085541	-1.224562	-0.265922
H	-6.085458	1.197587	-0.370992
H	-5.041207	-3.261417	0.278357
H	-3.226650	-3.427757	0.536711
H	3.449561	2.499135	-0.007673
C	5.840125	-1.441199	-0.427876
H	6.784067	-0.955316	-0.637455
H	5.811386	-2.521103	-0.512274
C	-4.066355	2.804001	0.063573
H	-3.225704	3.460427	0.243005
H	-5.040438	3.273809	-0.000820

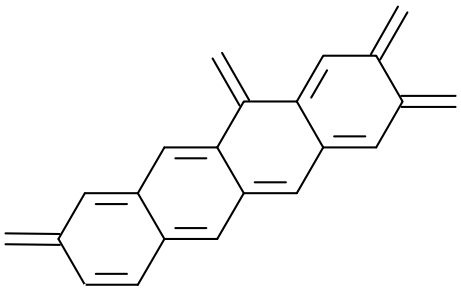
C	5.843363	1.439418	0.397803
H	6.788490	0.953189	0.601149
H	5.815602	2.519341	0.482274



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
Ci	0	-848,058523	-847,755968

C	4.780980	-1.181073	-0.491733
C	3.476430	-1.759581	-0.327313
C	2.398649	-0.996056	0.022964
C	2.548900	0.447561	0.113143
C	3.915188	1.015155	0.158668
C	4.996261	0.133924	-0.254730
C	1.058466	-1.567410	0.284544
C	-0.101786	-0.685422	0.044854
C	0.101786	0.685422	-0.044854
C	1.422893	1.225496	0.057327
C	4.190838	2.269158	0.593764
H	5.602144	-1.823069	-0.790273
H	3.348349	-2.819994	-0.509487
H	5.992074	0.556096	-0.332245
C	-1.422893	-1.225496	-0.057327
C	-1.058466	1.567410	-0.284544
H	1.534919	2.301507	0.042480
H	5.204311	2.650953	0.566421
H	3.432114	2.923870	1.002341
C	-2.548900	-0.447561	-0.113143
C	-2.398649	0.996056	-0.022964
C	-3.915188	-1.015155	-0.158668
C	-3.476430	1.759581	0.327313
C	-4.996261	-0.133924	0.254730
C	-4.780980	1.181073	0.491733
C	-4.190838	-2.269158	-0.593764
H	-1.534919	-2.301507	-0.042480
H	-3.348349	2.819994	0.509487
H	-5.992074	-0.556096	0.332245
H	-5.602144	1.823069	0.790273
H	-5.204311	-2.650953	-0.566421
H	-3.432114	-2.923870	-1.002341
C	-0.927870	2.806258	-0.805932
H	0.036724	3.245359	-1.021207
H	-1.796236	3.394448	-1.072529

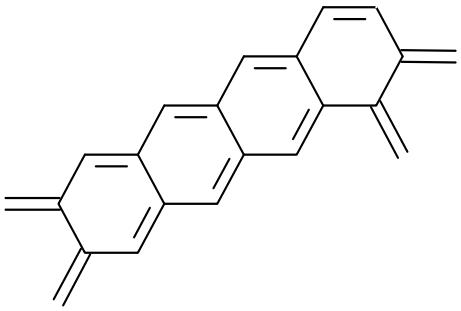
C	0.927870	-2.806258	0.805932
H	1.796236	-3.394448	1.072529
H	-0.036724	-3.245359	1.021207



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-848,079646	-847,776895

C	-3.278719	1.287542	-0.171044
C	-4.542154	0.612006	-0.430712
C	-4.601724	-0.845799	-0.115034
C	-3.331934	-1.513480	0.066746
C	-2.146051	-0.841969	0.178334
C	-2.139127	0.631327	0.149437
C	-5.571072	1.295867	-0.972834
C	-5.761719	-1.528146	0.025519
H	-3.265601	2.365048	-0.292213
H	-3.337364	-2.596465	0.139474
C	-0.896669	-1.529261	0.283878
C	-0.870966	1.325520	0.478269
H	-6.501963	0.818915	-1.250931
H	-5.488351	2.359135	-1.165102
H	-5.754951	-2.592856	0.226616
H	-6.728761	-1.046385	-0.034437
C	0.387967	0.572013	0.251072
C	0.319120	-0.887085	0.262702
H	-0.917317	-2.614792	0.296520
C	1.592049	1.178718	0.071419
C	1.550461	-1.621286	0.206710
C	2.828060	0.444157	-0.038909
C	2.764308	-1.010629	0.060292
H	1.648450	2.259964	0.007786
H	1.498630	-2.704835	0.256804
C	4.034843	1.064110	-0.216955
C	4.007607	-1.745655	-0.024924
C	5.279159	0.332085	-0.306608
C	5.190002	-1.119620	-0.196934
H	4.074082	2.146549	-0.291350
H	3.965075	-2.827475	0.051328
H	6.110328	-1.690445	-0.259740
C	-0.868393	2.540947	1.054232
C	6.471974	0.958235	-0.482176
H	7.397482	0.398980	-0.546742

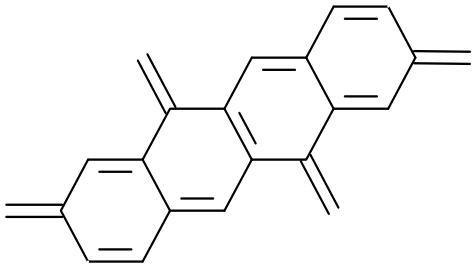
H	6.536823	2.036628	-0.563402
H	0.051512	3.031404	1.345081
H	-1.790212	3.059054	1.285439



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-848,074674	-847,77237

C	-3.459080	1.458783	0.164821
C	-4.780691	0.889186	0.039683
C	-4.884050	-0.601248	0.098396
C	-3.664042	-1.349859	-0.092825
C	-2.425889	-0.759638	-0.084562
C	-2.318912	0.700675	0.095628
C	-5.849841	1.689600	-0.191230
C	-6.041880	-1.244580	0.387092
H	-3.378312	2.538342	0.241851
H	-3.739636	-2.429780	-0.169817
C	-1.217092	-1.515969	-0.204622
C	-1.010561	1.280389	0.152486
H	-6.832308	1.291185	-0.408350
H	-5.744225	2.768031	-0.188546
H	-6.088702	-2.327133	0.382812
H	-6.946065	-0.713338	0.653953
C	0.128869	0.525036	0.032177
C	0.022474	-0.926328	-0.151071
H	-1.293780	-2.591343	-0.331702
H	-0.930021	2.355160	0.282549
C	1.441622	1.110157	0.065177
C	1.239673	-1.677834	-0.239217
C	2.577829	0.371041	-0.070705
C	2.470288	-1.085784	-0.181798
H	1.507966	2.183284	0.207643
H	1.170601	-2.757511	-0.330609
C	3.928337	0.980735	-0.138887
C	3.688388	-1.870054	-0.174212
C	5.079568	0.114495	0.248988
C	4.897297	-1.319248	0.055732
H	3.594144	-2.944676	-0.292780
H	5.776948	-1.949200	0.136798
C	6.229773	0.602017	0.750011
C	4.124468	2.215642	-0.630145

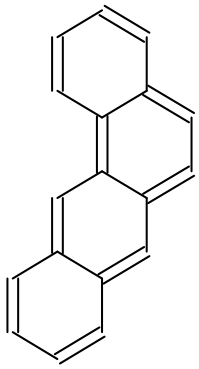
H	7.058345	-0.058268	0.979127
H	3.302146	2.824739	-0.983311
H	5.118676	2.632462	-0.727559
H	6.364939	1.654766	0.962451



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2	0	-848,077912	-847,775082

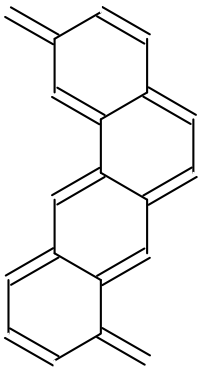
C	3.203227	-3.749360	-0.527360
C	3.123326	-2.325069	-0.264053
C	1.965194	-1.703621	0.090645
C	0.724596	-2.465318	0.111106
C	0.798633	-3.888870	-0.113955
C	1.965194	-4.503127	-0.406291
C	1.894449	-0.266708	0.456279
C	0.574582	0.391542	0.347916
C	-0.574582	-0.391542	0.347916
C	-0.471881	-1.815412	0.274847
H	1.998758	-5.574057	-0.574930
C	0.471881	1.815412	0.274847
C	-1.894449	0.266708	0.456279
H	-1.382183	-2.402206	0.247993
C	-0.724596	2.465318	0.111106
C	-1.965194	1.703621	0.090645
C	-0.798633	3.888870	-0.113955
C	-3.123326	2.325069	-0.264053
C	-1.965194	4.503127	-0.406291
C	-3.203227	3.749360	-0.527360
H	1.382183	2.402206	0.247993
H	-4.036198	1.749139	-0.369488
H	-1.998758	5.574057	-0.574930
H	0.122562	4.459681	-0.054258
H	4.036198	-1.749139	-0.369488
H	-0.122562	-4.459681	-0.054258
C	4.374319	-4.343420	-0.873897
C	2.964305	0.376592	0.967482
C	-4.374319	4.343420	-0.873897
H	-5.291184	3.773475	-0.964698
H	-4.429584	5.407195	-1.071205
H	3.898378	-0.139257	1.147395
H	2.924304	1.416179	1.262884
H	4.429584	-5.407195	-1.071205

H	5.291184	-3.773475	-0.964698
C	-2.964305	-0.376592	0.967482
H	-2.924304	-1.416179	1.262884
H	-3.898378	0.139257	1.147395



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
Cs	0	-693.3359192	-693.095916

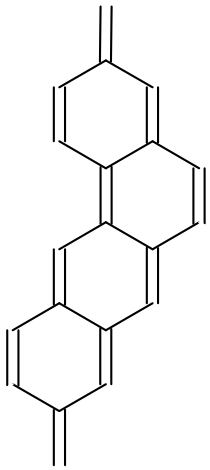
C	-0.854772	-4.673706	0.000000
C	-2.129158	-4.045994	0.000000
C	-2.228991	-2.680009	0.000000
C	-1.062903	-1.861332	0.000000
C	0.224384	-2.496802	0.000000
C	0.288657	-3.920041	0.000000
C	-1.134207	-0.457296	0.000000
C	0.000000	0.347904	0.000000
C	1.288964	-0.296379	0.000000
C	1.368865	-1.685666	0.000000
C	-0.058112	1.811225	0.000000
C	1.155132	2.553138	0.000000
C	2.417875	1.860615	0.000000
C	2.481304	0.509623	0.000000
C	-1.270499	2.529898	0.000000
C	-1.291570	3.912740	0.000000
C	-0.092309	4.638621	0.000000
C	1.111125	3.961984	0.000000
H	-0.793431	-5.756150	0.000000
H	-3.024650	-4.657143	0.000000
H	-3.202334	-2.200401	0.000000
H	1.262999	-4.397495	0.000000
H	-2.120576	-0.009694	0.000000
H	2.347728	-2.155515	0.000000
H	3.326176	2.454067	0.000000
H	3.440580	0.002882	0.000000
H	-2.213617	1.998919	0.000000
H	-2.241423	4.435422	0.000000
H	-0.110935	5.722472	0.000000
H	2.046777	4.511513	0.000000



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-770.6777547	-770.407600

C	2.514637	0.314037	0.000085
C	1.879079	-0.993881	-0.000220
C	3.996582	0.387539	0.000203
C	2.654051	-2.144695	-0.000409
C	4.712660	-0.871269	0.000017
C	4.069434	-2.073155	-0.000279
C	1.701961	1.418986	0.000208
C	0.282093	1.343334	0.000088
C	0.456563	-1.067362	-0.000309
C	-0.355777	0.040288	-0.000073
C	-0.498012	2.498193	0.000018
C	-1.894712	2.435345	-0.000216
C	-1.831670	-0.026380	-0.000041
C	-2.572036	1.224622	-0.000246
C	-2.534731	-1.204854	0.000246
C	-3.975649	-1.267260	0.000250
C	-4.007836	1.172480	-0.000370
C	-4.682188	-0.000512	-0.000117
C	4.700058	1.551384	0.000463
C	-4.640086	-2.459613	0.000568
H	-5.722369	-2.500285	0.000588
H	-4.107186	-3.402676	0.000792
H	-5.766666	-0.015320	-0.000240
H	-4.547822	2.113969	-0.000685
H	-2.469325	3.355818	-0.000331
H	-0.005289	3.464498	0.000103
H	2.135902	2.412477	0.000372
H	0.025210	-2.061643	-0.000598
H	2.165805	-3.112936	-0.000647
H	4.644463	-2.992587	-0.000416
H	5.796261	-0.831545	0.000115

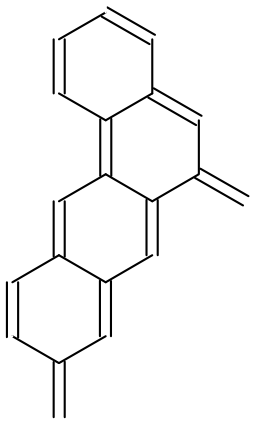
H	4.232830	2.526761	0.000617
H	5.782883	1.533705	0.000527
H	-2.011219	-2.153604	0.000600



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-770.6886749	-770.418012

C	-2.440669	0.600151	-0.000027
C	-1.953586	-0.773238	-0.000018
C	-3.792329	0.848647	0.000022
C	-2.936889	-1.834100	0.000060
C	-4.773297	-0.208384	0.000092
C	-4.260857	-1.574327	0.000109
C	-1.460230	1.642573	-0.000068
C	-0.112711	1.389127	-0.000087
C	-0.605460	-1.022248	-0.000076
C	0.378658	0.015866	-0.000125
C	0.848215	2.469784	-0.000077
C	2.174174	2.231353	0.000026
C	1.760538	-0.229791	-0.000144
C	2.698697	0.881656	0.000011
C	2.331013	-1.554151	-0.000340
C	3.667500	-1.768005	-0.000185
C	4.050844	0.654046	0.000131
C	4.618636	-0.670762	0.000060
C	-6.110170	0.046815	0.000143
C	5.963602	-0.885981	0.000470
H	6.666816	-0.061969	-0.000160
H	6.372584	-1.888955	0.000790
H	4.056155	-2.780825	-0.000403
H	1.672003	-2.412462	-0.000649
H	4.729195	1.501661	0.000300
H	2.884192	3.051659	0.000005
H	0.468789	3.486274	-0.000204
H	-1.805273	2.672137	-0.000082
H	-0.285576	-2.056649	-0.000034
H	-2.579299	-2.859004	0.000072
H	-4.980625	-2.385931	0.000160

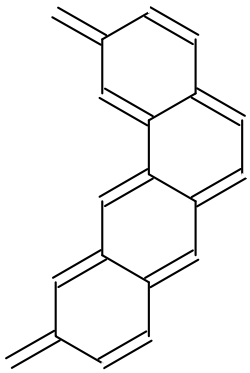
H	-6.490781	1.061063	0.000130
H	-6.836843	-0.756462	0.000197
H	-4.145416	1.875274	0.000013



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-770.6777485	-770.407442

C	2.121636	0.476462	-0.021903
C	1.725861	-0.916504	0.035628
C	3.457656	0.813722	-0.057664
C	2.770098	-1.913684	0.057500
C	4.501325	-0.177535	-0.035586
C	4.075971	-1.570615	0.024436
C	1.081374	1.455612	-0.037110
C	-0.251574	1.141285	0.010878
C	0.389971	-1.236896	0.057860
C	-0.647441	-0.262707	0.036010
C	-1.302175	2.194392	0.027195
C	-2.665895	1.752341	-0.039603
C	-2.016177	-0.619372	0.017009
C	-3.028750	0.426303	-0.038412
C	-2.477678	-1.973632	0.037136
C	-3.806477	-2.283796	0.001745
C	-4.419734	0.048684	-0.078458
C	-4.798345	-1.254902	-0.059117
C	5.822205	0.160580	-0.068362
C	-1.045347	3.528182	0.124233
H	-1.861820	4.239494	0.115757
H	-0.049552	3.937108	0.223522
H	-3.441428	2.510769	-0.064300
H	-5.159459	0.840963	-0.121452
H	-5.847918	-1.524520	-0.088001
H	-4.118036	-3.321953	0.019527
H	-1.760920	-2.782189	0.081847
H	0.128379	-2.286794	0.087929
H	2.478903	-2.958434	0.101069
H	4.845152	-2.335350	0.041575
H	6.138521	1.195638	-0.113126

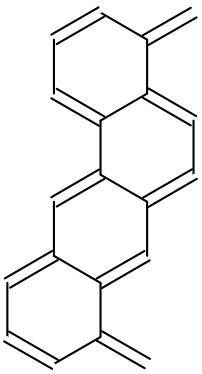
H	6.597228	-0.595788	-0.050375
H	3.743007	1.860187	-0.101382
H	1.388923	2.493340	-0.093090



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-770.6843358	-770.413963

C	2.369674	-0.968274	-0.000252
C	1.969787	0.430602	0.000152
C	3.783897	-1.265515	-0.000440
C	2.929500	1.417118	0.000359
C	4.712941	-0.286405	-0.000243
C	4.340320	1.123586	0.000170
C	1.401773	-1.938235	-0.000393
C	0.009470	-1.632545	-0.000182
C	0.568922	0.730553	0.000318
C	-0.404694	-0.234163	0.000034
C	-0.948504	-2.636488	-0.000023
C	-2.321275	-2.345542	0.000316
C	-1.853545	0.070224	0.000040
C	-2.790470	-1.044390	0.000327
C	-2.355098	1.345103	-0.000267
C	-3.767853	1.643170	-0.000258
C	-4.199605	-0.757147	0.000463
C	-4.673095	0.509353	0.000063
C	5.283005	2.106945	0.000364
C	-4.224856	2.927646	-0.000635
H	-5.285482	3.147158	0.000316
H	-3.543020	3.769338	-0.001108
H	-5.740445	0.701687	0.000169
H	-4.885800	-1.598069	0.000961
H	-1.684520	2.196341	-0.000720
H	-3.036998	-3.161033	0.000526
H	-0.623346	-3.671443	-0.000109
H	1.693147	-2.984417	-0.000623
H	4.085743	-2.308078	-0.000746
H	5.769680	-0.531479	-0.000391
H	5.005828	3.154161	0.000673

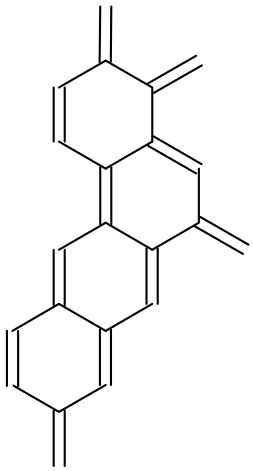
H	6.340574	1.873149	0.000212
H	2.623180	2.458656	0.000672
H	0.299699	1.780441	0.000698



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-770.6687943	-770.398799

C	2.488819	0.433043	-0.021042
C	2.050703	-0.950747	0.063028
C	3.943660	0.722328	-0.040151
C	2.989374	-1.972861	0.157313
C	4.836265	-0.409887	0.078996
C	4.375666	-1.691654	0.170661
C	1.523771	1.407614	-0.061538
C	0.131938	1.121768	-0.052689
C	0.657720	-1.233176	0.058404
C	-0.310306	-0.255888	-0.019579
C	-0.817071	2.142156	-0.064348
C	-2.183807	1.866609	-0.019532
C	-1.754743	-0.538766	-0.054597
C	-2.683926	0.569935	0.019720
C	-2.253616	-1.821463	-0.195163
C	-3.649045	-2.082276	-0.225473
C	-4.133845	0.296140	0.092075
C	-4.553501	-1.076544	-0.089169
C	4.466109	1.971838	-0.171865
C	-5.076239	1.248578	0.346366
H	3.858498	2.858988	-0.286842
H	5.539387	2.116431	-0.171003
H	5.902156	-0.211053	0.083451
H	5.080035	-2.512331	0.251172
H	2.648444	-3.000079	0.224289
H	0.375154	-2.276489	0.135641
H	1.807045	2.453622	-0.092635
H	-0.482216	3.173270	-0.102798
H	-2.873348	2.701517	-0.035818
H	-6.125975	0.983217	0.364247
H	-4.834126	2.281173	0.556445

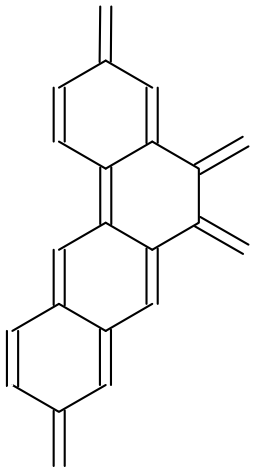
H	-5.617405	-1.285701	-0.090541
H	-3.987794	-3.104517	-0.352892
H	-1.577417	-2.658539	-0.311219



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-848.0799993	-847.777098

C	-2.687137	0.446912	0.014470
C	-2.251733	-0.939391	-0.015368
C	-4.025396	0.747286	0.083763
C	-3.270605	-1.964870	0.024909
C	-5.044724	-0.273344	0.123323
C	-4.582766	-1.656352	0.089414
C	-1.671257	1.456490	-0.038790
C	-0.337616	1.171705	-0.119289
C	-0.913400	-1.227707	-0.061186
C	0.103945	-0.220898	-0.080992
C	0.685283	2.236478	-0.252021
C	2.061689	1.842584	-0.045119
C	1.469534	-0.527348	-0.030123
C	2.449295	0.547678	0.090988
C	1.976901	-1.873940	-0.127877
C	3.298576	-2.158967	-0.206728
C	3.865518	0.190702	0.366190
C	4.328386	-1.139895	-0.113443
C	4.658144	0.980278	1.107725
C	5.607747	-1.405464	-0.442440
C	-6.369591	0.030920	0.188083
C	0.403530	3.519126	-0.583909
H	1.195972	4.255279	-0.643477
H	-0.595582	3.861086	-0.817977
H	5.673427	0.691146	1.348299
H	4.301540	1.913660	1.524757
H	6.373019	-0.639905	-0.438338
H	5.906688	-2.402246	-0.745774
H	3.618843	-3.181709	-0.375657
H	1.275312	-2.691712	-0.222269
H	-0.624362	-2.270720	-0.051885

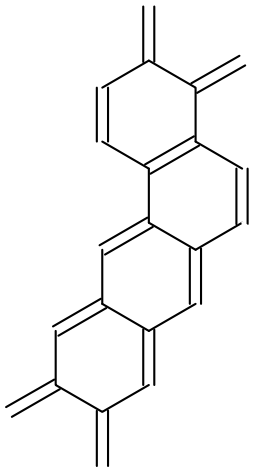
H	-2.951655	-3.002186	0.002800
H	-4.339509	1.786262	0.105934
H	-2.000391	2.489174	-0.012766
H	-5.330857	-2.441424	0.118504
H	-6.712043	1.058381	0.213516
H	-7.124773	-0.745107	0.216055
H	2.808440	2.628121	-0.051210



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-848.0864382	-847.783310

C	2.587027	0.416331	-0.023688
C	2.174608	-0.977078	0.020424
C	3.919739	0.739888	0.013345
C	3.209282	-1.982829	0.101781
C	4.956121	-0.261981	0.091242
C	4.517561	-1.651499	0.133853
C	1.549563	1.406064	-0.105148
C	0.224595	1.085290	-0.139310
C	0.839475	-1.292470	0.002158
C	-0.194890	-0.307877	-0.051126
C	-0.820463	2.124254	-0.284736
C	-2.126942	1.786224	0.332051
C	-1.563234	-0.640220	-0.036035
C	-2.576680	0.390266	0.115928
C	-2.035926	-1.996149	-0.154603
C	-3.353261	-2.309008	-0.174172
C	-3.901516	0.068514	0.077746
C	-4.376851	-1.288797	-0.069213
C	-5.703046	-1.589951	-0.108355
C	6.276396	0.065783	0.124384
C	-0.634786	3.263942	-0.965497
C	-2.807126	2.669922	1.074860
H	-1.437804	3.981363	-1.080179
H	0.306168	3.492681	-1.450746
H	-3.740116	2.409728	1.559630
H	-2.424358	3.669123	1.241834
H	-6.459393	-0.818245	-0.031153
H	-6.045148	-2.611995	-0.217271
H	-4.643263	0.855741	0.151873
H	-3.665783	-3.341641	-0.286840
H	-1.316164	-2.796419	-0.263323

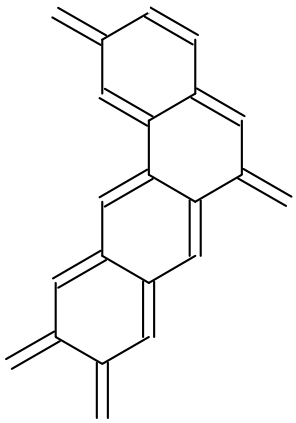
H	0.570460	-2.339215	0.064307
H	2.906519	-3.024592	0.136506
H	5.278490	-2.422299	0.193755
H	6.602662	1.098376	0.093684
H	7.044246	-0.696020	0.182905
H	4.217804	1.783325	-0.018192
H	1.847799	2.448376	-0.132136



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-848.0705112	-847.768145

C	2.381826	0.883699	-0.017091
C	2.023933	-0.543036	0.015417
C	3.700942	1.253061	-0.075196
C	3.016852	-1.487358	0.071768
C	4.773513	0.287902	-0.138299
C	4.417238	-1.138914	0.132905
C	1.313377	1.833407	-0.026509
C	-0.005332	1.456165	-0.009678
C	0.635942	-0.899198	0.025752
C	-0.372791	0.033451	0.019097
C	-1.060780	2.432563	-0.035910
C	-2.361310	2.061630	-0.005549
C	-1.791988	-0.319475	0.042484
C	-2.755322	0.674703	0.049637
C	-2.214300	-1.713272	0.061394
C	-3.505833	-2.073855	-0.063193
C	-4.184918	0.314316	0.161146
C	-4.561191	-1.081243	-0.196529
C	-5.782778	-1.423268	-0.650324
C	6.020880	0.675357	-0.501003
C	5.336417	-2.067615	0.493861
C	-5.100868	1.166897	0.660292
H	2.752629	-2.537103	0.150702
H	5.048649	-3.101389	0.644351
H	6.374117	-1.814687	0.668009
H	6.252537	1.723179	-0.651282
H	6.817654	-0.035453	-0.677031
H	3.958843	2.304316	-0.154077
H	1.562883	2.889510	-0.055929
H	-0.788641	3.481107	-0.092113
H	-3.132796	2.819344	-0.054095

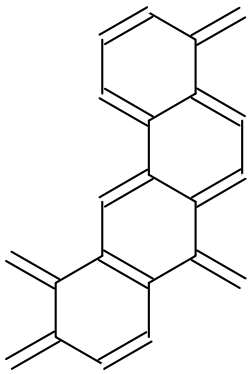
H	-6.120931	0.849177	0.834189
H	-4.853963	2.180317	0.946979
H	-6.548147	-0.685504	-0.854949
H	-6.030029	-2.460098	-0.847901
H	-3.780988	-3.121562	-0.120778
H	-1.464325	-2.489105	0.131416
H	0.411465	-1.957553	0.045669



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-848.0726715	-847.770371

C	-2.133660	0.738692	-0.018093
C	-1.716129	-0.665770	0.006905
C	-3.463230	1.054177	0.014265
C	-2.659673	-1.655715	-0.014336
C	-4.497946	0.046135	0.104971
C	-4.077051	-1.375678	-0.091344
C	-1.102702	1.736601	-0.043980
C	0.227599	1.440894	-0.036843
C	-0.308861	-0.942271	0.019070
C	0.650486	0.029428	0.000239
C	1.257891	2.510766	-0.065028
C	2.641645	2.094068	-0.054976
C	2.093513	-0.304332	0.013239
C	3.054657	0.798530	-0.019165
C	2.568441	-1.579816	0.054971
C	3.980969	-1.912207	0.065627
C	4.468973	0.474793	-0.010169
C	4.913240	-0.794894	0.029315
C	-5.765612	0.401749	0.421474
C	0.977831	3.834480	-0.100035
C	4.407763	-3.198015	0.107639
C	-4.949580	-2.366261	-0.394295
H	-6.037852	1.445786	0.521420
H	-6.542118	-0.328588	0.607789
H	-4.609767	-3.390357	-0.493872
H	-6.000660	-2.177788	-0.569742
H	-3.768122	2.095513	0.042341
H	-2.347208	-2.694772	-0.044174
H	-1.428660	2.769320	-0.065966
H	-0.026471	-1.987469	0.039337
H	1.885659	-2.420156	0.082898

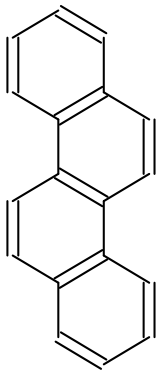
H	5.463520	-3.440913	0.115425
H	3.708731	-4.025430	0.134994
H	5.976061	-1.011380	0.035713
H	5.170525	1.302373	-0.036148
H	3.390305	2.879949	-0.077032
H	1.782039	4.559765	-0.119608
H	-0.027359	4.232032	-0.110084



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-848.0621767	-847.759603

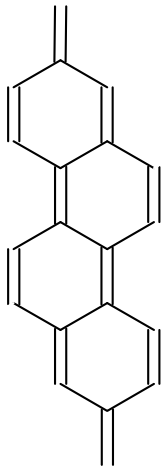
C	2.110151	0.992391	-0.003961
C	1.857050	-0.369467	0.079020
C	3.472894	1.472423	0.094250
C	2.981569	-1.301106	0.341225
C	4.531384	0.634032	0.095605
C	4.351813	-0.807485	0.028647
C	0.994029	1.922142	-0.226191
C	-0.372613	1.388607	-0.046351
C	0.526699	-0.863851	-0.041684
C	-0.575309	-0.039485	-0.126215
C	-1.459718	2.191243	0.215153
C	-2.767907	1.668553	0.318959
C	-1.946438	-0.555329	-0.214903
C	-3.045085	0.332364	0.131202
C	-2.231232	-1.828658	-0.661039
C	-3.566657	-2.323593	-0.706286
C	-4.416542	-0.218829	0.214122
C	-4.611792	-1.564600	-0.287537
C	5.368239	-1.623347	-0.314559
C	-5.467621	0.451262	0.757350
C	2.800142	-2.493821	0.936305
C	1.191436	3.192175	-0.658518
H	1.818982	-2.864563	1.202641
H	3.644456	-3.113014	1.211315
H	5.226799	-2.686513	-0.462018
H	6.365085	-1.229066	-0.476106
H	5.543468	1.023952	0.102476
H	3.645674	2.539935	0.141365
H	0.360107	3.834499	-0.916052
H	2.179086	3.603940	-0.809852
H	0.380846	-1.935338	-0.019850

H	-1.433049	-2.465679	-1.021753
H	-3.738904	-3.327905	-1.077355
H	-5.621230	-1.960495	-0.296066
H	-6.454559	0.005205	0.764785
H	-5.371166	1.426283	1.215613
H	-3.575783	2.360988	0.522705
H	-1.316757	3.254044	0.370595



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2h	0	-693.3390497	-693.098737

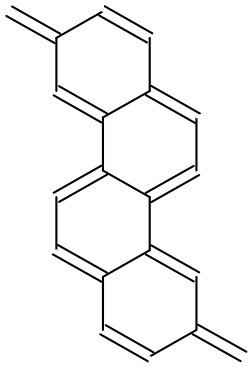
C	3.752217	-2.774206	0.000000
C	3.713493	-1.399134	0.000000
C	2.547615	-3.501820	0.000000
C	2.481042	-0.704855	0.000000
C	1.256077	-1.433432	0.000000
C	1.334362	-2.847717	0.000000
C	2.439121	0.719704	0.000000
C	1.256077	1.392025	0.000000
C	0.001002	0.707588	0.000000
C	-0.001002	-0.707588	0.000000
C	-2.481042	0.704855	0.000000
C	-1.256077	1.433432	0.000000
C	-3.752217	2.774206	0.000000
C	-3.713493	1.399134	0.000000
C	-2.547615	3.501820	0.000000
C	-1.334362	2.847717	0.000000
C	-2.439121	-0.719704	0.000000
C	-1.256077	-1.392025	0.000000
H	4.633256	-0.823412	0.000000
H	2.572740	-4.585741	0.000000
H	3.376341	1.266317	0.000000
H	-3.376341	-1.266317	0.000000
H	4.702150	-3.296465	0.000000
H	0.430255	-3.441450	0.000000
H	1.274711	2.473147	0.000000
H	-1.274711	-2.473147	0.000000
H	-4.633256	0.823412	0.000000
H	-4.702150	3.296465	0.000000
H	-2.572740	4.585741	0.000000
H	-0.430255	3.441450	0.000000



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
Cs	0	-770.6865876	-770.415818

C	0.720035	-2.478635	0.000000
C	1.434397	-1.214289	0.000000
C	1.399318	-3.672218	0.000000
C	2.876243	-1.294027	0.000000
C	2.836629	-3.747020	0.000000
C	3.536770	-2.475119	0.000000
C	-0.720034	-2.441481	0.000000
C	-1.398692	-1.273853	0.000000
C	0.726064	-0.003555	0.000000
C	-0.726058	0.003559	0.000000
C	1.398695	1.273859	0.000000
C	0.720035	2.441487	0.000000
C	-1.434393	1.214291	0.000000
C	-0.720034	2.478638	0.000000
C	-2.876239	1.294023	0.000000
C	-3.536769	2.475113	0.000000
C	-1.399322	3.672219	0.000000
C	-2.836633	3.747016	0.000000
C	3.504527	-4.935300	0.000000
C	-3.504535	4.935294	0.000000
H	2.974525	-5.880038	0.000000
H	4.587029	-4.972226	0.000000
H	4.621507	-2.489680	0.000000
H	3.458193	-0.382377	0.000000
H	0.836281	-4.600372	0.000000
H	-1.255605	-3.385014	0.000000
H	-2.479355	-1.302812	0.000000
H	-3.458183	0.382369	0.000000
H	-4.621507	2.489671	0.000000
H	-4.587038	4.972216	0.000000
H	-2.974537	5.880034	0.000000

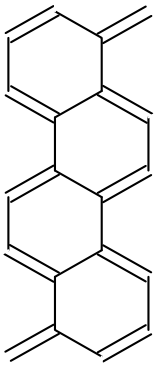
H	-0.836288	4.600375	0.000000
H	1.255605	3.385020	0.000000
H	2.479357	1.302822	0.000000



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-770.6769173	-770.406749

C	2.245535	1.308645	-0.096816
C	1.929568	-0.107354	-0.012169
C	3.625863	1.712541	-0.094685
C	2.968351	-0.999577	0.117587
C	4.631052	0.814701	0.008670
C	4.353780	-0.604496	0.131683
C	1.219756	2.231170	-0.163597
C	-0.126968	1.841182	-0.134411
C	0.513359	-0.510107	-0.056846
C	-0.513357	0.510124	-0.056836
C	0.126977	-1.841160	-0.134480
C	-1.219744	-2.231158	-0.163644
C	-1.929569	0.107364	-0.012173
C	-2.245526	-1.308641	-0.096807
C	-2.968366	0.999579	0.117549
C	-4.353790	0.604484	0.131672
C	-3.625851	-1.712551	-0.094642
C	-4.631047	-0.814720	0.008711
C	5.358399	-1.520775	0.258098
C	-5.358419	1.520754	0.258065
H	-6.398006	1.217321	0.268887
H	-5.148333	2.579309	0.350615
H	-2.769458	2.058822	0.226772
H	-0.878518	2.617897	-0.192881
H	1.462140	3.286489	-0.233068
H	3.842529	2.773000	-0.174562
H	5.665843	1.139715	0.009405
H	5.148301	-2.579323	0.350691
H	6.397990	-1.217353	0.268895
H	2.769426	-2.058812	0.226860
H	0.878531	-2.617864	-0.193011

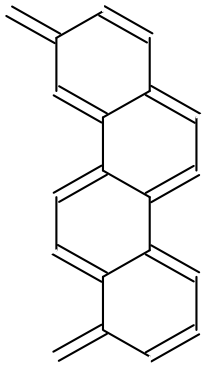
H	-1.462125	-3.286474	-0.233164
H	-3.842507	-2.773014	-0.174485
H	-5.665834	-1.139746	0.009481



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-770.6617248	-770.391853

C	-2.538931	0.586830	-0.018838
C	-1.811468	-0.659432	0.003189
C	-4.014259	0.578444	0.022357
C	-2.530781	-1.851299	-0.036129
C	-4.662797	-0.708398	-0.036845
C	-3.942907	-1.866727	-0.065375
C	-1.811784	1.767541	-0.113789
C	-0.421534	1.791606	-0.131704
C	-0.346807	-0.629308	0.034032
C	0.346786	0.629403	-0.034063
C	0.421440	-1.791471	0.132600
C	1.811693	-1.767438	0.115120
C	1.811474	0.659471	-0.003774
C	2.538893	-0.586817	0.019472
C	2.530877	1.851346	0.033596
C	3.943002	1.866758	0.062597
C	4.014240	-0.578543	-0.021461
C	4.662833	0.708356	0.035768
C	-4.780493	1.704674	0.132615
C	4.780503	-1.704958	-0.129653
H	-4.365990	2.698219	0.230477
H	-5.860479	1.627032	0.140017
H	-2.334859	2.712013	-0.196504
H	0.061513	2.754659	-0.229878
H	2.014604	2.801174	0.060290
H	4.455329	2.821794	0.101761
H	5.746760	0.732657	0.041305
H	5.860486	-1.627296	-0.137102
H	4.366055	-2.698701	-0.225700
H	2.334706	-2.711873	0.198621
H	-0.061693	-2.754412	0.231462

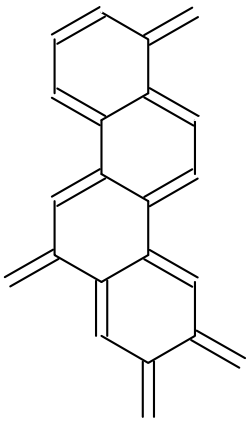
H	-2.014414	-2.801033	-0.064456
H	-4.455188	-2.821722	-0.106122
H	-5.746723	-0.732740	-0.042458



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-770.6690349	-770.398947

C	2.370016	1.221558	-0.151339
C	1.861416	-0.128895	-0.004424
C	3.791785	1.426200	-0.178129
C	2.765227	-1.155908	0.151395
C	4.662797	0.399604	-0.044954
C	4.191357	-0.959779	0.139502
C	1.479178	2.277259	-0.255892
C	0.096232	2.083471	-0.195652
C	0.403851	-0.329009	-0.020191
C	-0.469851	0.818673	-0.040547
C	-0.175379	-1.590434	-0.051697
C	-1.561687	-1.776841	-0.083602
C	-1.918304	0.621483	0.060432
C	-2.453878	-0.719042	-0.052695
C	-2.793685	1.668709	0.309120
C	-4.194982	1.468185	0.380936
C	-3.917758	-0.919285	-0.083603
C	-4.741836	0.236098	0.189380
C	5.059196	-2.004142	0.297629
C	-4.514010	-2.109947	-0.377072
H	4.702783	-3.017616	0.435508
H	6.131168	-1.850384	0.289541
H	2.418118	-2.170631	0.304339
H	0.451606	-2.472656	-0.076553
H	-1.935491	-2.793054	-0.109851
H	-5.593340	-2.196564	-0.360430
H	-3.960442	-2.996944	-0.652466
H	-5.816766	0.097892	0.220831
H	-4.834836	2.319002	0.587804
H	-2.411064	2.665257	0.486797
H	-0.545060	2.949084	-0.301199

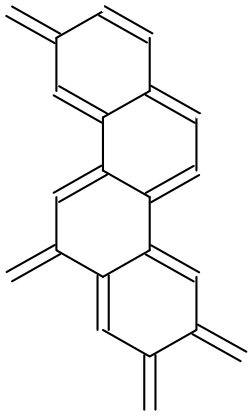
H	1.867085	3.282394	-0.385263
H	4.155286	2.441023	-0.304492
H	5.732834	0.575451	-0.066159



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-848.0591754	-847.756884

C	1.469991	-0.412737	-0.041730
C	2.086518	0.923972	-0.148609
C	2.266883	-1.489360	0.200889
C	3.436408	1.034841	-0.094003
C	3.707134	-1.411796	0.337974
C	4.335064	-0.100033	0.020540
C	0.008372	-0.537652	-0.122875
C	-0.802540	0.663165	0.015915
C	1.198945	2.104248	-0.302127
C	-0.218621	1.891521	-0.120629
C	-0.633785	-1.726763	-0.362939
C	-2.048330	-1.828127	-0.414170
C	-2.256249	0.508892	0.199952
C	-2.872295	-0.755538	-0.173876
C	-3.033987	1.488539	0.765339
C	-4.450987	1.336247	0.896951
C	-4.348663	-0.851344	-0.199510
C	-5.082154	0.228396	0.437704
C	5.657219	0.063597	-0.201493
C	4.401154	-2.480930	0.789805
C	1.643728	3.345747	-0.611366
C	-5.024982	-1.857255	-0.810530
H	5.463779	-2.440332	0.990587
H	3.901211	-3.422446	0.983906
H	6.351330	-0.766767	-0.209268
H	6.066588	1.046295	-0.403866
H	3.903654	2.009061	-0.173643
H	2.683853	3.569775	-0.804207
H	0.947857	4.172294	-0.687803
H	-0.847826	2.772738	-0.171058
H	-0.056816	-2.624748	-0.547021

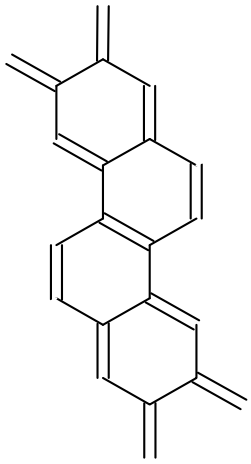
H	1.820248	-2.460231	0.378561
H	-2.479761	-2.802573	-0.610675
H	-4.529862	-2.636179	-1.375072
H	-6.106634	-1.896742	-0.767418
H	-6.160319	0.135542	0.508165
H	-5.019600	2.132231	1.364936
H	-2.570637	2.386289	1.156605



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-848.0685821	-847.766016

C	1.553969	-0.428031	-0.072739
C	2.003872	0.975669	-0.136003
C	2.467124	-1.401049	0.197589
C	3.325727	1.252721	-0.019733
C	3.878951	-1.147397	0.401429
C	4.352650	0.235899	0.122551
C	0.125064	-0.733256	-0.226455
C	-0.837518	0.355723	-0.101744
C	0.982806	2.037954	-0.312316
C	-0.403964	1.646718	-0.190083
C	-0.340544	-1.988029	-0.533812
C	-1.726360	-2.278313	-0.633016
C	-2.273271	0.017594	0.002442
C	-2.684914	-1.333802	-0.358766
C	-3.219716	0.903574	0.432638
C	-4.634103	0.595710	0.459380
C	-4.093910	-1.638787	-0.368212
C	-5.020673	-0.731922	0.009270
C	5.652607	0.563670	-0.040940
C	4.679753	-2.127250	0.878410
C	-5.552551	1.502540	0.887653
C	1.278341	3.329964	-0.588541
H	5.718469	-1.956523	1.129468
H	4.293098	-3.126035	1.043030
H	6.442971	-0.175646	-0.026023
H	5.946039	1.591840	-0.216885
H	3.670745	2.278739	-0.066321
H	2.136749	-2.422013	0.346670
H	2.288568	3.685748	-0.737554
H	0.487284	4.063776	-0.683567
H	-1.131671	2.448069	-0.244979

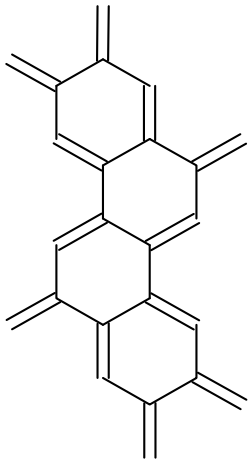
H	-2.924434	1.884999	0.786698
H	-5.257576	2.489106	1.224270
H	-6.609832	1.267478	0.905611
H	-6.075950	-0.982503	-0.000983
H	-4.393748	-2.634804	-0.678140
H	-2.032723	-3.284064	-0.901003
H	0.361973	-2.787562	-0.734312



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-848.0673503	-847.765179

C	1.900395	0.228631	0.001968
C	2.335788	-1.178435	-0.037411
C	2.859834	1.197452	0.091154
C	3.661871	-1.493002	-0.082489
C	4.279295	0.910207	0.160862
C	4.704975	-0.491523	-0.116913
C	0.461849	0.517901	-0.015666
C	-0.461872	-0.517924	-0.015680
C	1.320432	-2.200843	-0.055486
C	0.007505	-1.889653	-0.038795
C	-0.007515	1.889628	-0.038866
C	-1.320443	2.200829	-0.055461
C	-1.900409	-0.228644	0.001887
C	-2.335789	1.178415	-0.037308
C	-2.859869	-1.197476	0.090876
C	-4.279299	-0.910197	0.160822
C	-3.661882	1.493002	-0.082271
C	-4.704968	0.491539	-0.116909
C	5.144862	1.884263	0.526912
C	5.972098	-0.833181	-0.445775
C	-5.972045	0.833160	-0.446001
C	-5.144843	-1.884166	0.527172
H	6.196534	1.690349	0.693059
H	4.800538	2.898980	0.688628
H	6.753261	-0.096848	-0.582962
H	6.240402	-1.870709	-0.606300
H	3.958205	-2.534580	-0.156367
H	1.638751	-3.237402	-0.088174
H	-0.715568	-2.692868	-0.063719
H	-2.587013	-2.240057	0.185722
H	-4.800547	-2.898908	0.688810

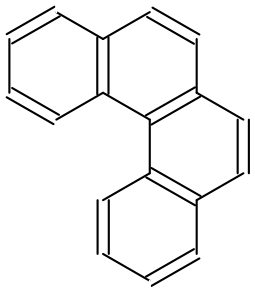
H	-6.196449	-1.690151	0.693630
H	-6.240369	1.870700	-0.606429
H	-6.753126	0.096789	-0.583455
H	-3.958197	2.534591	-0.156112
H	-1.638764	3.237382	-0.088248
H	0.715564	2.692832	-0.064006
H	2.586967	2.240011	0.186190



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-925.4661642	-925.131494

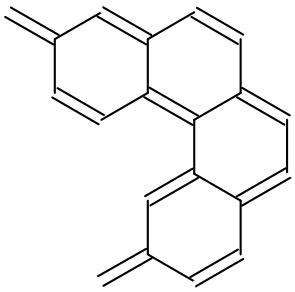
C	-1.888507	-0.343968	-0.008828
C	-2.430450	1.003983	-0.258673
C	-2.718383	-1.320101	0.443417
C	-3.763578	1.213044	-0.133368
C	-4.138896	-1.125897	0.666050
C	-4.713890	0.164847	0.196714
C	-0.444772	-0.581623	-0.189180
C	0.444816	0.581528	-0.189409
C	-1.482878	2.089861	-0.612680
C	-0.068758	1.814617	-0.430659
C	0.068831	-1.814766	-0.430113
C	1.482931	-2.089906	-0.612534
C	1.888540	0.343938	-0.008983
C	2.430512	-1.004013	-0.258668
C	2.718324	1.320108	0.443366
C	4.138811	1.125900	0.666148
C	3.763625	-1.213092	-0.133200
C	4.713884	-0.164799	0.196733
C	-1.863827	3.296095	-1.086654
C	1.863858	-3.295979	-1.086935
C	-4.854568	-2.066333	1.321430
C	-6.037093	0.378091	0.031474
C	6.037085	-0.377829	0.031290
C	4.854429	2.066225	1.321729
H	6.406059	-1.345544	-0.287568
H	6.773169	0.400655	0.184682
H	4.395219	3.000586	1.622203
H	5.894128	1.923986	1.586533
H	2.310919	2.283883	0.725605
H	0.603384	2.653972	-0.567365
H	-2.895726	3.551320	-1.286482

H	-1.125483	4.059397	-1.300695
H	-4.177150	2.198424	-0.312420
H	-6.773310	-0.400243	0.184987
H	-6.405951	1.345860	-0.287358
H	-5.894311	-1.924198	1.586123
H	-4.395356	-3.000706	1.621864
H	-2.311067	-2.283916	0.725652
H	-0.603252	-2.654225	-0.566456
H	1.125556	-4.059359	-1.300840
H	2.895726	-3.550949	-1.287257
H	4.177180	-2.198524	-0.312010



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2	0	-693.3295069	-693.088964

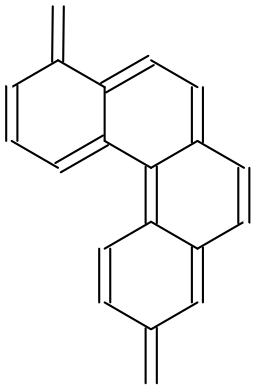
C	-0.412921	-2.391822	1.890066
C	-0.226284	-1.210510	2.534042
C	0.000000	0.000000	1.810123
C	0.000000	0.000000	0.394688
C	-0.255669	-2.473827	0.474621
C	0.019364	-1.288924	-0.279811
C	0.226284	1.210510	2.534042
C	0.412921	2.391822	1.890066
C	0.255669	2.473827	0.474621
C	-0.019364	1.288924	-0.279811
C	0.294766	3.730661	-0.173230
C	-0.396401	1.470137	-1.636137
C	-0.385096	2.712030	-2.235738
C	0.000000	3.853515	-1.511183
C	0.396401	-1.470137	-1.636137
C	0.385096	-2.712030	-2.235738
C	0.000000	-3.853515	-1.511183
C	-0.294766	-3.730661	-0.173230
H	-0.625499	-3.299688	2.444383
H	-0.268976	-1.159387	3.616827
H	0.268976	1.159387	3.616827
H	0.625499	3.299688	2.444383
H	0.534201	4.608056	0.418568
H	-0.756516	0.627863	-2.206779
H	-0.695585	2.808037	-3.270167
H	0.024158	4.824229	-1.993041
H	0.756516	-0.627863	-2.206779
H	0.695585	-2.808037	-3.270167
H	-0.024158	-4.824229	-1.993041
H	-0.534201	-4.608056	0.418568



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-770.6762464	-770.405414

C	-0.109001	2.155667	0.124296
C	-0.093745	0.711128	0.024789
C	1.121415	2.856983	0.377578
C	1.143151	0.059150	-0.091363
C	2.300484	2.202792	0.448125
C	2.376692	0.787384	0.183583
C	-1.289253	2.853786	-0.085269
C	-2.495302	2.194347	-0.369860
C	-1.400770	0.032181	0.016271
C	-2.584145	0.817104	-0.310974
C	-1.583307	-1.275812	0.399498
C	-2.858520	-1.951076	0.328695
C	-3.844367	0.135493	-0.454745
C	-3.981962	-1.178369	-0.169906
C	1.302424	-1.305892	-0.538639
C	2.505540	-1.925197	-0.571596
C	3.586188	0.135438	0.183944
C	3.723503	-1.257703	-0.150138
C	4.926300	-1.898813	-0.125719
C	-2.993659	-3.250805	0.717093
H	-3.948356	-3.759243	0.659317
H	-2.151594	-3.815805	1.097940
H	-4.942423	-1.671152	-0.274274
H	-4.701131	0.720835	-0.773223
H	-3.387183	2.774757	-0.581470
H	-1.266588	3.937928	-0.057315
H	1.075058	3.932495	0.512503
H	3.221182	2.735395	0.660889
H	4.483840	0.694177	0.430140
H	5.011753	-2.944617	-0.394404
H	5.834750	-1.382675	0.160247
H	2.582202	-2.938974	-0.950184
H	0.433886	-1.830240	-0.911661

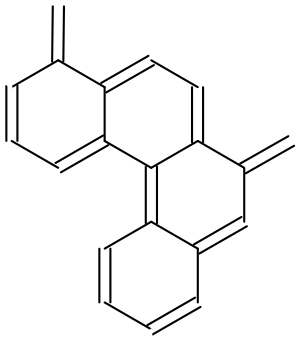
H	-0.755389	-1.839607	0.807515



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-770.6687872	-770.398174

C	0.224162	1.941200	-0.127891
C	0.043677	0.507468	-0.095987
C	1.495439	2.476557	0.009114
C	1.254128	-0.316003	-0.198698
C	2.622978	1.660827	0.188996
C	2.536323	0.283239	0.127101
C	-0.926001	2.795059	-0.266929
C	-2.176270	2.286361	-0.296739
C	-1.256699	-0.005725	0.052061
C	-2.405729	0.875069	-0.106088
C	-1.550167	-1.369021	0.425049
C	-2.815081	-1.847569	0.497378
C	-3.683468	0.369038	-0.064473
C	-3.966639	-1.016867	0.198512
C	1.253651	-1.596566	-0.725245
C	2.443088	-2.377137	-0.802053
C	3.725901	-0.583108	0.251357
C	3.623870	-1.910879	-0.317548
C	4.866907	-0.197624	0.882910
C	-5.238768	-1.508967	0.219878
H	1.615048	3.554629	-0.001923
H	3.591901	2.129292	0.314296
H	-0.759277	3.863825	-0.350511
H	-3.037691	2.933613	-0.422257
H	-0.728681	-2.015060	0.702762
H	-2.990067	-2.869646	0.816224
H	-4.520566	1.042758	-0.219393
H	0.344403	-2.004319	-1.144221
H	2.387524	-3.367825	-1.239624
H	4.512536	-2.532322	-0.326919
H	4.954968	0.748824	1.399747
H	5.729832	-0.851992	0.906144
H	-6.093177	-0.871144	0.028639

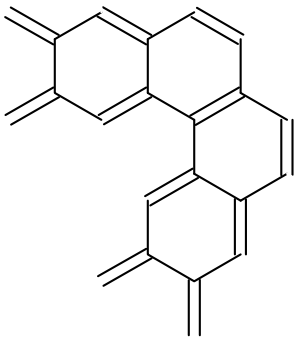
H	-5.434570	-2.552745	0.432805



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-770.6583814	-770.388038

C	0.342105	1.611415	0.036104
C	0.226207	0.180236	0.083902
C	-0.794377	2.358818	-0.242269
C	-1.116032	-0.382411	0.224243
C	-2.055799	1.771537	-0.387271
C	-2.255258	0.420296	-0.167785
C	1.661712	2.251093	0.229156
C	2.806828	1.392954	0.177617
C	1.395930	-0.608925	-0.073811
C	2.704037	0.031808	0.003038
C	1.378065	-1.998380	-0.410826
C	2.527628	-2.727097	-0.542881
C	3.885366	-0.787077	-0.090311
C	3.803739	-2.121383	-0.336220
C	-1.357521	-1.612744	0.825414
C	-2.668183	-2.148237	0.924783
C	-3.593777	-0.200810	-0.230832
C	-3.740701	-1.492771	0.400655
C	-4.657696	0.372630	-0.859004
C	1.817312	3.578948	0.503987
H	-0.703240	3.428505	-0.385250
H	-2.900072	2.409482	-0.619337
H	3.787363	1.840232	0.303846
H	0.428342	-2.473549	-0.612809
H	2.472978	-3.769584	-0.834992
H	4.848966	-0.301059	0.019711
H	4.702714	-2.721994	-0.416565
H	-0.540797	-2.154793	1.281111
H	-2.804429	-3.104870	1.417178
H	-4.730522	-1.934228	0.434527
H	-4.581911	1.299039	-1.412122
H	-5.628014	-0.108266	-0.840757
H	0.982224	4.249966	0.650627

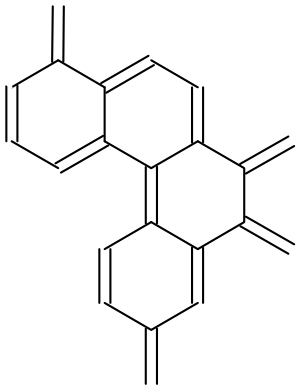
H	2.808865	4.001719	0.608701



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-848.0610511	-847.758677

C	0.000000	2.343569	0.000000
C	0.000000	0.954427	0.000000
C	-1.229154	3.087415	-0.170096
C	-1.293144	0.258590	0.058762
C	-2.417821	2.469505	-0.329255
C	-2.523497	1.037138	-0.207226
C	1.229153	3.087415	0.170096
C	2.417821	2.469505	0.329255
C	1.293144	0.258590	-0.058762
C	2.523497	1.037138	0.207226
C	1.445795	-1.038732	-0.465957
C	2.732958	-1.698659	-0.552451
C	3.735484	0.414135	0.279716
C	3.890378	-1.010295	0.083349
C	-1.445795	-1.038732	0.465957
C	-2.732958	-1.698659	0.552451
C	-3.735484	0.414135	-0.279717
C	-3.890377	-1.010295	-0.083350
C	-5.006123	-1.656997	-0.489580
C	2.859046	-2.859322	-1.236841
C	-2.859047	-2.859321	1.236844
C	5.006124	-1.656996	0.489579
H	-1.162662	4.169386	-0.212048
H	-3.322704	3.037992	-0.514724
H	1.162662	4.169386	0.212049
H	3.322703	3.037992	0.514725
H	0.595959	-1.594961	-0.835295
H	4.620013	0.997384	0.515140
H	-0.595959	-1.594960	0.835294
H	-4.620014	0.997384	-0.515141
H	-5.841378	-1.110624	-0.912016
H	-5.098483	-2.733991	-0.431799
H	3.822300	-3.321861	-1.409412

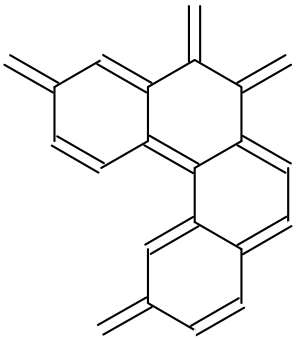
H	1.990444	-3.353997	-1.655579
H	-3.822301	-3.321859	1.409415
H	-1.990445	-3.353996	1.655581
H	5.841379	-1.110622	0.912013
H	5.098485	-2.733990	0.431797



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-848.0661026	-847.763177

C	-0.217489	1.663755	-0.082619
C	-0.211762	0.227197	0.021614
C	-1.421083	2.325873	-0.208231
C	-1.498073	-0.445439	0.202245
C	-2.648738	1.637505	-0.270601
C	-2.720547	0.271055	-0.116561
C	1.072447	2.387759	-0.097456
C	2.203313	1.648660	0.517615
C	1.013940	-0.466835	-0.117145
C	2.267665	0.221366	0.130160
C	1.105135	-1.835366	-0.549836
C	2.291338	-2.483256	-0.669987
C	3.455469	-0.441292	0.023546
C	3.545798	-1.834241	-0.352052
C	-1.610561	-1.691862	0.795927
C	-2.871546	-2.334179	0.955151
C	-4.002516	-0.464248	-0.143113
C	-4.016286	-1.765412	0.492402
C	-5.123479	0.013452	-0.745374
C	4.742468	-2.478709	-0.443456
C	1.247159	3.596193	-0.653578
C	3.054386	2.224428	1.376458
H	-1.430076	3.407239	-0.268249
H	-3.559713	2.212844	-0.385553
H	0.194611	-2.343685	-0.838233
H	2.318317	-3.500482	-1.045789
H	4.380919	0.093368	0.207270
H	-0.730608	-2.174413	1.198627
H	-2.904037	-3.303109	1.441056
H	-4.964758	-2.285421	0.569854
H	-5.132676	0.937150	-1.308737
H	-6.053248	-0.540059	-0.694632
H	5.674605	-1.970010	-0.229614

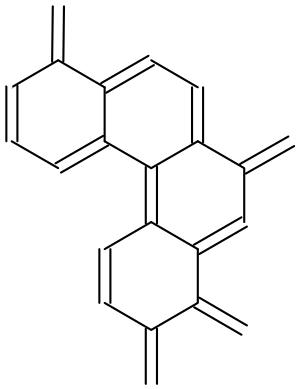
H	4.799682	-3.520004	-0.736327
H	2.948816	3.266054	1.653826
H	3.854943	1.664768	1.845042
H	2.222220	4.066831	-0.662296
H	0.438785	4.130493	-1.136905



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-848.0732593	-847.770184

C	0.026098	1.880076	-0.111450
C	-0.233011	0.460625	-0.071671
C	1.423831	2.354719	-0.011242
C	0.851652	-0.436050	-0.184197
C	2.357639	1.396210	0.631582
C	2.191815	-0.000329	0.170516
C	-1.020162	2.757109	-0.313185
C	-2.348004	2.313231	-0.475919
C	-1.633525	0.026154	0.003922
C	-2.679697	0.986448	-0.318968
C	-2.013477	-1.213870	0.463140
C	-3.386177	-1.661628	0.483999
C	-4.045761	0.528283	-0.363469
C	-4.387885	-0.726653	-0.000325
C	0.725292	-1.778145	-0.690235
C	1.780822	-2.624799	-0.778481
C	3.243898	-0.864467	0.099854
C	3.106794	-2.232859	-0.347357
C	4.168840	-3.082636	-0.399915
C	-3.720576	-2.901383	0.940622
C	1.857237	3.530587	-0.491288
C	3.236188	1.769485	1.570723
H	-0.819195	3.820173	-0.362103
H	-3.129869	3.038253	-0.676413
H	-1.269064	-1.894483	0.855349
H	-4.806389	1.237140	-0.674947
H	-5.422370	-1.050883	-0.032851
H	-0.237936	-2.096225	-1.065467
H	1.651057	-3.610393	-1.212595
H	4.235467	-0.518787	0.370758
H	5.160210	-2.765746	-0.099421
H	4.056619	-4.102837	-0.746396
H	-4.749686	-3.239251	0.949056

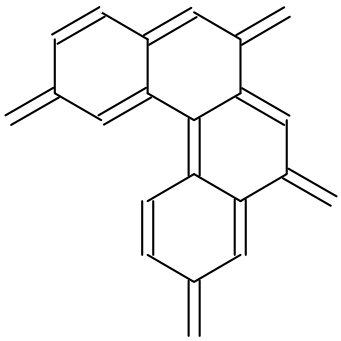
H	-2.968664	-3.587512	1.311087
H	1.199275	4.227531	-0.994949
H	2.900679	3.808838	-0.414697
H	3.300093	2.799990	1.897868
H	3.888790	1.053530	2.055801



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-848.0590085	-847.756242

C	0.383987	1.752388	-0.122880
C	0.289123	0.308818	-0.101962
C	1.603069	2.340795	0.141495
C	1.548973	-0.437382	-0.219536
C	2.772211	1.581706	0.347917
C	2.780828	0.213193	0.193237
C	-0.834304	2.544009	-0.373020
C	-2.092458	1.850887	-0.229818
C	-0.961843	-0.292981	0.090490
C	-2.175333	0.522555	0.047026
C	-1.128242	-1.696381	0.391291
C	-2.330906	-2.316334	0.366889
C	-3.489395	-0.130643	0.291575
C	-3.564319	-1.602330	0.078591
C	1.638308	-1.681473	-0.814146
C	2.875078	-2.390185	-0.887162
C	4.014216	-0.592203	0.316271
C	4.007987	-1.888679	-0.331742
C	5.106277	-0.182195	1.012733
C	-0.817266	3.844481	-0.761508
C	-4.534502	0.543436	0.797886
C	-4.684601	-2.240850	-0.307659
H	1.666850	3.419135	0.222828
H	3.696269	2.103364	0.567072
H	-2.996672	2.429221	-0.378867
H	-0.245176	-2.274996	0.626896
H	-2.394391	-3.382151	0.559674
H	0.767290	-2.114372	-1.286489
H	2.892241	-3.355723	-1.380577
H	4.930400	-2.458815	-0.339920
H	5.121600	0.736685	1.583847
H	6.003710	-0.788494	1.034317
H	0.099871	4.383369	-0.957912

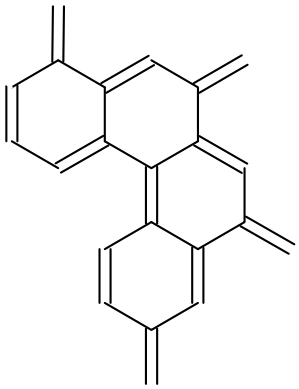
H	-1.744260	4.385604	-0.907438
H	-4.473993	1.597079	1.039440
H	-5.468886	0.043766	1.019306
H	-5.590879	-1.706305	-0.562620
H	-4.705312	-3.321162	-0.395358



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-848.0676416	-847.764739

C	-0.092317	1.836135	0.014004
C	-0.162215	0.369472	-0.025631
C	-1.290061	2.620206	-0.390875
C	-1.492639	-0.251420	0.033783
C	-2.529115	1.895188	-0.562367
C	-2.653754	0.558602	-0.351191
C	1.062658	2.441105	0.393130
C	2.270244	1.698863	0.681854
C	1.028229	-0.347479	-0.119102
C	2.302904	0.307613	0.173544
C	1.101927	-1.712562	-0.596515
C	2.274470	-2.364927	-0.759898
C	3.475555	-0.363494	-0.006435
C	3.544606	-1.735695	-0.454904
C	-1.715759	-1.503929	0.529614
C	-3.023215	-2.134307	0.547225
C	-3.946632	-0.095277	-0.422480
C	-4.128208	-1.362408	-0.005600
C	-1.257970	3.947916	-0.645822
C	3.276623	2.272628	1.380230
C	4.731411	-2.379511	-0.612253
C	-3.200935	-3.380911	1.048874
H	-3.405915	2.470227	-0.843729
H	1.098085	3.515432	0.526165
H	0.186487	-2.198093	-0.902801
H	2.283560	-3.370872	-1.166017
H	4.415289	0.143305	0.182763
H	-0.896195	-2.072436	0.949387
H	-4.783102	0.487462	-0.794693
H	-5.108434	-1.825023	-0.046504
H	-0.353885	4.538501	-0.588613
H	-2.161064	4.469721	-0.938639
H	3.209067	3.308153	1.691950

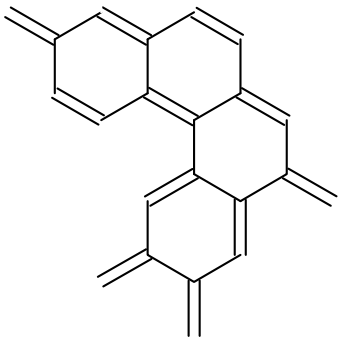
H	4.165749	1.730563	1.674179
H	5.672775	-1.887940	-0.398139
H	4.773923	-3.405311	-0.957900
H	-4.175913	-3.853406	1.051673
H	-2.375273	-3.945120	1.465821



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-848.0593714	-847.756659

C	-0.209545	1.663753	0.040409
C	-0.087105	0.203896	0.127353
C	-1.559907	2.260073	-0.154003
C	-1.318845	-0.570976	0.306682
C	-2.667250	1.346343	-0.356529
C	-2.575964	0.004694	-0.184088
C	0.904055	2.437095	0.120012
C	2.231640	1.894107	0.297002
C	1.171045	-0.380181	-0.002936
C	2.379861	0.442445	0.041541
C	1.364137	-1.787402	-0.285707
C	2.586040	-2.337363	-0.460858
C	3.602659	-0.129054	-0.153087
C	3.795333	-1.542528	-0.380631
C	-1.390090	-1.738777	1.016800
C	-2.622296	-2.469632	1.154012
C	-3.754289	-0.886433	-0.319113
C	-3.746247	-2.083608	0.506995
C	-4.771748	-0.632208	-1.171485
C	-1.807925	3.588648	-0.153649
C	3.241668	2.704655	0.691879
C	5.033150	-2.079633	-0.547800
H	-3.633015	1.788979	-0.574326
H	0.822343	3.516394	0.090415
H	0.489111	-2.406716	-0.418492
H	2.677448	-3.390083	-0.706589
H	4.489666	0.494222	-0.154984
H	-0.511608	-2.116991	1.522682
H	-2.623643	-3.368809	1.760116
H	-4.651168	-2.679376	0.554620
H	-4.745884	0.197192	-1.866750
H	-5.645148	-1.273300	-1.198699
H	3.072253	3.766118	0.827119

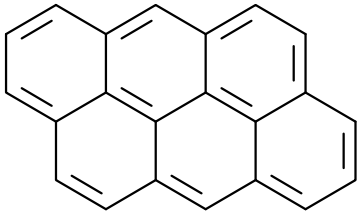
H	4.235988	2.338474	0.910003
H	5.924952	-1.465946	-0.506182
H	5.167429	-3.139271	-0.728646
H	-1.045874	4.336721	0.016050
H	-2.813095	3.954909	-0.323137



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-848.0687765	-847.765897

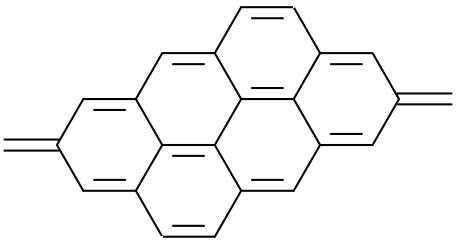
C	0.281627	2.076654	0.331580
C	0.316811	0.634746	0.103931
C	1.515273	2.754887	0.667144
C	1.544784	0.012350	-0.088629
C	2.697303	2.111123	0.637816
C	2.784894	0.729672	0.216741
C	-0.869245	2.786646	0.138414
C	-2.108915	2.197567	-0.313887
C	-0.984066	-0.051816	0.097531
C	-2.211552	0.721786	-0.195347
C	1.704777	-1.322657	-0.632146
C	2.911906	-1.916618	-0.756629
C	3.995192	0.101980	0.120251
C	4.139814	-1.259793	-0.339449
C	-1.117917	-1.349948	0.492072
C	-2.385588	-2.052004	0.531489
C	-3.401419	0.077166	-0.265905
C	-3.548305	-1.356119	-0.080882
C	-4.675087	-1.986905	-0.473055
C	-2.478144	-3.250479	1.149851
C	-3.090993	2.989506	-0.802368
C	5.348018	-1.876316	-0.414490
H	1.460826	3.806423	0.928275
H	3.617377	2.626263	0.892857
H	-0.838531	3.867007	0.238914
H	0.826733	-1.834492	-1.000656
H	2.987188	-2.902039	-1.204324
H	4.894574	0.647218	0.389870
H	-0.258563	-1.886128	0.872286
H	-4.307208	0.633913	-0.475089
H	-5.508198	-1.429186	-0.884582
H	-4.783995	-3.062383	-0.415830
H	-2.967612	4.065520	-0.822707

H	-4.014889	2.598984	-1.206873
H	6.259345	-1.370324	-0.119171
H	5.438842	-2.894652	-0.772666
H	-3.423173	-3.762586	1.276834
H	-1.597721	-3.732105	1.558665



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2h	0	-845,827725	-845,562234

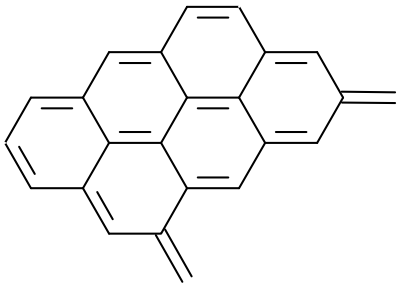
C	-1.254353	1.418741	0.000000
C	-0.002043	0.707568	0.000000
C	0.002043	-0.707568	0.000000
C	-1.223044	-1.421537	0.000000
C	-2.463446	-0.708609	0.000000
C	-2.440797	0.706963	0.000000
C	1.254353	-1.418741	0.000000
C	1.217563	-2.859783	0.000000
C	0.044529	-3.537625	0.000000
C	-1.223188	-2.851108	0.000000
C	-3.670171	-1.446737	0.000000
C	-3.653751	-2.828075	0.000000
C	-2.440797	-3.529767	0.000000
C	1.223044	1.421537	0.000000
C	2.463446	0.708609	0.000000
C	2.440797	-0.706963	0.000000
C	-1.217563	2.859783	0.000000
H	0.038695	-4.622622	0.000000
H	2.160915	-3.395770	0.000000
H	-3.384202	1.244162	0.000000
H	-2.443699	-4.614553	0.000000
H	-4.613329	-0.910935	0.000000
H	3.384202	-1.244162	0.000000
C	1.223188	2.851108	0.000000
H	-4.588332	-3.377811	0.000000
C	3.670171	1.446737	0.000000
C	3.653751	2.828075	0.000000
H	4.613329	0.910935	0.000000
H	4.588332	3.377811	0.000000
C	2.440797	3.529767	0.000000
C	-0.044529	3.537625	0.000000
H	-2.160915	3.395770	0.000000
H	-0.038695	4.622622	0.000000
H	2.443699	4.614553	0.000000



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2h	0	-923,16893	-922,873318

C	1.906952	0.002024	0.000000
C	1.099609	2.321089	0.000000
C	2.155036	1.348465	0.000000
C	-0.537130	0.480352	0.000000
C	0.537130	-0.480352	0.000000
C	0.269333	-1.840140	0.000000
C	-1.099609	-2.321089	0.000000
C	-0.269333	1.840140	0.000000
C	2.968860	-0.981137	0.000000
C	2.706484	-2.305342	0.000000
C	1.348254	-2.809403	0.000000
C	1.066386	-4.148226	0.000000
C	-0.289484	-4.652243	0.000000
C	-1.348254	-3.673558	0.000000
C	1.348254	3.673558	0.000000
H	3.993196	-0.623266	0.000000
H	3.516744	-3.026879	0.000000
H	1.879478	-4.867215	0.000000
H	2.374273	4.027421	0.000000
H	3.180681	1.704393	0.000000
C	-1.906952	-0.002024	0.000000
C	-2.155036	-1.348465	0.000000
C	-1.348254	2.809403	0.000000
C	0.289484	4.652243	0.000000
C	-2.968860	0.981137	0.000000
C	-2.706484	2.305342	0.000000
C	-1.066386	4.148226	0.000000
H	-1.879478	4.867215	0.000000
H	-3.516744	3.026879	0.000000
H	-3.993196	0.623266	0.000000
H	-3.180681	-1.704393	0.000000
H	-2.374273	-4.027421	0.000000
C	0.551900	5.993407	0.000000
C	-0.551900	-5.993407	0.000000
H	1.568097	6.367952	0.000000

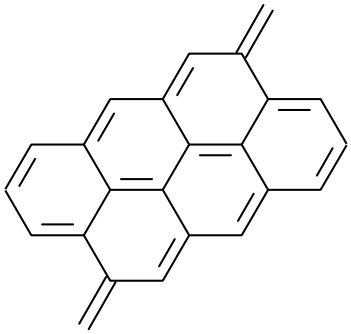
H	-0.248304	6.723201	0.000000
H	0.248304	-6.723201	0.000000
H	-1.568097	-6.367952	0.000000



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
Cs	0	-923,162172	-922,866912

C	1.451114	0.907278	0.000000
C	1.635434	-1.547166	0.000000
C	2.204956	-0.232376	0.000000
C	-0.594908	-0.521163	0.000000
C	0.000000	0.787190	0.000000
C	-0.812375	1.919875	0.000000
C	-2.250383	1.792753	0.000000
C	0.198670	-1.665122	0.000000
C	2.053928	2.269045	0.000000
C	1.150202	3.385369	0.000000
C	-0.220385	3.248505	0.000000
C	-1.093381	4.383214	0.000000
C	-2.454591	4.226488	0.000000
C	-3.036839	2.939887	0.000000
C	2.420155	-2.681507	0.000000
H	1.580087	4.381560	0.000000
H	-0.652605	5.374044	0.000000
H	-3.098753	5.098715	0.000000
H	3.500910	-2.582897	0.000000
H	3.286845	-0.170003	0.000000
C	-2.039000	-0.643154	0.000000
C	-2.818674	0.485943	0.000000
C	-0.391957	-2.986267	0.000000
C	1.854302	-4.004448	0.000000
C	-2.610825	-1.971392	0.000000
C	-1.836365	-3.077589	0.000000
C	0.412767	-4.096065	0.000000
H	-0.037760	-5.083466	0.000000
H	-2.285689	-4.065067	0.000000
H	-3.692430	-2.057741	0.000000
H	-3.900121	0.391603	0.000000
H	-4.116715	2.839614	0.000000
C	2.644629	-5.123995	0.000000
H	3.724950	-5.049582	0.000000
H	2.213046	-6.117116	0.000000

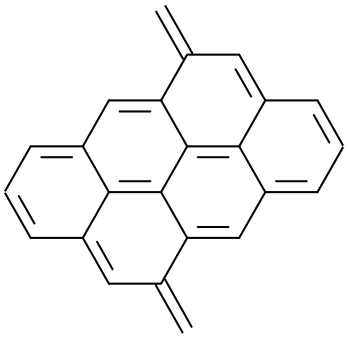
C	3.395629	2.504749	0.000000
H	3.768065	3.521513	0.000000
H	4.137555	1.718502	0.000000



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2h	0	-923,153404	-922,858587

C	1.779802	-0.640898	0.000000
C	1.823139	1.817882	0.000000
C	2.478478	0.569022	0.000000
C	-0.332919	0.608532	0.000000
C	0.332919	-0.608532	0.000000
C	-0.390422	-1.858322	0.000000
C	-1.823139	-1.817882	0.000000
C	0.390422	1.858322	0.000000
C	2.432462	-1.881444	0.000000
C	1.757853	-3.129604	0.000000
C	0.278696	-3.103656	0.000000
C	-0.477303	-4.279979	0.000000
C	-1.875935	-4.241767	0.000000
C	-2.543868	-3.034764	0.000000
C	2.543868	3.034764	0.000000
H	3.517789	-1.891711	0.000000
H	0.015744	-5.242266	0.000000
H	-2.434496	-5.171055	0.000000
H	3.628004	3.003565	0.000000
H	3.563672	0.549961	0.000000
C	-1.779802	0.640898	0.000000
C	-2.478478	-0.569022	0.000000
C	-0.278696	3.103656	0.000000
C	1.875935	4.241767	0.000000
C	-2.432462	1.881444	0.000000
C	-1.757853	3.129604	0.000000
C	0.477303	4.279979	0.000000
H	2.434496	5.171055	0.000000
H	-0.015744	5.242266	0.000000
H	-3.517789	1.891711	0.000000
H	-3.563672	-0.549961	0.000000
H	-3.628004	-3.003565	0.000000
C	-2.478478	4.295746	0.000000
C	2.478478	-4.295746	0.000000
H	-2.021760	5.274064	0.000000

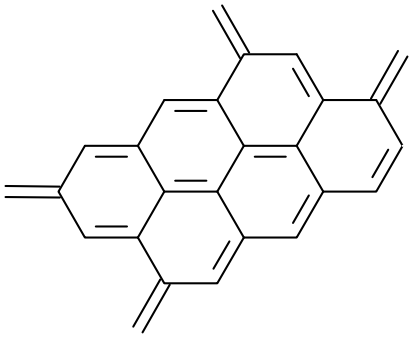
H	-3.561007	4.264310	0.000000
H	3.561007	-4.264310	0.000000
H	2.021760	-5.274064	0.000000



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
Ci	0	-923,158517	-922,863421

C	1.825684	-0.563151	0.033009
C	1.724716	1.884785	0.021110
C	2.444947	0.658742	0.038259
C	-0.375192	0.609974	-0.008798
C	0.375192	-0.609974	0.008798
C	-0.294254	-1.843209	0.002749
C	-1.724716	-1.884785	-0.021110
C	0.294254	1.843209	-0.002749
C	2.589359	-1.839593	0.051115
C	1.833552	-3.054656	0.043804
C	0.450859	-3.086044	0.020574
C	-0.276978	-4.312834	0.013646
C	-1.652673	-4.322285	-0.009438
C	-2.379801	-3.120613	-0.026757
C	2.379801	3.120613	0.026757
H	2.380864	-3.991398	0.057251
H	0.278321	-5.244325	0.027069
H	-2.185273	-5.266748	-0.014291
H	3.463783	3.144090	0.044575
H	3.526202	0.722933	0.055893
C	-1.825684	0.563151	-0.033009
C	-2.444947	-0.658742	-0.038259
C	-0.450859	3.086044	-0.020574
C	1.652673	4.322285	0.009438
C	-2.589359	1.839593	-0.051115
C	-1.833552	3.054656	-0.043804
C	0.276978	4.312834	-0.013646
H	2.185273	5.266748	0.014291
H	-0.278321	5.244325	-0.027069
H	-2.380864	3.991398	-0.057251
H	-3.526202	-0.722933	-0.055893
H	-3.463783	-3.144090	-0.044575
C	-3.953380	1.904084	-0.074289
C	3.953380	-1.904084	0.074289

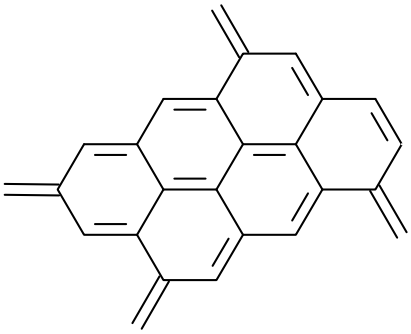
H	-4.590581	1.031228	-0.081148
H	-4.450169	2.866071	-0.086926
H	4.450169	-2.866071	0.086926
H	4.590581	-1.031228	0.081148



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-1000,553358	-1000,226065

C	0.387371	-2.000899	0.055138
C	-2.050816	-1.789981	-0.007113
C	-0.925187	-2.566485	0.027172
C	-0.689990	0.257472	0.071307
C	0.507335	-0.546082	0.058934
C	1.765032	0.037796	0.025822
C	1.885368	1.476761	-0.041791
C	-1.945047	-0.343128	0.007758
C	1.512007	-2.784221	0.090876
C	2.845890	-2.243426	0.147335
C	2.976903	-0.767574	0.007045
C	4.180604	-0.147823	-0.158014
C	4.326781	1.288538	-0.249860
C	3.122545	2.066530	-0.166610
C	-3.369110	-2.389457	-0.046844
H	1.403900	-3.863610	0.117513
H	5.087197	-0.737038	-0.233240
H	-3.428737	-3.472605	-0.021455
H	-1.020462	-3.647633	0.029607
C	-0.557285	1.703260	0.118854
C	0.685750	2.258203	0.024566
C	-3.153918	0.473354	-0.037946
C	-4.490550	-1.651243	-0.131110
C	-1.788626	2.515409	0.255854
C	-3.047300	1.823419	0.096366
C	-4.473430	-0.196123	-0.199968
H	-5.459271	-2.136926	-0.180448
H	-3.939883	2.435609	0.133495
H	0.797798	3.335806	-0.011297
H	3.197999	3.148050	-0.213106
C	-5.627955	0.463111	-0.432095
C	-1.791508	3.838110	0.553763
C	5.557510	1.864711	-0.406020
C	3.897187	-3.077862	0.356114
H	-6.558353	-0.083266	-0.529489

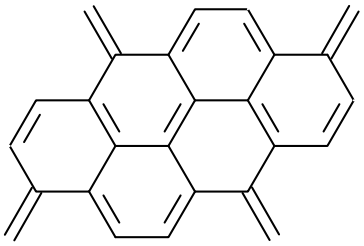
H	-5.684980	1.537148	-0.546096
H	-0.887848	4.398277	0.752657
H	-2.725574	4.382533	0.619611
H	3.739920	-4.147081	0.427818
H	4.913064	-2.726960	0.476349
H	6.456436	1.263856	-0.466175
H	5.671421	2.939631	-0.472934



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-1000,554078	-1000,227054

C	0.021373	-1.841240	0.006499
C	-2.368500	-1.285513	-0.023977
C	-1.358318	-2.207829	-0.016855
C	-0.700649	0.544367	0.018873
C	0.363633	-0.425606	0.017075
C	1.697529	-0.042786	0.014163
C	2.034148	1.360937	-0.011610
C	-2.030827	0.126506	-0.004986
C	1.013112	-2.790631	0.027180
C	2.414496	-2.467259	0.074930
C	2.773000	-1.023079	0.011428
C	4.063501	-0.585591	-0.059159
C	4.427423	0.813440	-0.091877
C	3.350660	1.761486	-0.056405
C	-3.799107	-1.694719	-0.050730
H	0.738432	-3.840315	0.034381
H	4.877557	-1.299935	-0.097331
H	-1.583453	-3.266987	-0.029075
C	-0.354175	1.958530	0.034194
C	0.963182	2.312332	0.006135
C	-3.092015	1.125954	-0.018310
C	-4.793199	-0.630626	-0.072344
C	-1.446204	2.965292	0.069276
C	-2.795647	2.454117	0.012068
C	-4.467109	0.673993	-0.057634
H	-5.835418	-0.930263	-0.098957
H	-5.243580	1.431760	-0.072352
H	-3.605145	3.176907	0.009909
H	1.243815	3.358859	-0.010661
H	3.588325	2.820132	-0.072820
C	-4.218290	-2.977852	-0.054972
C	3.322994	-3.471280	0.196590
C	5.739017	1.199948	-0.153539
C	-1.248380	4.302384	0.164774
H	-3.547045	-3.825410	-0.036604

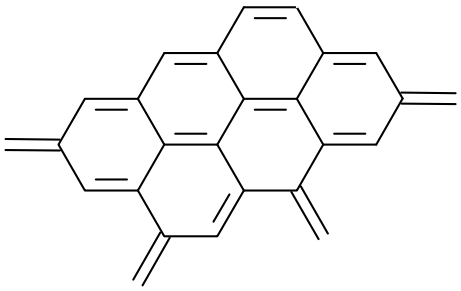
H	-5.277451	-3.204186	-0.076420
H	2.994098	-4.502739	0.224425
H	4.387321	-3.300039	0.280731
H	6.539630	0.471261	-0.179150
H	6.016762	2.246455	-0.177125
H	-0.268964	4.754778	0.238245
H	-2.094774	4.978056	0.178084



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2	0	-1000,552437	-1000,224756

C	-1.845273	0.336663	0.133493
C	-1.457978	-2.134520	0.074467
C	-2.364460	-1.026913	0.366756
C	0.447132	-0.557864	0.123967
C	-0.447132	0.557864	0.123967
C	0.069087	1.897893	0.003679
C	1.457978	2.134520	0.074467
C	-0.069087	-1.897893	0.003679
C	-2.695767	1.416410	-0.091484
C	-2.205416	2.710961	-0.239587
C	-0.846340	2.994747	-0.176825
C	-0.326040	4.369798	-0.304804
C	1.110177	4.518390	-0.295307
C	1.944008	3.463042	-0.106629
C	-1.944008	-3.463042	-0.106629
H	-3.761634	1.246557	-0.181543
H	-2.914048	3.508901	-0.421352
H	1.516969	5.512797	-0.442004
H	-3.014136	-3.628420	-0.119987
C	1.845273	-0.336663	0.133493
C	2.364460	1.026913	0.366756
C	0.846340	-2.994747	-0.176825
C	-1.110177	-4.518390	-0.295307
C	2.695767	-1.416410	-0.091484
C	2.205416	-2.710961	-0.239587
C	0.326040	-4.369798	-0.304804
H	-1.516969	-5.512797	-0.442004
H	2.914048	-3.508901	-0.421352
H	3.761634	-1.246557	-0.181543
H	3.014136	3.628420	-0.119987
C	1.110177	-5.477032	-0.425605
C	-3.594042	-1.223735	0.904808
C	-1.110177	5.477032	-0.425605
C	3.594042	1.223735	0.904808
H	0.656197	-6.455000	-0.526705
H	2.190710	-5.444480	-0.420588

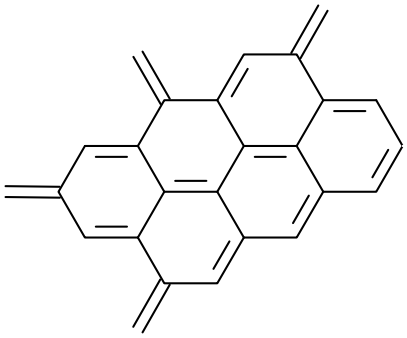
H	-4.219435	-0.392669	1.201531
H	-3.979008	-2.213226	1.109071
H	-2.190710	5.444480	-0.420588
H	-0.656197	6.455000	-0.526705
H	3.979008	2.213226	1.109071
H	4.219435	0.392669	1.201531



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-1000,558027	-1000,230124

C	-0.082865	1.634674	0.121741
C	2.350438	0.959727	0.120668
C	1.321314	1.977806	0.443835
C	0.585467	-0.781188	0.096221
C	-0.452045	0.220515	0.076551
C	-1.785643	-0.141337	-0.008999
C	-2.168344	-1.541283	0.050157
C	1.931750	-0.427378	0.063675
C	-1.025954	2.581255	-0.107452
C	-2.423730	2.269997	-0.339749
C	-2.834817	0.859292	-0.129189
C	-4.139464	0.473405	-0.053434
C	-4.546838	-0.911756	0.060895
C	-3.495663	-1.893999	0.080453
C	3.659063	1.282027	-0.074428
H	-0.737888	3.624733	-0.163630
H	-4.926829	1.217930	-0.081868
H	3.961680	2.322872	-0.089424
C	0.199382	-2.181264	0.075938
C	-1.125328	-2.523418	0.078871
C	2.956687	-1.448415	-0.057220
C	4.691454	0.283382	-0.261634
C	1.243479	-3.181482	0.043321
C	2.544554	-2.836310	-0.030619
C	4.270251	-1.094562	-0.208332
H	5.024374	-1.868577	-0.309205
H	3.316706	-3.596676	-0.080112
H	0.948187	-4.225328	0.056409
H	-1.408124	-3.571395	0.089299
H	-3.768680	-2.943013	0.133288
C	5.993588	0.632430	-0.463769
C	1.632601	3.107622	1.102301
C	-3.262608	3.243416	-0.761957
C	-5.865013	-1.259043	0.133797
H	6.299148	1.670861	-0.501852

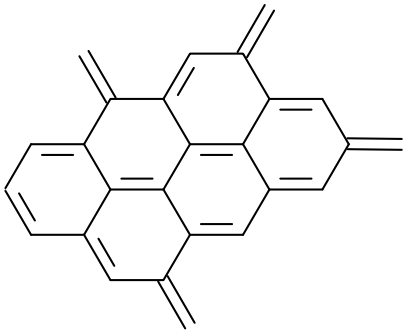
H	6.763999	-0.117923	-0.592955
H	0.870641	3.814124	1.405389
H	2.650443	3.335317	1.391046
H	-2.908850	4.260830	-0.877745
H	-4.297650	3.056213	-1.015079
H	-6.646534	-0.509493	0.115359
H	-6.170908	-2.295157	0.211223



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-1000,547243	-1000,219712

C	0.188117	2.080882	0.060948
C	-2.251776	1.861907	-0.022347
C	-1.115891	2.645275	0.017421
C	-0.870304	-0.178079	0.106801
C	0.315705	0.625850	0.126893
C	1.587642	0.041929	0.106346
C	1.746269	-1.393839	0.132438
C	-2.131307	0.413039	-0.017088
C	1.315532	2.876172	0.073876
C	2.642126	2.336318	0.136259
C	2.773740	0.864929	-0.028825
C	3.963728	0.273846	-0.349251
C	4.120038	-1.156077	-0.452874
C	2.954869	-1.955360	-0.156337
C	-3.560636	2.443779	-0.060511
H	1.201024	3.954887	0.091061
H	4.831198	0.889038	-0.559675
H	-3.646264	3.524935	-0.052852
H	-1.212734	3.725977	0.009647
C	-0.760628	-1.627870	0.200153
C	0.566002	-2.206106	0.511243
C	-3.327716	-0.390661	-0.121124
C	-4.670322	1.654328	-0.095345
C	-1.859655	-2.401272	0.010549
C	-3.182182	-1.860521	-0.228126
C	-4.552206	0.238372	-0.125808
H	-5.658634	2.099809	-0.106987
H	-5.460200	-0.351305	-0.154577
H	-1.759635	-3.480508	-0.004074
H	3.056111	-3.034109	-0.187140
C	-4.191855	-2.701128	-0.560562
C	0.697217	-3.356416	1.193368
C	5.313227	-1.719381	-0.804084
C	3.702702	3.151424	0.389341
H	-5.188087	-2.358002	-0.804766

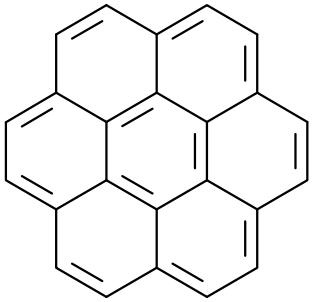
H	-4.021431	-3.769825	-0.606446
H	1.670204	-3.746675	1.462799
H	-0.165136	-3.915090	1.533801
H	6.182311	-1.109250	-1.017237
H	5.428758	-2.793725	-0.878274
H	3.565888	4.223655	0.459578
H	4.702009	2.772162	0.555020



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-1000,548171	-1000,220628

C	-0.604909	1.920807	0.088301
C	1.815589	1.507913	0.005607
C	0.681085	2.379408	0.028651
C	0.282989	-0.404511	0.088215
C	-0.841696	0.488578	0.091048
C	-2.148957	-0.011850	-0.016279
C	-2.418744	-1.424160	0.032812
C	1.580632	0.080859	0.000009
C	-1.769640	2.842461	0.119400
C	-3.055319	2.264129	-0.155536
C	-3.259901	0.905680	-0.221983
C	-4.566133	0.358601	-0.473757
C	-4.762993	-0.986416	-0.499711
C	-3.685972	-1.882399	-0.235929
C	3.100316	2.003420	-0.006709
H	-3.902703	2.933340	-0.261599
H	-5.386918	1.045979	-0.646698
H	-5.746282	-1.392429	-0.708669
H	3.258935	3.076869	0.004027
H	0.874587	3.444587	-0.023130
C	0.057026	-1.848972	0.147463
C	-1.315210	-2.329172	0.421691
C	2.725842	-0.809382	-0.093367
C	4.246752	1.138418	-0.012219
C	1.095489	-2.700681	-0.034463
C	2.463919	-2.263996	-0.234977
C	3.983986	-0.284024	-0.062948
H	4.845818	-0.940943	-0.083253
H	0.911490	-3.768253	-0.072035
H	-3.877143	-2.948509	-0.252146
C	5.524243	1.625419	0.017837
C	3.407178	-3.174521	-0.567757
C	-1.673860	4.166492	0.417588
C	-1.543033	-3.478465	1.081930
H	4.432737	-2.907867	-0.785237

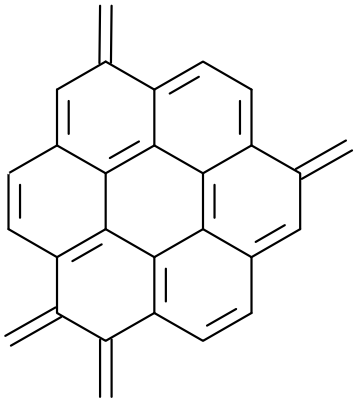
H	3.152622	-4.224899	-0.641005
H	5.719519	2.690235	0.047467
H	6.379960	0.961750	0.012698
H	-2.553220	4.798108	0.388758
H	-0.745814	4.635811	0.714462
H	-2.545958	-3.804968	1.324325
H	-0.729689	-4.100615	1.432540



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
D2h	0	-922,093109	-921,814536

C	0.000000	2.844330	0.000000
C	0.000000	-2.844330	0.000000
C	0.000000	1.425334	0.000000
C	0.000000	-1.425334	0.000000
C	1.246654	3.528636	0.000000
C	-1.246654	-3.528636	0.000000
C	-1.246654	3.528636	0.000000
C	1.246654	-3.528636	0.000000
C	1.234375	0.712667	0.000000
C	-1.234375	-0.712667	0.000000
C	-1.234375	0.712667	0.000000
C	1.234375	-0.712667	0.000000
C	-2.432561	-2.843952	0.000000
C	2.432561	2.843952	0.000000
C	-2.432561	2.843952	0.000000
C	2.432561	-2.843952	0.000000
C	2.463262	-1.422165	0.000000
C	2.463262	1.422165	0.000000
C	-2.463262	-1.422165	0.000000
C	-2.463262	1.422165	0.000000
C	-3.679215	0.684684	0.000000
C	3.679215	-0.684684	0.000000
C	3.679215	0.684684	0.000000
C	-3.679215	-0.684684	0.000000
H	-1.244167	-4.613536	0.000000
H	1.244167	4.613536	0.000000
H	1.244167	-4.613536	0.000000
H	-1.244167	4.613536	0.000000
H	-4.617523	-1.229288	0.000000
H	4.617523	1.229288	0.000000
H	-4.617523	1.229288	0.000000
H	4.617523	-1.229288	0.000000
H	-3.373356	3.384248	0.000000
H	3.373356	-3.384248	0.000000

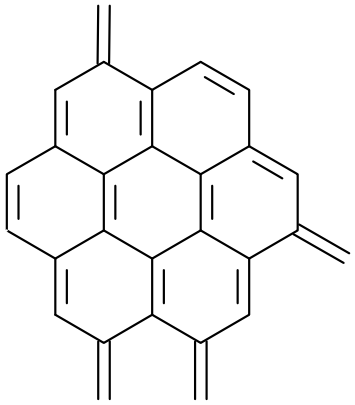
H	-3.373356	-3.384248	0.000000
H	3.373356	3.384248	0.000000



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2	0	-1076,801131	-1076,460988

C	-0.000384	1.423880	-0.089087
C	0.013083	0.718355	-1.324677
C	-0.013083	-0.718355	-1.324677
C	0.000384	-1.423880	-0.089087
C	0.019150	-0.727635	1.149315
C	-0.019150	0.727635	1.149315
C	0.034339	1.431710	-2.563262
C	0.015960	0.694172	-3.742935
C	-0.015960	-0.694172	-3.742935
C	-0.034339	-1.431710	-2.563262
C	-0.070804	-2.910295	-2.565545
C	-0.022553	-3.558571	-1.294911
C	0.019150	-2.867288	-0.096726
C	0.078191	-3.549843	1.155579
C	0.144714	-2.859111	2.331510
C	0.125665	-1.441452	2.359020
C	0.260188	-0.695876	3.616142
C	-0.260188	0.695876	3.616142
C	-0.125665	1.441452	2.359020
C	-0.019150	2.867288	-0.096726
C	0.022553	3.558571	-1.294911
C	0.070804	2.910295	-2.565545
C	-0.078191	3.549843	1.155579
C	-0.144714	2.859111	2.331510
C	-0.148747	-3.666127	-3.704673
C	0.884088	-1.197619	4.700293
C	-0.884088	1.197619	4.700293
C	0.148747	3.666127	-3.704673
H	-0.203190	-3.242885	-4.697358
H	-0.165118	-4.746585	-3.636913
H	1.268558	-2.209196	4.727042
H	1.056072	-0.583976	5.575303

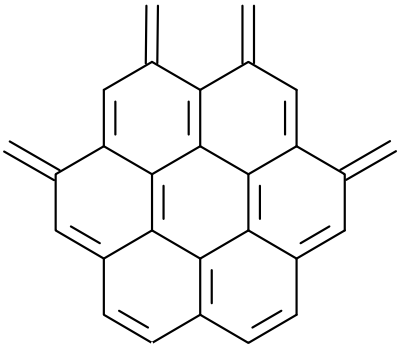
H	-1.056072	0.583976	5.575303
H	-1.268558	2.209196	4.727042
H	0.165118	4.746585	-3.636913
H	0.203190	3.242885	-4.697358
H	0.022900	1.204522	-4.697333
H	-0.022900	-1.204522	-4.697333
H	-0.023263	-4.643280	-1.275041
H	0.068939	-4.634302	1.155734
H	0.180912	-3.401533	3.268307
H	-0.180912	3.401533	3.268307
H	-0.068939	4.634302	1.155734
H	0.023263	4.643280	-1.275041



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-1076,794599	-1076,454117

C	1.640649	0.309816	0.014449
C	0.594335	1.303332	-0.004454
C	-0.745090	0.932995	-0.013572
C	-1.131761	-0.460055	-0.003119
C	-0.075839	-1.451508	-0.043524
C	1.257742	-1.080089	-0.012992
C	0.956414	2.716069	0.002570
C	-0.008765	3.684759	-0.080163
C	-1.406377	3.370725	-0.211517
C	-1.784996	1.948587	-0.021148
C	-3.066896	1.564715	0.215457
C	-3.471907	0.184804	0.368651
C	-2.472846	-0.839648	0.052238
C	-2.828400	-2.245653	-0.189182
C	-1.753335	-3.211179	-0.135246
C	-0.440483	-2.857097	-0.065331
C	0.616939	-3.845042	-0.049942
C	1.914515	-3.482598	-0.018354
C	2.305155	-2.089886	0.003247
C	2.982866	0.690786	0.058334
C	3.307768	2.090209	0.091396
C	2.352217	3.050796	0.065038
C	4.039148	-0.331921	0.069516
C	3.614046	-1.712369	0.042215
C	-2.295896	4.341412	-0.544862
C	-4.708103	-0.062004	0.888279
C	-4.065707	-2.680343	-0.557027
C	5.369464	-0.047788	0.102705
H	-1.974634	5.371860	-0.636309
H	-3.336006	4.132053	-0.755985
H	-5.367347	0.765239	1.123222
H	-5.052190	-1.052614	1.142120

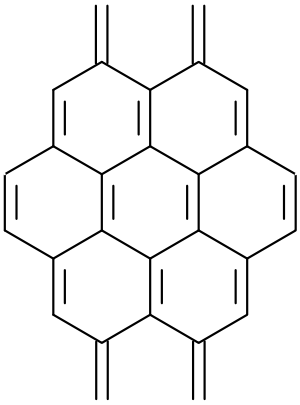
H	-4.895931	-2.013711	-0.731744
H	-4.229093	-3.733569	-0.752821
H	5.764092	0.957671	0.122170
H	6.096328	-0.850730	0.109284
H	4.346612	2.388514	0.134413
H	2.628246	4.099630	0.081892
H	0.285944	4.728644	-0.109568
H	-3.835349	2.315096	0.361042
H	-2.019705	-4.260768	-0.208590
H	0.334055	-4.892206	-0.068108
H	2.699357	-4.231437	-0.007939
H	4.386476	-2.474624	0.054954



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2	0	-1076,789535	-1076,449422

C	0.000000	0.000000	-0.972176
C	-0.015379	1.240156	-0.229423
C	-0.015663	1.236421	1.160309
C	0.000000	0.000000	1.886439
C	0.015663	-1.236421	1.160309
C	0.015379	-1.240156	-0.229423
C	-0.031060	2.498931	-0.955688
C	0.107801	3.770688	-0.200389
C	0.000000	3.688618	1.233398
C	-0.037654	2.494536	1.901860
C	-0.062281	2.435665	3.340197
C	-0.039008	1.248160	3.996003
C	0.000000	0.000000	3.287611
C	0.039008	-1.248160	3.996003
C	0.062281	-2.435665	3.340197
C	0.037654	-2.494536	1.901860
C	0.000000	-3.688618	1.233398
C	-0.107801	-3.770688	-0.200389
C	0.031060	-2.498931	-0.955688
C	0.000000	0.000000	-2.371577
C	-0.312667	1.247720	-3.070087
C	-0.230105	2.468838	-2.299861
C	0.312667	-1.247720	-3.070087
C	0.230105	-2.468838	-2.299861
C	0.379948	4.963769	-0.789213
C	-0.379948	-4.963769	-0.789213
C	0.757327	-1.334232	-4.357244
C	-0.757327	1.334232	-4.357244
H	0.569394	5.063571	-1.849487
H	0.440720	5.866996	-0.194416
H	-0.440720	-5.866996	-0.194416
H	-0.569394	-5.063571	-1.849487

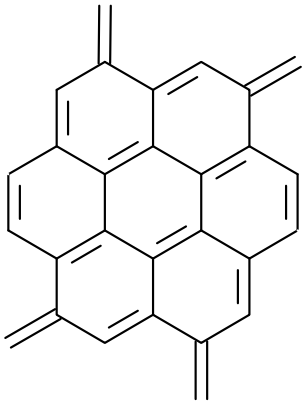
H	0.946417	-0.468207	-4.972677
H	0.996560	-2.302757	-4.779882
H	-0.946417	0.468207	-4.972677
H	-0.996560	2.302757	-4.779882
H	-0.383456	3.394277	-2.842842
H	0.383456	-3.394277	-2.842842
H	-0.011578	-4.615244	1.798003
H	0.085950	-3.369916	3.890574
H	0.046903	-1.222873	5.080663
H	-0.046903	1.222873	5.080663
H	-0.085950	3.369916	3.890574
H	0.011578	4.615244	1.798003



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
D2	0	-1076,792774	-1076,451809

C	-0.182208	2.478996	-2.777821
C	-0.066310	2.492944	-1.421535
C	-0.026164	1.237298	-0.691845
C	0.000000	0.000000	-1.446701
C	0.000000	0.000000	-2.838282
C	-0.275864	1.259338	-3.548472
C	0.026164	1.237298	0.691845
C	0.000000	0.000000	1.446701
C	-0.026164	-1.237298	0.691845
C	0.026164	-1.237298	-0.691845
C	0.275864	-1.259338	-3.548472
C	0.182208	-2.478996	-2.777821
C	0.066310	-2.492944	-1.421535
C	0.030381	-3.730546	-0.672739
C	-0.030381	-3.730546	0.672739
C	-0.066310	-2.492944	1.421535
C	-0.182208	-2.478996	2.777821
C	-0.275864	-1.259338	3.548472
C	0.000000	0.000000	2.838282
C	0.275864	1.259338	3.548472
C	0.182208	2.478996	2.777821
C	0.066310	2.492944	1.421535
C	0.030381	3.730546	0.672739
C	-0.030381	3.730546	-0.672739
H	0.058069	-4.662075	-1.227950
H	-0.058069	-4.662075	1.227950
H	-0.274381	-3.417818	3.314319
C	-0.716899	-1.344917	4.833752
C	0.716899	1.344917	4.833752
H	0.274381	3.417818	3.314319
H	0.058069	4.662075	1.227950
H	-0.058069	4.662075	-1.227950

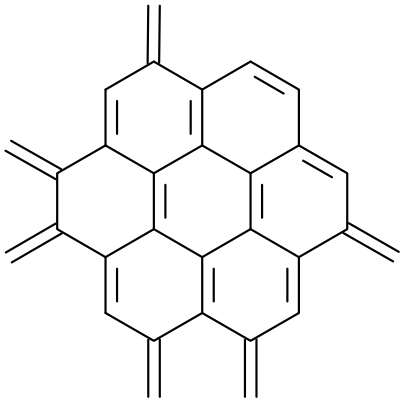
C	0.716899	-1.344917	-4.833752
H	0.274381	-3.417818	-3.314319
C	-0.716899	1.344917	-4.833752
H	-0.274381	3.417818	-3.314319
H	-0.934748	-2.316056	5.262363
H	-0.929545	-0.480454	5.442912
H	0.929545	0.480454	5.442912
H	0.934748	2.316056	5.262363
H	-0.929545	0.480454	-5.442912
H	-0.934748	2.316056	-5.262363
H	0.929545	-0.480454	-5.442912
H	0.934748	-2.316056	-5.262363



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2	0	-1076,79458	-1076,454803

C	-2.454536	1.404332	-0.106540
C	2.454536	-1.404332	-0.106540
C	-1.246052	0.702468	-0.021212
C	1.246052	-0.702468	-0.021212
C	-2.430919	2.838555	-0.120161
C	2.430919	-2.838555	-0.120161
C	-3.716011	0.666408	-0.193062
C	3.716011	-0.666408	-0.193062
C	0.008284	1.416363	0.015714
C	-0.008284	-1.416363	0.015714
C	-1.219661	-0.734874	0.031176
C	1.219661	0.734874	0.031176
C	1.271653	-3.539407	-0.060939
C	-1.271653	3.539407	-0.060939
C	-3.643026	-0.772557	-0.090322
C	3.643026	0.772557	-0.090322
C	2.481906	1.463785	0.059089
C	-0.001334	2.874502	0.010672
C	0.001334	-2.874502	0.010672
C	-2.481906	-1.463785	0.059089
C	-2.454536	-2.941179	0.217540
C	2.454536	2.941179	0.217540
C	1.170659	3.578834	0.096763
C	-1.170659	-3.578834	0.096763
H	3.367045	-3.378733	-0.169386
H	-3.367045	3.378733	-0.169386
H	-1.136704	-4.662936	0.126333
H	1.136704	4.662936	0.126333
H	-4.583258	-1.307843	-0.151798
H	4.583258	1.307843	-0.151798
H	1.284592	-4.623945	-0.062938
H	-1.284592	4.623945	-0.062938

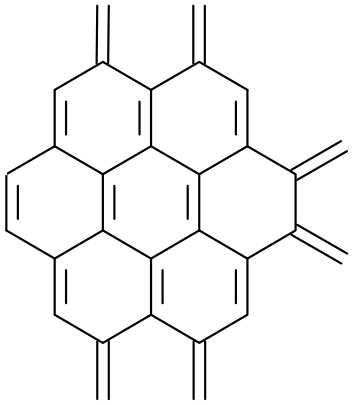
C	-4.935018	1.250046	-0.366877
C	4.935018	-1.250046	-0.366877
C	-3.551779	-3.688500	0.506163
C	3.551779	3.688500	0.506163
H	-5.075626	2.316996	-0.463419
H	-5.827555	0.639065	-0.420338
H	-4.525846	-3.256878	0.691859
H	-3.473816	-4.766159	0.581655
H	3.473816	4.766159	0.581655
H	4.525846	3.256878	0.691859
H	5.827555	-0.639065	-0.420338
H	5.075626	-2.316996	-0.463419



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-1154,192781	-1153,819901

C	-0.012040	3.422991	0.073805
C	0.892697	2.423135	-0.052553
C	0.448444	1.040038	0.015682
C	-0.978163	0.775752	0.001978
C	-1.903705	1.819167	-0.023707
C	-1.434836	3.188425	0.218543
C	1.368423	0.000168	0.025226
C	0.930523	-1.373646	-0.033520
C	-0.487935	-1.641152	-0.013362
C	-1.410869	-0.603833	0.017197
C	-3.307511	1.505724	-0.302383
C	-3.710877	0.124842	-0.162905
C	-2.835636	-0.893348	0.045388
C	-3.286219	-2.295232	0.228029
C	-2.286552	-3.315396	0.060617
C	-0.951863	-3.024139	-0.038420
C	0.035019	-4.063467	-0.133530
C	1.358163	-3.775376	-0.172507
C	1.845671	-2.425370	-0.114855
C	3.285430	-2.143133	-0.145250
C	3.682494	-0.757953	-0.000707
C	2.798943	0.263797	0.108103
C	3.241692	1.660161	0.320880
C	2.336381	2.692453	-0.239405
H	4.745886	-0.547864	0.007102
C	-4.226085	2.396200	-0.773772
C	-2.217549	4.212860	0.650985
H	0.327209	4.451326	0.123898
H	-3.265441	4.094938	0.880800
H	-1.776818	5.184780	0.839527
H	-3.983802	3.421286	-1.008025
H	-5.235800	2.065356	-0.986254

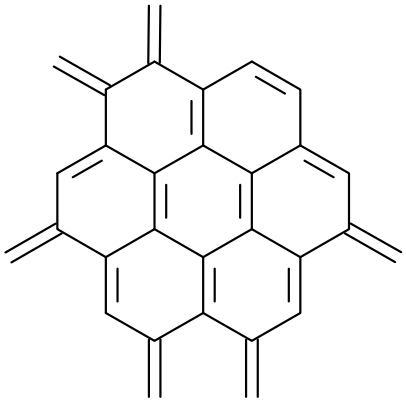
C	2.799457	3.755036	-0.912004
C	4.340370	1.981154	1.018172
H	3.862042	3.900214	-1.062596
H	2.131620	4.483371	-1.355569
H	4.973815	1.224106	1.463992
H	4.611196	3.015924	1.187382
H	-0.304635	-5.093183	-0.161721
H	-2.605385	-4.352434	0.077423
H	-4.765857	-0.089144	-0.289635
H	2.069300	-4.588017	-0.234307
C	4.245363	-3.092895	-0.295276
C	-4.552211	-2.631575	0.586469
H	4.029820	-4.145052	-0.413859
H	5.291211	-2.811399	-0.306387
H	-5.306520	-1.894079	0.825737
H	-4.839958	-3.672458	0.670980



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C2	0	-1154,191774	-1153,818224

C	-0.528050	2.787361	-0.353767
C	0.528050	-2.787361	-0.353767
C	-0.282578	1.417354	-0.347955
C	0.282578	-1.417354	-0.347955
C	-0.400107	3.529836	0.907688
C	0.898643	-3.445407	-1.616008
C	-0.898643	3.445407	-1.616008
C	0.400107	-3.529836	0.907688
C	-0.135404	0.680629	0.893532
C	0.153522	-0.674718	-1.586473
C	-0.153522	0.674718	-1.586473
C	0.135404	-0.680629	0.893532
C	0.670858	-2.701001	-2.833015
C	-0.436561	2.748728	2.128071
C	-0.670858	2.701001	-2.833015
C	0.436561	-2.748728	2.128071
C	0.338177	-1.398361	2.142934
C	-0.338177	1.398361	2.142934
C	0.320487	-1.385842	-2.842900
C	-0.320487	1.385842	-2.842900
C	-0.149928	0.656342	-4.080485
C	0.398548	-0.624786	3.403121
C	-0.398548	0.624786	3.403121
C	0.149928	-0.656342	-4.080485
H	0.275915	-1.198101	-5.011833
H	-0.275915	1.198101	-5.011833
H	-0.849627	3.211944	-3.773654
H	0.481024	-3.294275	3.063713
H	0.849627	-3.211944	-3.773654
H	-0.481024	3.294275	3.063713
C	-1.534957	4.646065	-1.705782
C	-0.149928	4.862142	1.004029

C	0.149928	-4.862142	1.004029
C	1.534957	-4.646065	-1.705782
C	-1.156601	0.988397	4.446709
C	1.156601	-0.988397	4.446709
H	-1.847900	5.213248	-0.843283
H	-1.807385	5.037192	-2.679037
H	0.001861	5.496245	0.144202
H	-0.030448	5.317295	1.980335
H	-0.001861	-5.496245	0.144202
H	0.030448	-5.317295	1.980335
H	1.807385	-5.037192	-2.679037
H	1.847900	-5.213248	-0.843283
H	1.769214	-1.881353	4.421122
H	1.205868	-0.378453	5.340234
H	-1.205868	0.378453	5.340234
H	-1.769214	1.881353	4.421122



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C1	0	-1154,187294	-1153,814539

C	-2.660876	2.458036	-0.039846
C	-2.566724	1.116997	0.121062
C	-1.269698	0.451225	0.005894
C	-0.111031	1.205676	-0.078085
C	-0.178600	2.657989	-0.167678
C	-1.510440	3.306132	-0.275136
C	-1.217929	-0.989885	0.011329
C	0.074461	-1.629357	-0.011519
C	1.240296	-0.875733	-0.003686
C	1.191797	0.570301	-0.003089
C	0.977942	3.367491	-0.185620
C	2.293759	2.768912	-0.161343
C	2.360875	1.325807	0.085477
C	3.608000	0.643742	0.444586
C	3.639606	-0.791825	0.277634
C	2.535827	-1.535802	0.006950
C	2.603187	-3.003813	-0.198323
C	1.361601	-3.722071	-0.104756
C	0.149243	-3.086639	-0.033902
C	-1.080981	-3.825033	-0.015611
C	-2.281111	-3.191006	-0.020679
C	-2.382338	-1.761767	-0.024322
C	-3.700997	-1.114370	-0.078285
C	-3.748669	0.282469	0.424223
H	-3.192228	-3.774994	0.005273
C	3.358171	3.562877	-0.466500
C	-1.701862	4.607428	-0.591501
H	-3.635212	2.932835	-0.031082
H	-0.892132	5.286055	-0.823377
H	-2.703768	5.017021	-0.633435
H	3.201801	4.615779	-0.669269
H	4.361061	3.183907	-0.586247

C	-4.769629	0.725916	1.172894
C	-4.798652	-1.716411	-0.572301
H	-5.607010	0.083945	1.415936
H	-4.774731	1.725178	1.590394
H	-4.780799	-2.729405	-0.952564
H	-5.738446	-1.184386	-0.644431
H	-1.031260	-4.908373	-0.002006
H	4.592777	-1.280961	0.442344
H	0.947514	4.447508	-0.267331
H	1.392089	-4.805537	-0.155464
C	4.693317	1.243399	1.010379
C	3.749412	-3.660611	-0.514658
H	4.683510	-3.147660	-0.700317
H	3.752934	-4.738895	-0.617947
H	4.716696	2.289467	1.273841
H	5.559457	0.648054	1.274152

Full citation of Ref. [23].

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