Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic supplementary information

Generalized kekulenes and clarenes as novel families of cycloarenes: structures, stability, and spectroscopic properties

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Contents

1 DFT refinement calculations and comparison between xTB and DFT relative energies

We performed geometry optimizations and vibrational frequency analyses, which verify the energy minima on the potential energy surface using the GFN2-xTB method[1,2] implemented in the XTB program (version 6.3.3).[1,3,4] We refined the xTB results at DFT level for all kekulene isomers containing up to 32 rings and all clarene isomers containing up to 54 rings. For larger size isomers of kekulene and clarene, we determined the lowest-energy structures by considering only those with xTB relative energies lower than 10 kcal/mol. Our assessment calculations showed that the relative isomer energies obtained from the GFN2-xTB calculations are consistent with those obained at the B3LYP-D3(BJ)/6-31G* level (see Fig. S1).

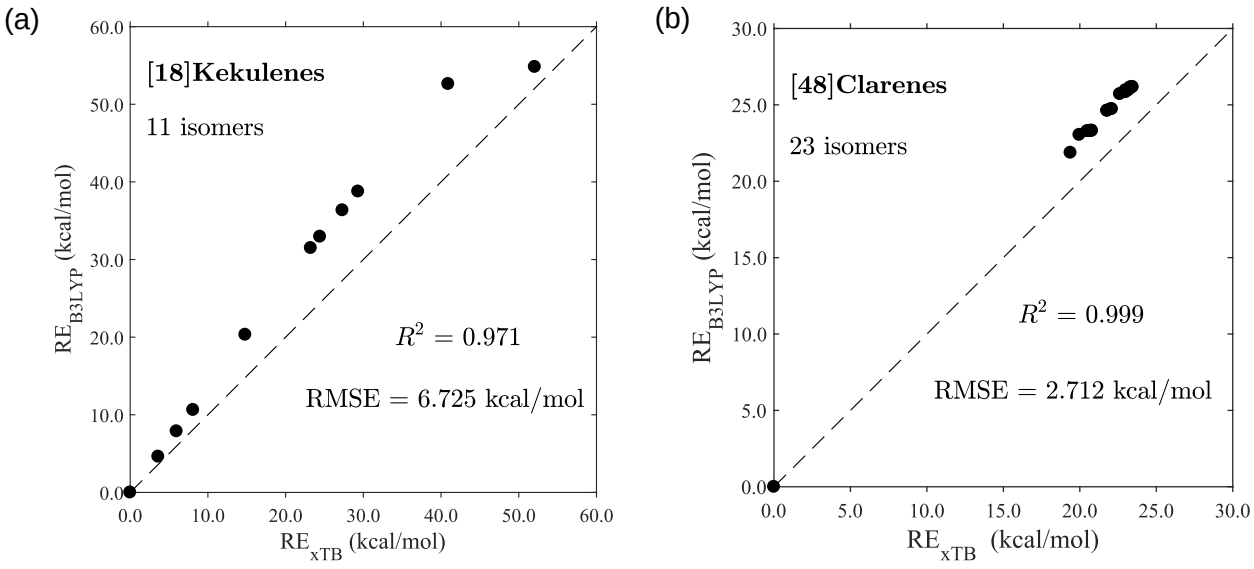
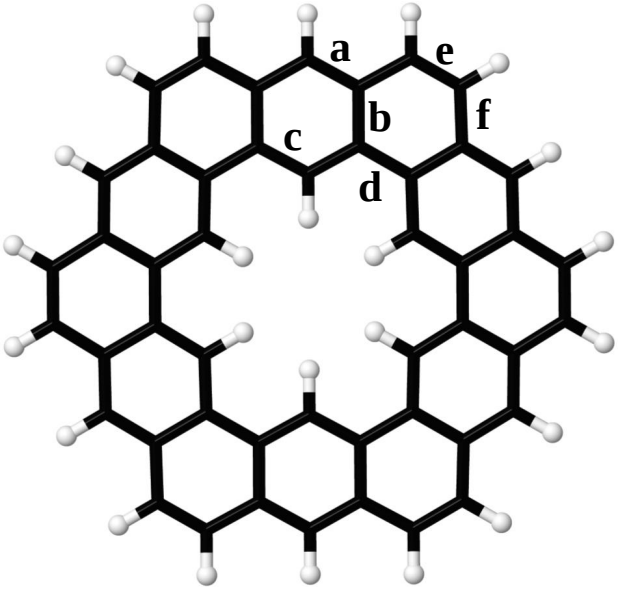


Figure S1. DFT relative energies, RE_{B3YLP}, versus xTB relative energies, RE_{xTB}, for (a) all 11 isomers of [18]kekulenes and (b) all 23 isomers of [48]clarenes. Squared correlation coefficient (R^2) and root mean square error (RMSE) are provided in each plot.

2 Comparison between DFT and experimental structures of [12]kekulene

Fig. S2 shows the molecular structure of the experimentally synthesized [12]kekulene, [2,2,2,2,2,2][5–8] computed at the ωB97XD/cc-pVDZ level in vacuum. The representative CC bonds are labeled by small letters. The bond lengths are compared between the X-ray crystallographic measurements[6,8] and the DFT predictions, as summarized in table. As we can see, the DFT predicted geometry is consistent with the experimental values measured from XRD.



Label	Bond Length (Å)	
	DFT [a]	Exp
a	1.40	1.40
b	1.42	1.42
c	1.39	1.38
d	1.46	1.45
e	1.36	1.35
f	1.45	1.44

[a]: ωB97XD/cc-pVDZ

Figure S2. ωB97XD/cc-pVDZ optimized structure of the experimentally synthesized [12]kekulene.[5–8] The representative CC bonds are labeled by small letters. Bond lengths of calculation and experiment are given in table.

3 Relative energies and free energies of looped polyarenes at the B3LYP-D3(BJ)/6-31G* level

Fig. S3-S4 show the relative energies and relative Gibbs free energies (at 298.15 K and 1 atm) of different forms of looped polyarenes with a varying number of rings at the B3LYP-D3(BJ)/6-31G* level of theory.[9,10] Compared with Fig. 5 in the main text, both the B3LYP-D3(BJ)/6-31G* and the ωB97XD/cc-pVDZ methods[11,12] give essentially consistent results. In addition, the relative Gibbs free energies also follow almost the same tendencies as those for the relative energies among looped polyarenes. Therefore, the B3LYP-D3(BJ)/6-31G* and the ωB97XD/cc-pVDZ methods lead to consistent results.

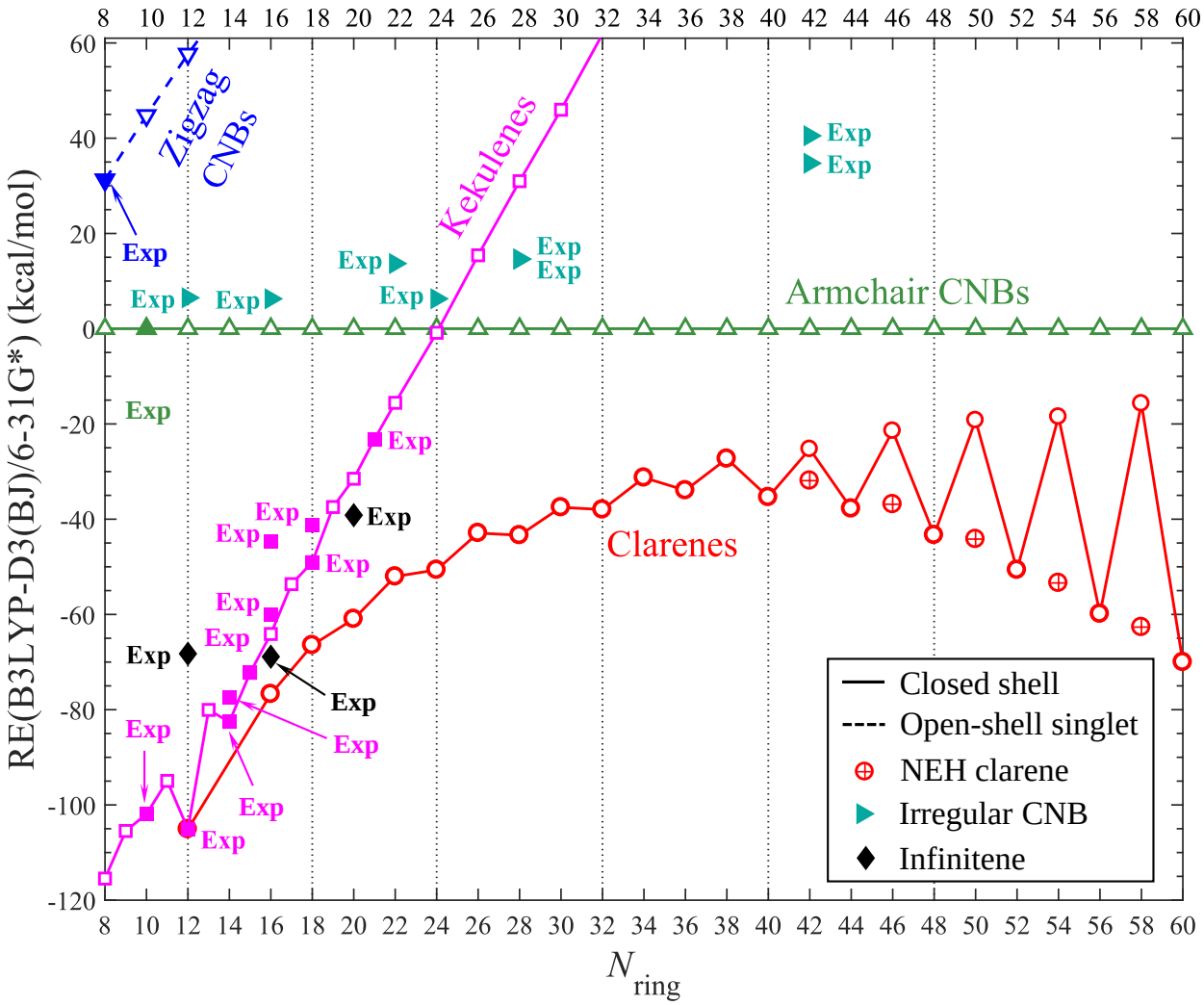


Figure S3. Idem Fig. 5 in the main text for the results obtained at the B3LYP-D3(BJ)/6-31G* level.

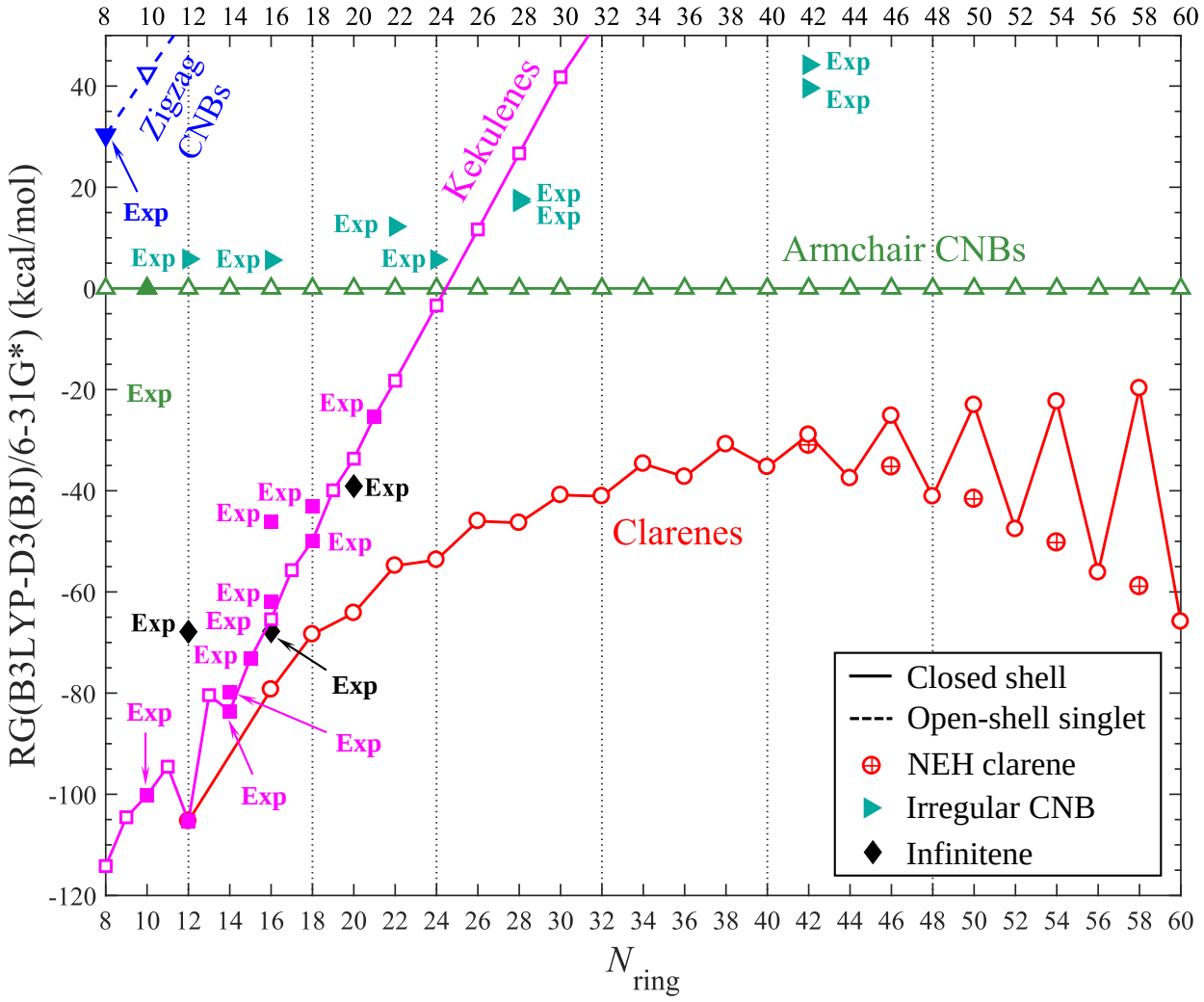
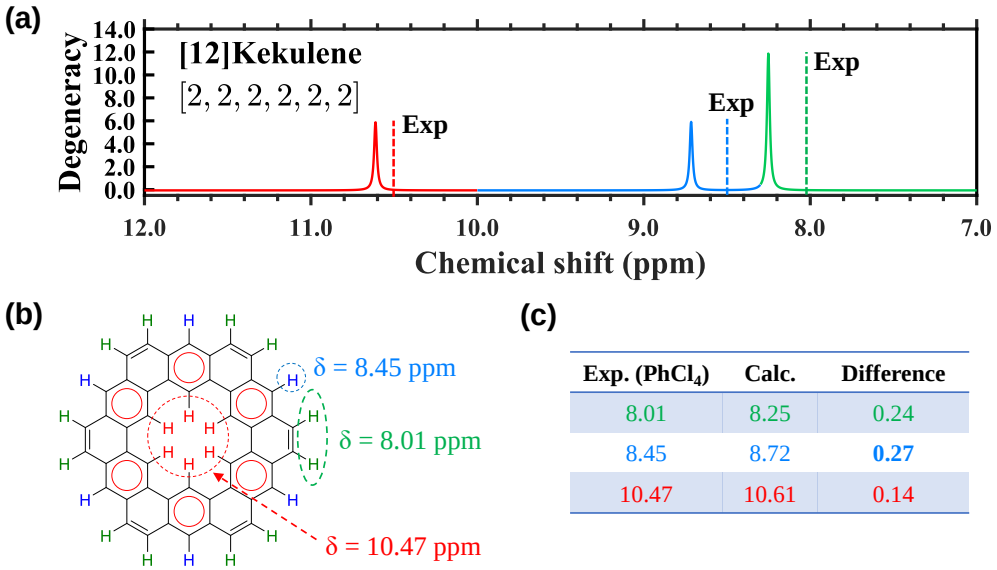


Figure S4. Idem Fig. S3 for relative Gibbs free energies at 298.15 K and 1 atm, calculated at the B3LYP-D3(BJ)/6-31G* level.

4 Simulated ^{1}H NMR spectra of kekulenes and clarenes

^{1}H NMR spectrum for synthesized [12]kekulene, [2,2,2,2,2,2],[5–8] was simulated in l,2,4,5-tetrachlorobenze solvent with SMD model at the GIAO-DFT level. As shown in Fig. S5, the simulated result is in good agreement with the experimental one. Obviously, there are three groups of peaks corresponding to three types of H atoms in both kekulene and clarene structures.



Exp. ($PhCl_4$)	Calc.	Difference
8.01	8.25	0.24
8.45	8.72	**0.27**
10.47	10.61	0.14

Figure S5. ^{1}H NMR spectrum for the synthesized [12]kekulene. (a) Simulated ^{1}H NMR chemical shift for [12]kekulene in l,2,4,5-tetrachlorobenz at the GIAO-DFT (B3LYP/6-311+G(2d,p)($PHCl_4$-SMD)//ωB97XD/cc-pVDZ) level. Low-field, medium-field and high-field peaks are colored in red, blue and green, respectively. Experimental value are indicated by vertical lines. (b) Different types of H atoms are colored in red, blue and green, respectively, corresponding to peaks indicated by the same color in (a). (c) Comparison of chemical shifts between experimental measurements and our calculations.

In the following, we present in Fig. S6–S12 the simulated ^{1}H NMR spectra for the lowest-energy isomers of kekulenes and clarenes of varing sizes (with 8 to 60 benzene rings). In each spectrum, the ^{1}H NMR peaks shown in distinct colors originate from the H atoms in the illustrated structure on the left, which are highlighted in the same color. The rings are colored in orange and light yellow represent sextets and migrated sextets, respectively. For [8]kekulene (see Fig. S6(a)), H atoms colored in red fall in high-field regions which is obviously different from other kekulenes. The reason is that [8]kekulene has a non-planar structure, and the H atoms colored in red fall into the shielding regions of the benzene rings on the opposite side.

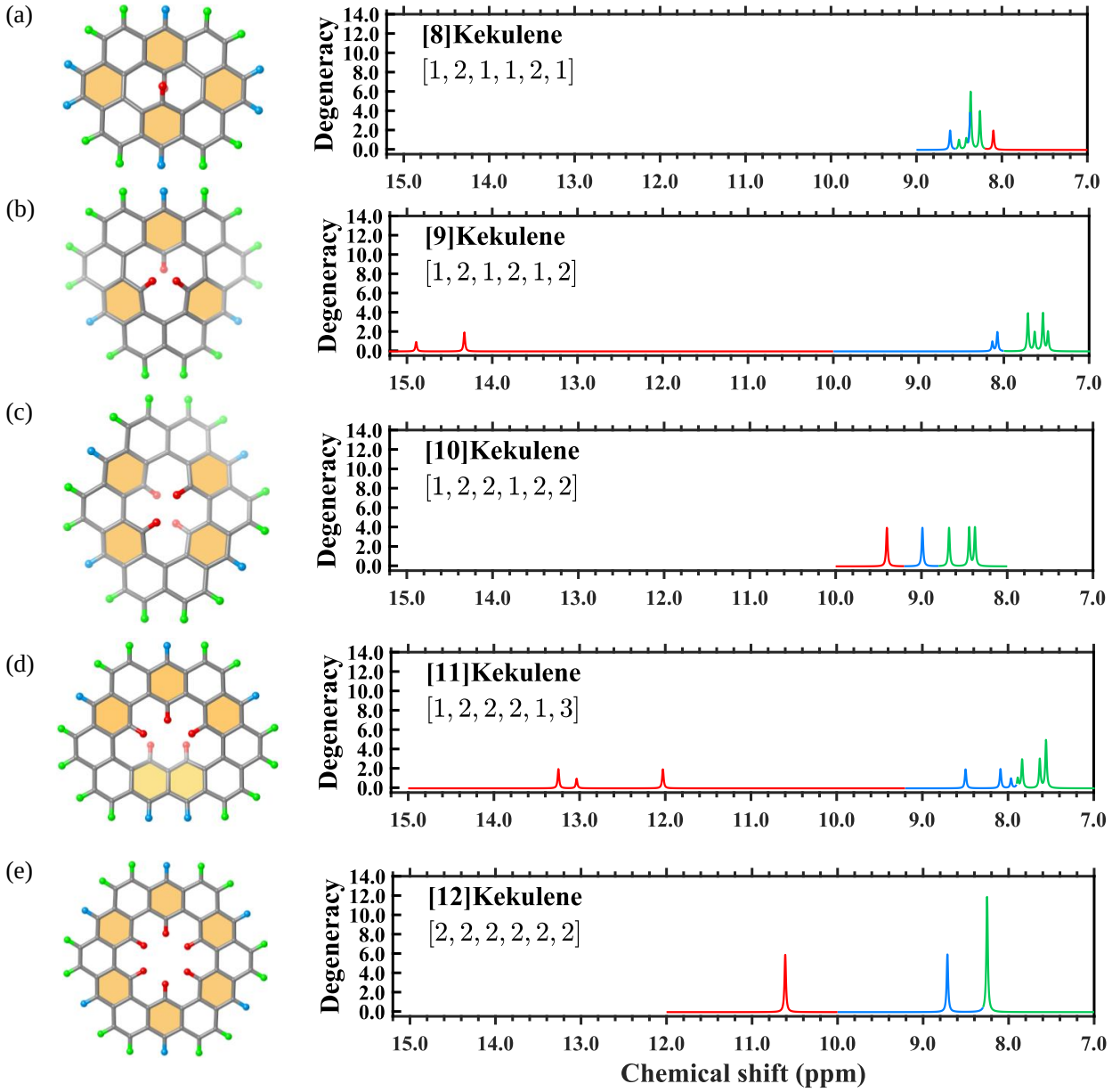


Figure S6. Simulated ^{1}H NMR spectra for the lowest-energy isomers of kekulenes containing 8 to 12 rings in $PHCl_4$ solvent. NMR peaks in different colors originate from the corresponding H atoms in the illustrated structure on the left, which are highlighted in the same color. The rings are colored in orange and light yellow represent sextets and migrating sextets, respectively.

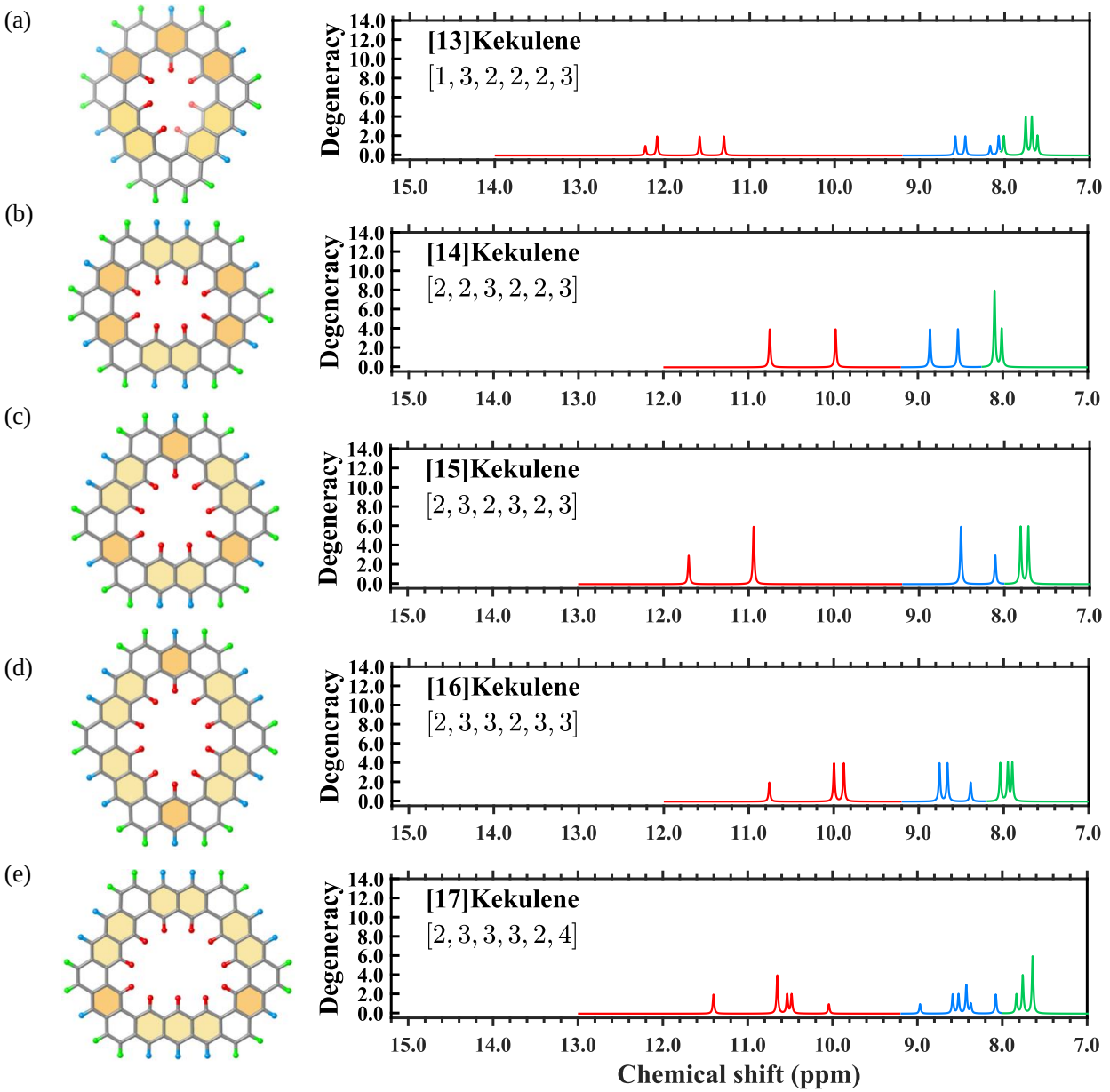


Figure S7. Idem Fig. S6 for the lowest-energy isomers of kekulenes containing 13 to 17 rings.

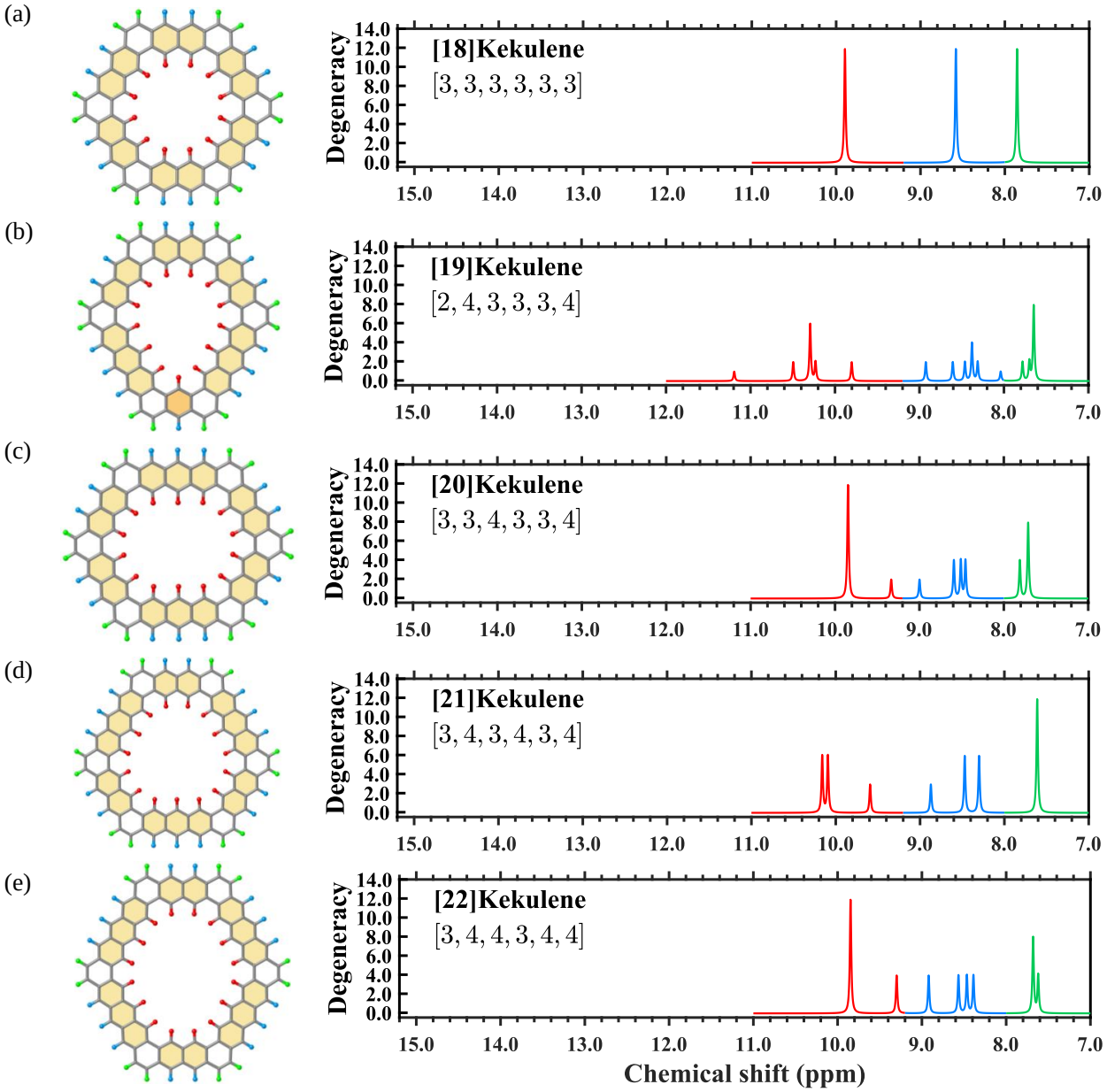


Figure S8. Idem Fig. S6 for the lowest-energy isomers of kekulenes containing 18 to 22 rings.

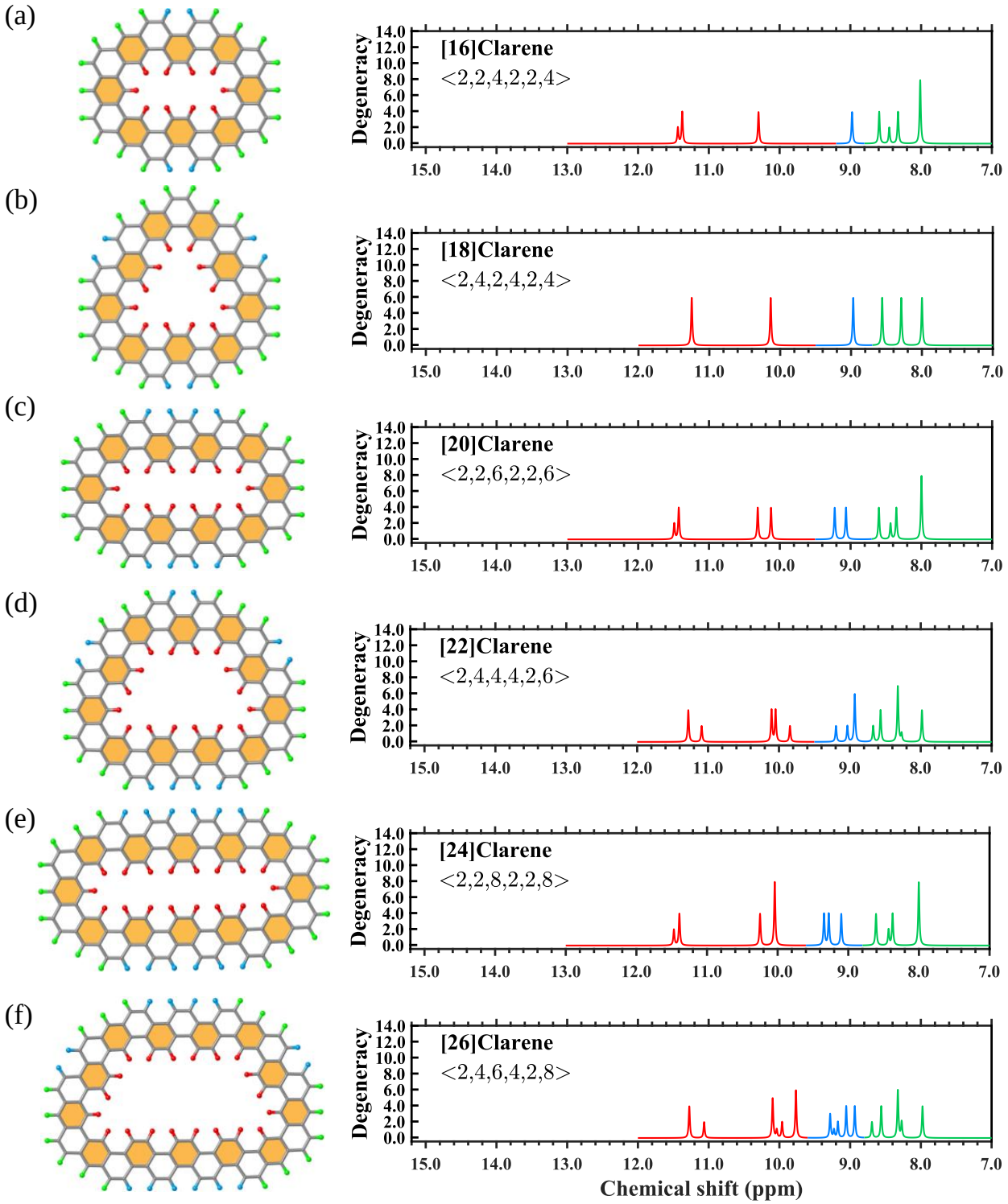


Figure S9. Idem Fig. S6 for the lowest-energy isomers of clarenes containing 18 to 26 rings.

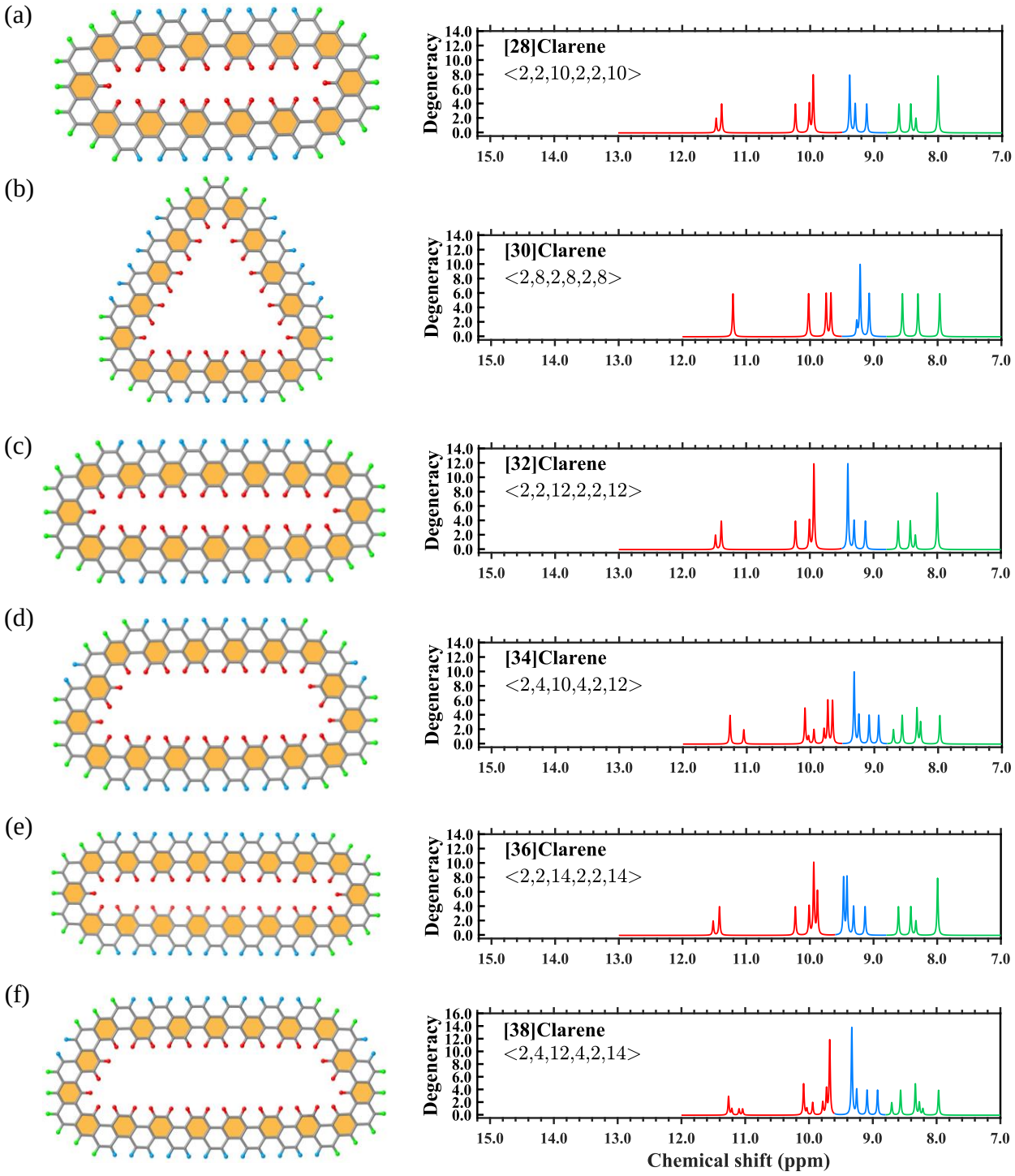


Figure S10. Idem Fig. S6 for the lowest-energy isomers of clarenes containing 28 to 38 rings.

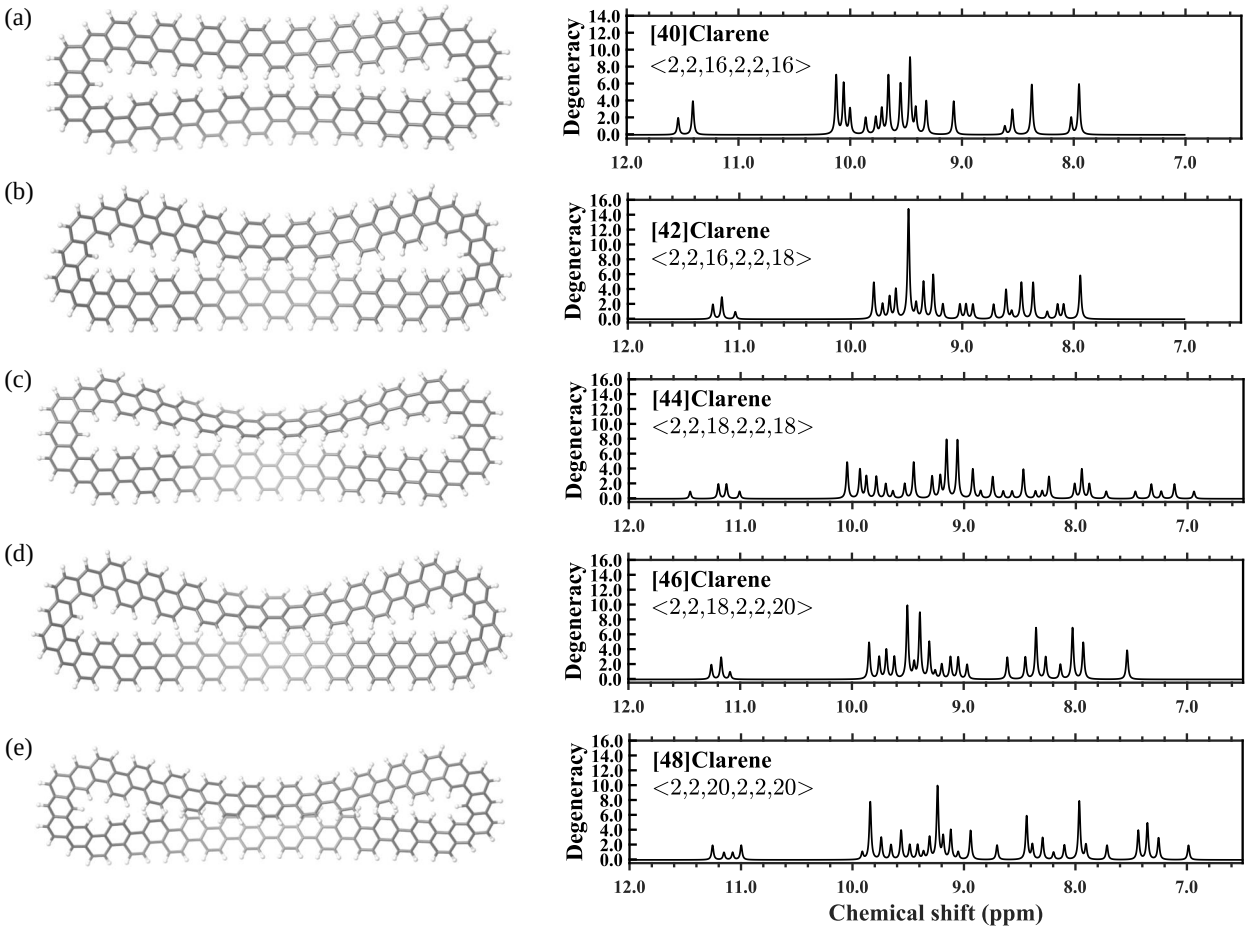


Figure S11. Simulated ^{1}H NMR spectra for the lowest-energy isomers of clarenes containing 40 to 48 rings.

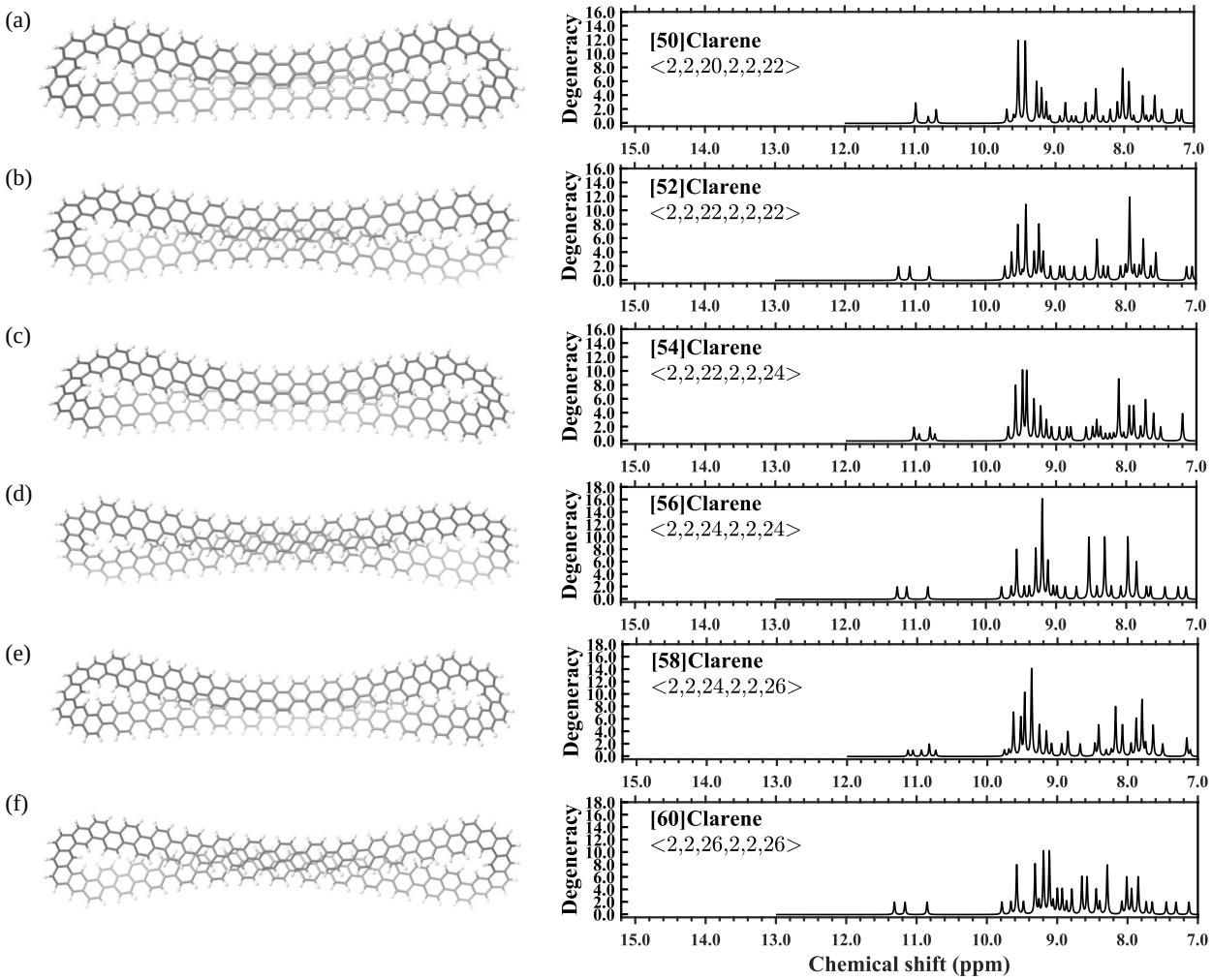


Figure S12. Idem Fig. S11 for the lowest-energy isomers of clarenes containing 50 to 60 rings.

5 Simulated UV-vis spectra of kekulenes and clarenes

We performed TD DFT calculations at the B3P86/6-311G(d,p)//ωB97XD/cc-pVDZ level to simulate the UV-vis absorption for the lowest-energy isomers of kekulenes and clarenes from 8 to 60 rings (see Fig. S15-S19). We also tried a larger basis set, 6-311++G(2d,p), but the results did not improve significantly. From the assessment for [12]kekulene and [16]clarene, we can see that the 6-311G(d,p) basis set results in a UV-vis spectrum very similar to that given by the 6- 311++G(2d,p) basis set, as shown in Fig. S13, indicating that the 6-311G(d,p) is sufficient to describe the considered compounds.

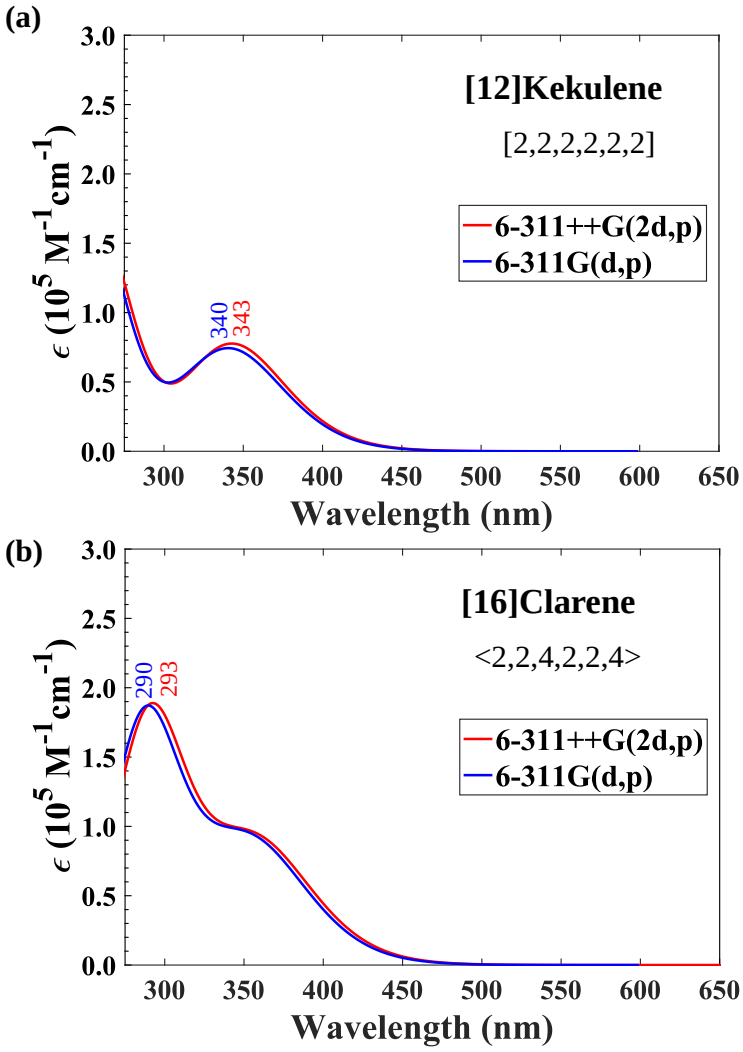


Figure S13. Comparison of the UV-vis absorption spectra simulated with basis sets 6-311++G(2d,p) and 6-311G(d,p) for (a) the experimentally synthesized [12]kekulene and (b) the lowest-energy isomer of [16]clarene.

We also simulate UV-vis absorption spectra for the experimentally synthesized [12]kekulene in order to verify the feasibility of the method. As shown in Fig. S14, simulated spectrum is in reasonable agreement with the experimental one,[13] in terms of prediction of maximum absorption peak wavelength (340 nm vs. 327 nm).

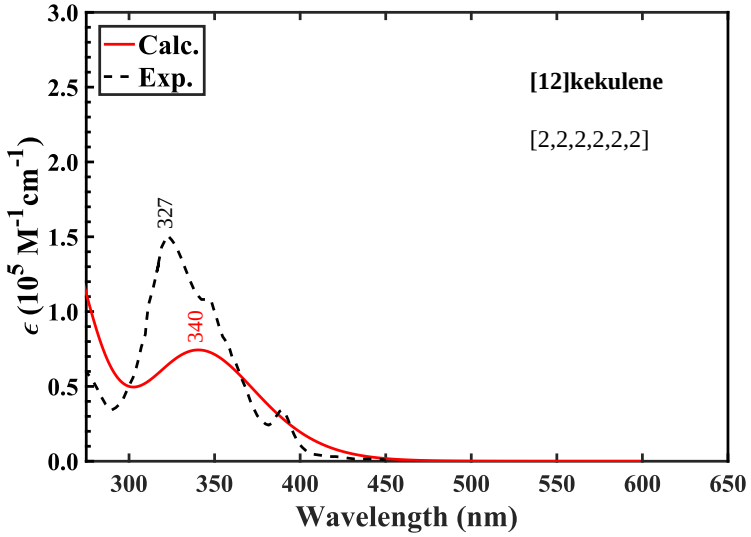


Figure S14. Comparison of the UV-vis spectra between experiment and calculation for experimentally synthesized [12]kekulene.[5–8,13]

In the following, we present in Fig. S15-S19 the simulated UV-vis absorption spectra for the lowest-energy isomers of kekulenes and clarenes of varing sizes (with 8 to 60 benzene rings).

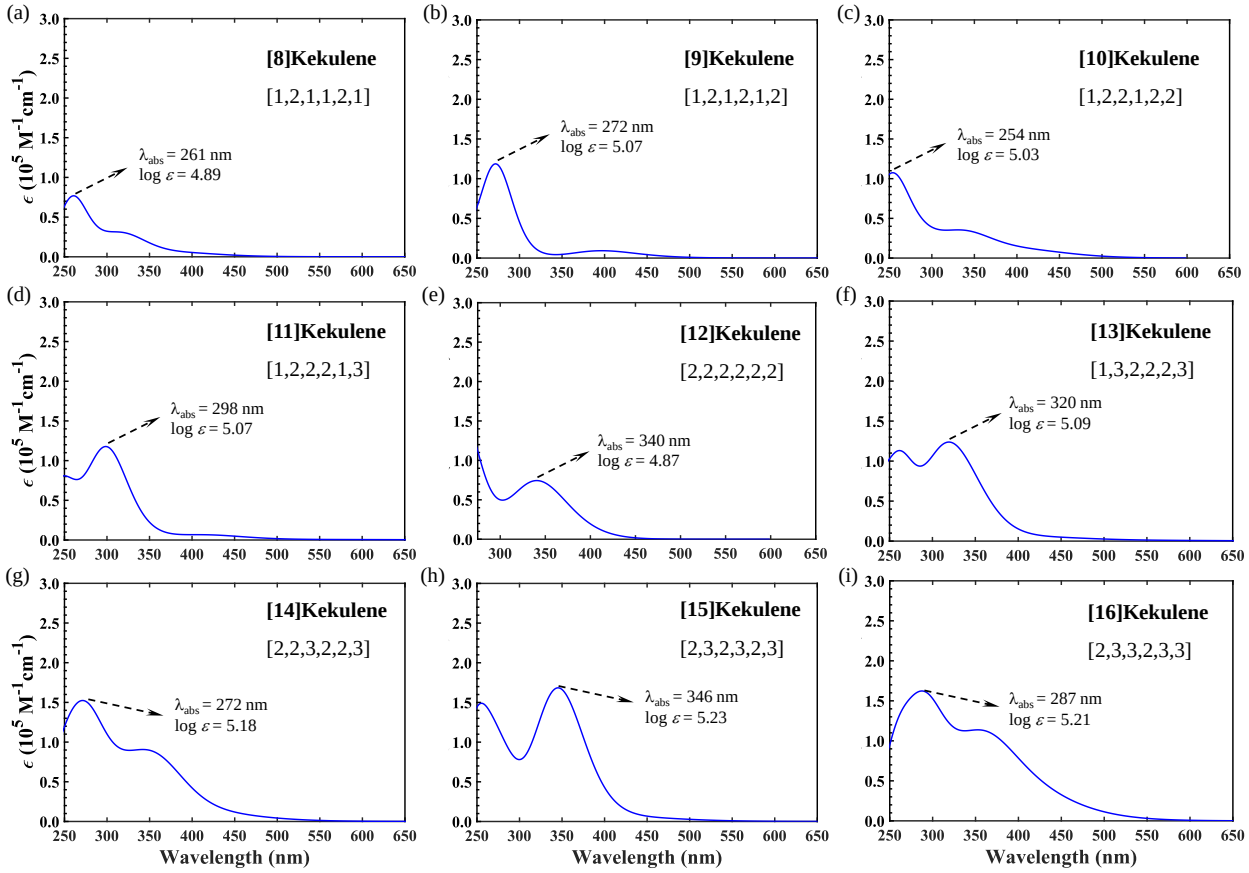


Figure S15. Simulated UV-vis spectra for lowest-energy isomers of kekulenes containing 8 to 16 rings

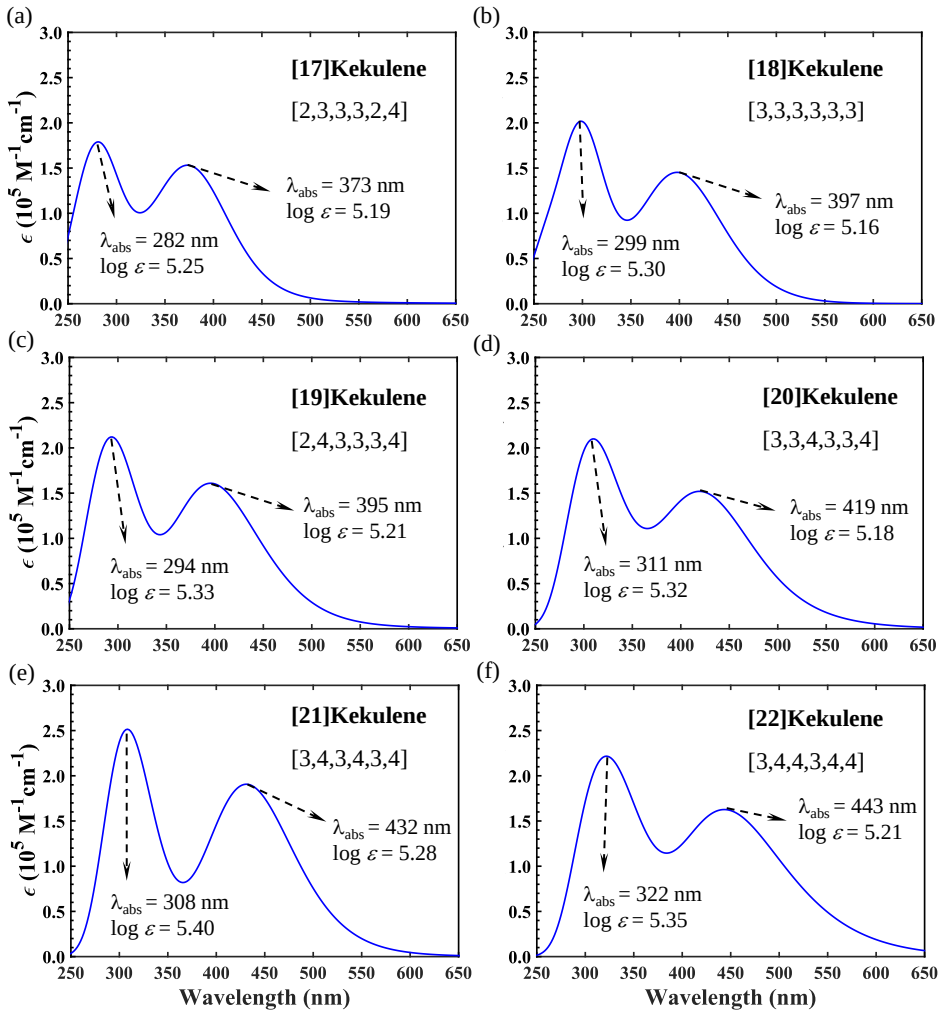


Figure S16. Idem Fig. S15 for the lowest-energy isomers of kekulenes containing 17 to 22 rings.

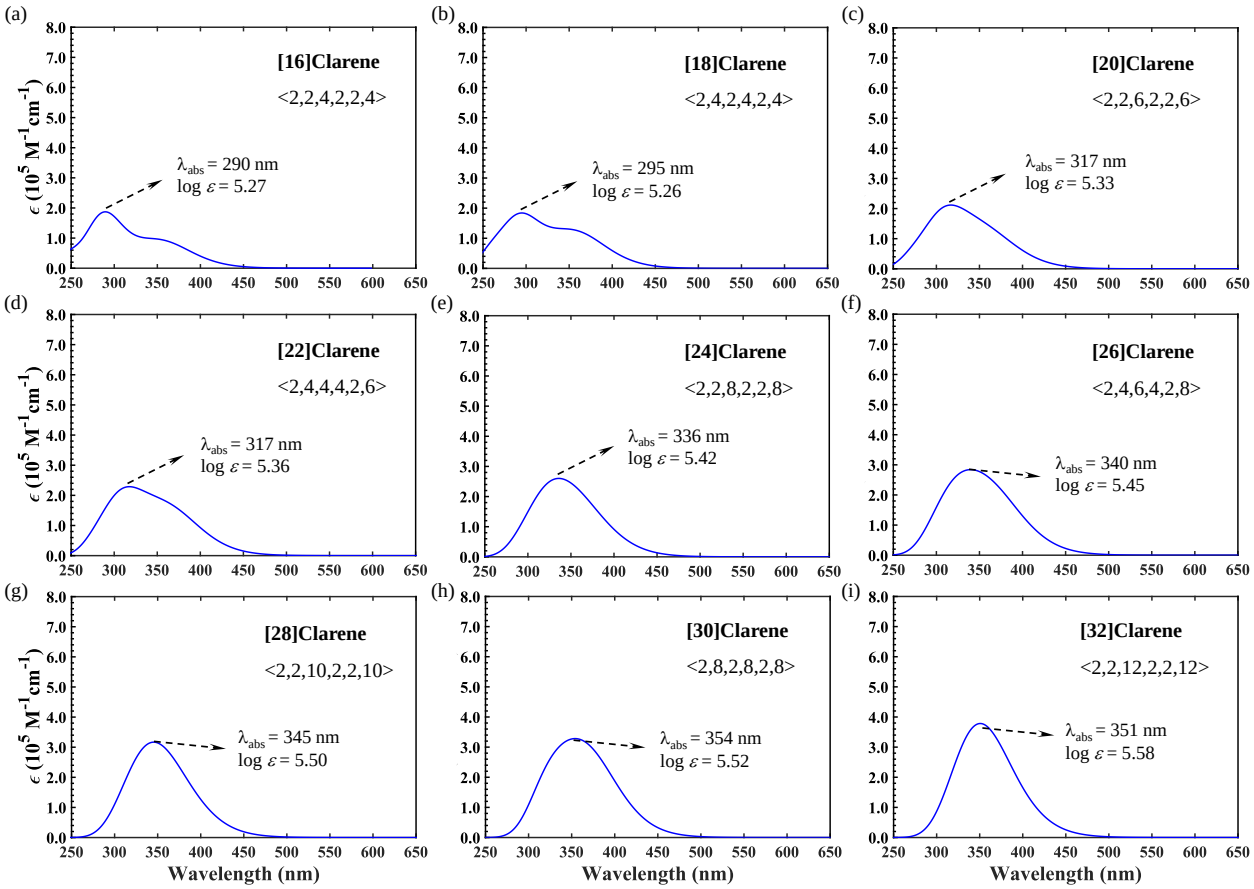


Figure S17. Idem Fig. S15 for the lowest-energy isomers of clarenes containing 16 to 32 rings.

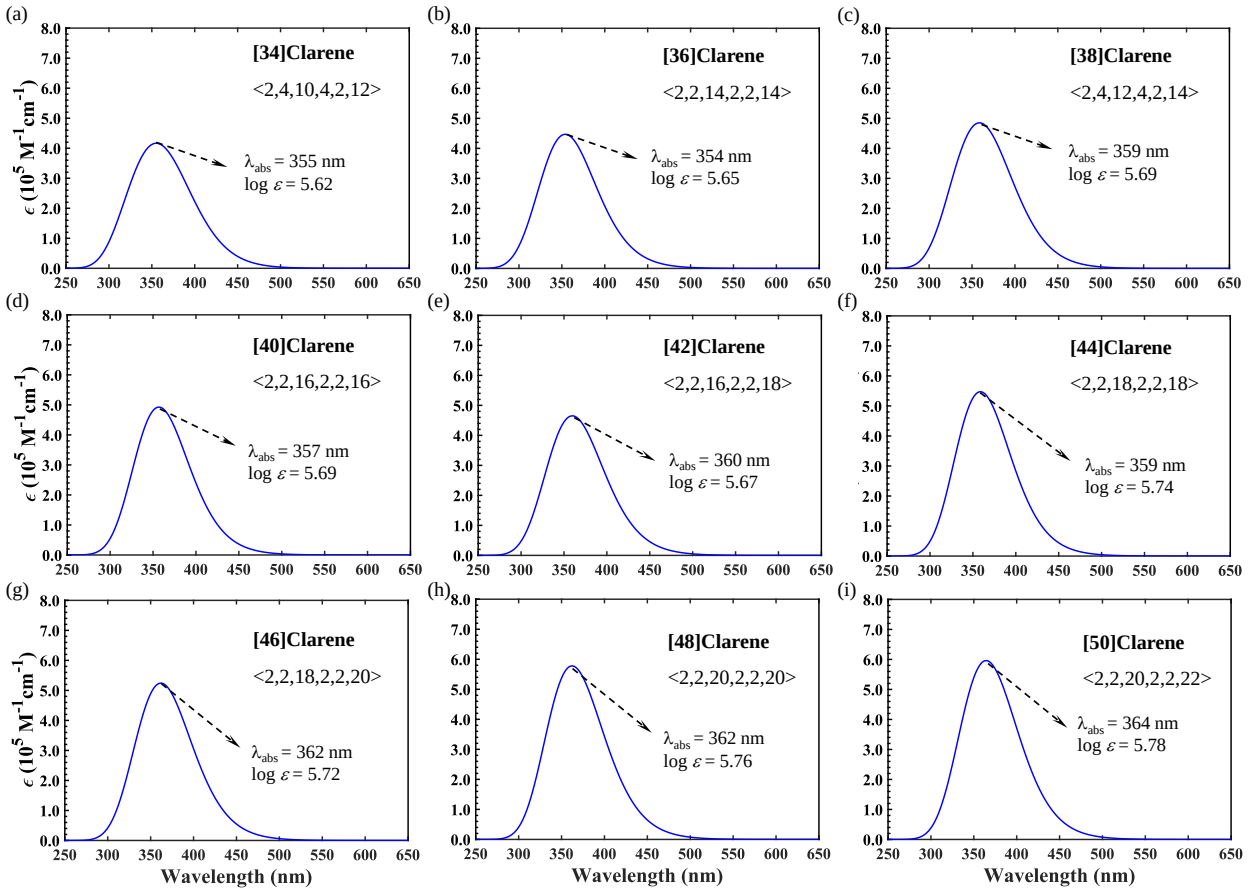


Figure S18. Idem Fig. S15 for the lowest-energy isomers of clarenes containing 34 to 50 rings.

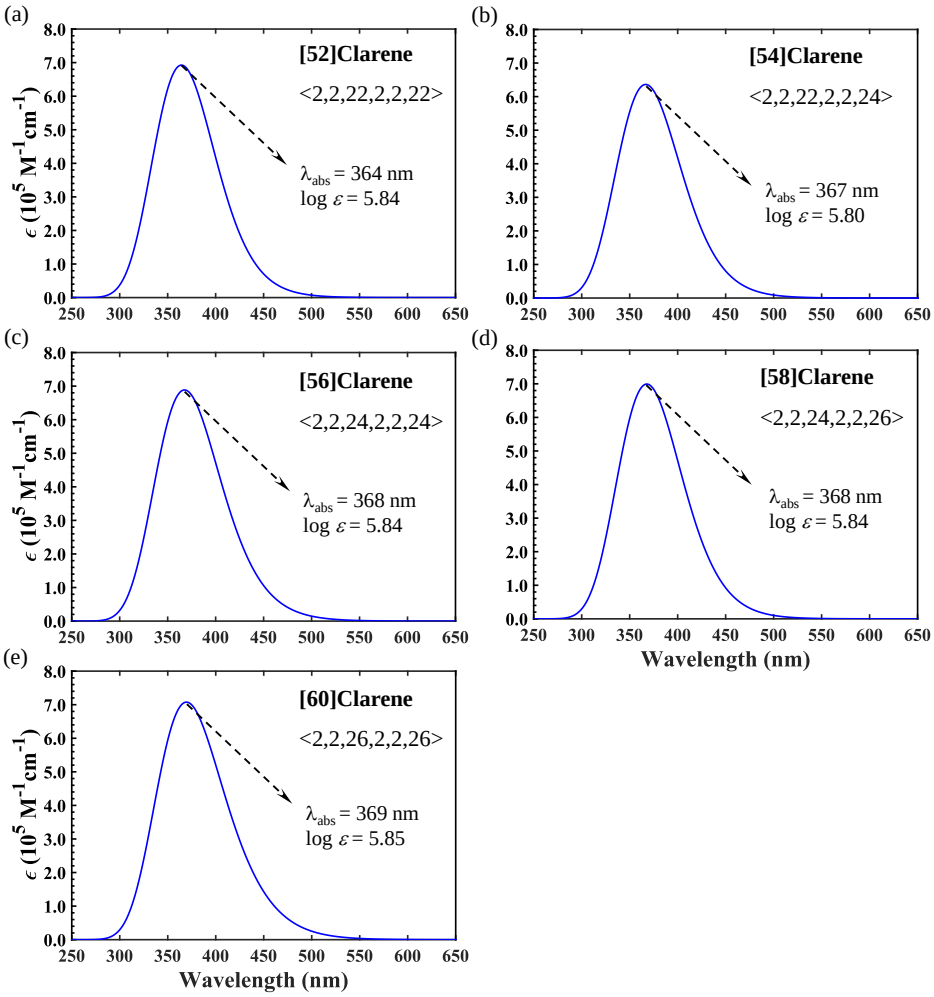


Figure S19. Idem Fig. S15 for the lowest-energy isomers of clarenes containing 52 to 60 rings.

As shown in Fig. S20, the molar extinction coefficients (ε) gradually increases as the increasing of melocular size, which is caused by the increase of transition probability as a result of the increasing the number of frontier molecular orbitals as the π-conjugated system grows.

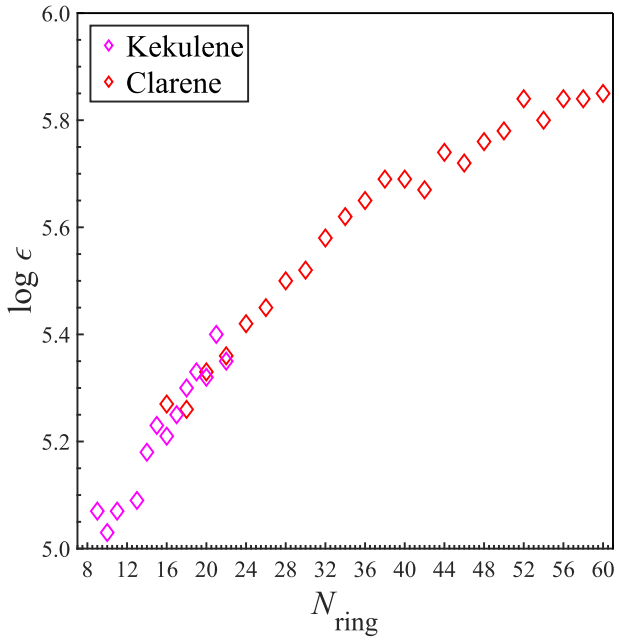


Figure S20. The molar extinction coefficients, log ε, of kekulenes and clarenes, versus the number of rings, N_{ring}.

6 Details on the construction of equiangular hexagons

Equiangular hexagons[14] can be constructed from the intersection between two appropriate equilateral triangles with the side lengths of a_0 and a_1, as shown in Fig. S21(a). Without losing generality, let $a_0 \geq a_1$. Obviously, the smaller triangle cannot be too small to ensure the intersection of the two triangles to form a hexagon. The extreme case is that the smaller triangle is inscribed in the larger one, in which $a_1 = a_0/2$ (see the Fig. S21(c)).

As we can see, the equiangular hexagon can be obtained by the intersection of the two equilateral triangles, as shown by the green lines in Fig. S21(b), where the side lengths of the equiangular hexagon, h_1, h_2, h_3, h_4, h_5, and h_6, are all positive integers. Evidently,

$$\begin{cases} a_0 = h_6 + h_1 + h_2 = h_2 + h_3 + h_4 = h_4 + h_5 + h_6 \\ a_1 = h_1 + h_2 + h_3 = h_3 + h_4 + h_5 = h_5 + h_6 + h_1 \\ a_0 + a_1 = h_1 + h_2 + h_3 + h_4 + h_5 + h_6 = L \end{cases} \tag{S1}$$

where L is the integer perimeter of the given equiangular hexagon. Since h_1, h_2, h_3, h_4, h_5, and h_6, are all positive integers, according to Eq. (S1), both a_0 and a_1 are positive integers as well.

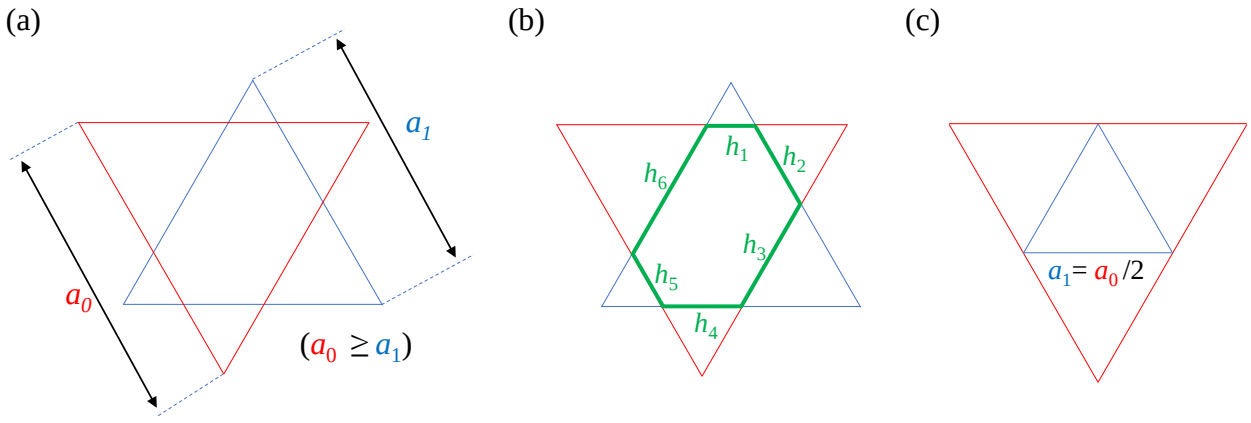


Figure S21. Schematic diagram of the construction of equiangular hexagon. (a) Equiangular hexagons constructed from the intersection between two appropriate equilateral triangles with the side lengths of a_0 and a_1 (let $a_0 \geq a_1$). (b) Equiangular hexagon surrounded by green lines indicates the superhexagon formed by benzene rings, the side lengths of which (h_1, h_2, h_3, h_4, h_5, and h_6) define the structural notation of a kekulene or a clarene. (c) Limit for the side lengths of equilateral triangles to ensure a valid equiangular hexagon. Equiangular hexagon can not be constructed when a_1 is less than or equal to half of a_0.

To sum up, the side lengths of the two equilateral triangles have the following constraint.

$$\begin{cases} a_0/2 < a_1 \leq a_0 \\ a_0 + a_1 = L \\ a_0, a_1 \in \mathbb{Z}^+ \end{cases} \tag{S2}$$

Next, we determine the value of the side lengths of the equiangular hexagon, h_1, h_2, h_3, h_4, h_5, and h_6, which can be achieved by the following steps.

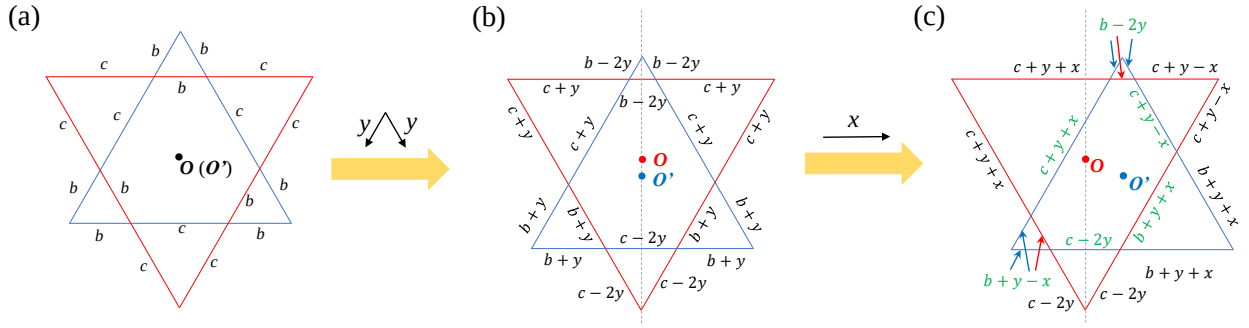


Figure S22. Construction steps of equiangular hexagons of any shape. (a) Two equiangular triangles with their centers, O and O', coincide each other. (b) Slide the smaller triangle vertically by amount of y ($y > 0$ for downward slide and $y < 0$ for upward slide). (c) Slide the smaller triangle horizontally to the right by amount of x (let $x \geq 0$).

Step 1: Place the two equiangular triangles in such a way that their centers, O and O', coincide each other, as shown in Fig. S22(a). As we can see:

$$\begin{cases} b + 2c = a_0 \\ 2b + c = a_1 \end{cases} \tag{S3}$$

And then we can deduce the value of b, and c,

$$\begin{cases} b = \dfrac{2a_1 - a_0}{3} \\ c = \dfrac{2a_0 - a_1}{3} \end{cases} \tag{S4}$$

Since $a_0 \geq a_1$, it is easy to show that $b \leq c$. As a_0 and a_1 are positive integers, both b and c are positive multiples of $1/3$.

Step 2: Slide the smaller triangle vertically by amount of y ($y > 0$ for downward slide and $y < 0$ for upward slide), as shown in the Fig. S22(b). We can see that the downward

slide ($y > 0$) and the upward slide ($y < 0$) give rise to different results. So, y can be positive, negative or zero.

Step 3: Slide the smaller triangle horizontally to the right by amount of x, as shown by the Fig. S22(c). Because of bilateral symmetry, the rightward slide and the leftward slide by the same amount lead to equivalent results. Hence, we only need to consider the case with $x \geq 0$.

As a result, the six side lengths of the equiangular hexagon are:

$$\begin{cases} h_1 = b - 2y \\ h_2 = c - x + y \\ h_3 = b + x + y \\ h_4 = c - 2y \\ h_5 = b - x + y \\ h_6 = c + x + y \end{cases} \tag{S5}$$

We can quickly check that: $L = (b - 2y) + (c + y - x) + (b + y + x) + (c - 2y) + (b + y - x) + (c + y + x) = 3(b + c)$. Plugging Eq. (S4) into this equation, we verify that $L = (2a_1 - a_0) + (2a_0 - a_1) = a_0 + a_1$.

The parameters b, c, x and y in Eq. (S5) are subject to some constraints, which can be worked out as follows.

From $a_0 + a_1 = L$ and $a_0/2 < a_1 \leq a_0$, we have

$$\frac{L}{2} < a_0 \leq \frac{2L}{3} \tag{S6}$$

As $h_1 = b - 2y \geq 1$, it follows that $y \leq (b-1)/2$. As $h_5 = b - x + y \geq 1$, then $x \leq b + y - 1$. Thereby, we also have that $y \geq x - b + 1 \geq -b + 1$ (since x is nonnegative as mentioned before). Therefore, x and y are subject to the following constraints:

$$\begin{cases} -(b-1) \leq y \leq \dfrac{b-1}{2} \\ 0 \leq x \leq b + y - 1 \end{cases} \tag{S7}$$

Note that just as the values of b, c are multiples of $1/3$, the values of y are multiples of $1/6$ since the upper boundary of y is $(b-1)/2$. Likewise, x values are also multiples of $1/6$. We should also be aware that the minimum value of y is exactly $-(b-1)$ when $x = 0$ and $h_5 = 1$, while the maximum value of y is exactly $(b-1)/2$ when $h_1 = 1$. By varying continually y value from $-(b-1)$ to $(b-1)/2$, we obtain a series of side lengths of the hexagon, h_1, h_2, h_3,

h_4, h_5, and h_6, which are all integers. Therefore, the variation stepsize of y value between $-(b-1)$ and $(b-1)/2$ must be an integer, otherwise h_5 and h_1 are not integer numbers. That is to say, the valid y values are $-(b-1), -(b-1)+1, -(b-1)+2, -(b-1)+3, \ldots, (b-1)/2$. For the same reason, the valid values for x are $0, 1, 2, \ldots, b+y-1$.

Based on the above discussion, we can propose a simple algorithm for enumeration of all possible equiangular hexagons with a given integer perimeter, as follow:

1. Given an integer number, L, for the perimeter of equiangular hexagons, we choose all eligible values of a_0 and a_1, as follows (Eq. (S6)):

$$\begin{cases} \dfrac{L}{2} < a_0 \leq \dfrac{2L}{3} \quad (\text{a}_0 \text{ being an integer}) \\ a_1 = L - a_0 \end{cases} \tag{S8}$$

Once a_0 and a_1 are chosen, we then have the corresponding values of b and c (Eq. (S4)):

$$\begin{cases} b = \dfrac{2a_1 - a_0}{3} \\ c = \dfrac{2a_0 - a_1}{3} \end{cases} \tag{S9}$$

2. For every selection of a_0, a_1, b and c values, we choose all eligible values of y by running over the following range (Eq. (S7)):

$$y = -(b-1), -(b-1)+1, -(b-1)+2, ..., \frac{b-1}{2} \tag{S10}$$

3. And for every selection of y, we choose all eligible values of x by running over the following range (Eq. (S7)):

$$x = 0, 1, 2, ..., b+y-1 \tag{S11}$$

4. For each selection of values of b, c, y and x, we obtain the side lengths of a possible equiangular hexagon using Eq. (S5)

5. From all equiangular hexagons generated using the above procedures, we remove the duplicate or symmetrically equivalent ones. Thus, all possible equiangular hexagons with a given perimeter of L is enumerated.

7 Simple HMO model for predicting relative energies of clarenes

Fig. S23-S24 show the good correlation between π energy predicted by HMO, E_{HMO} and the DFT relative energies of clarene isomers, $\mathrm{RE_{B3LYP}}$.

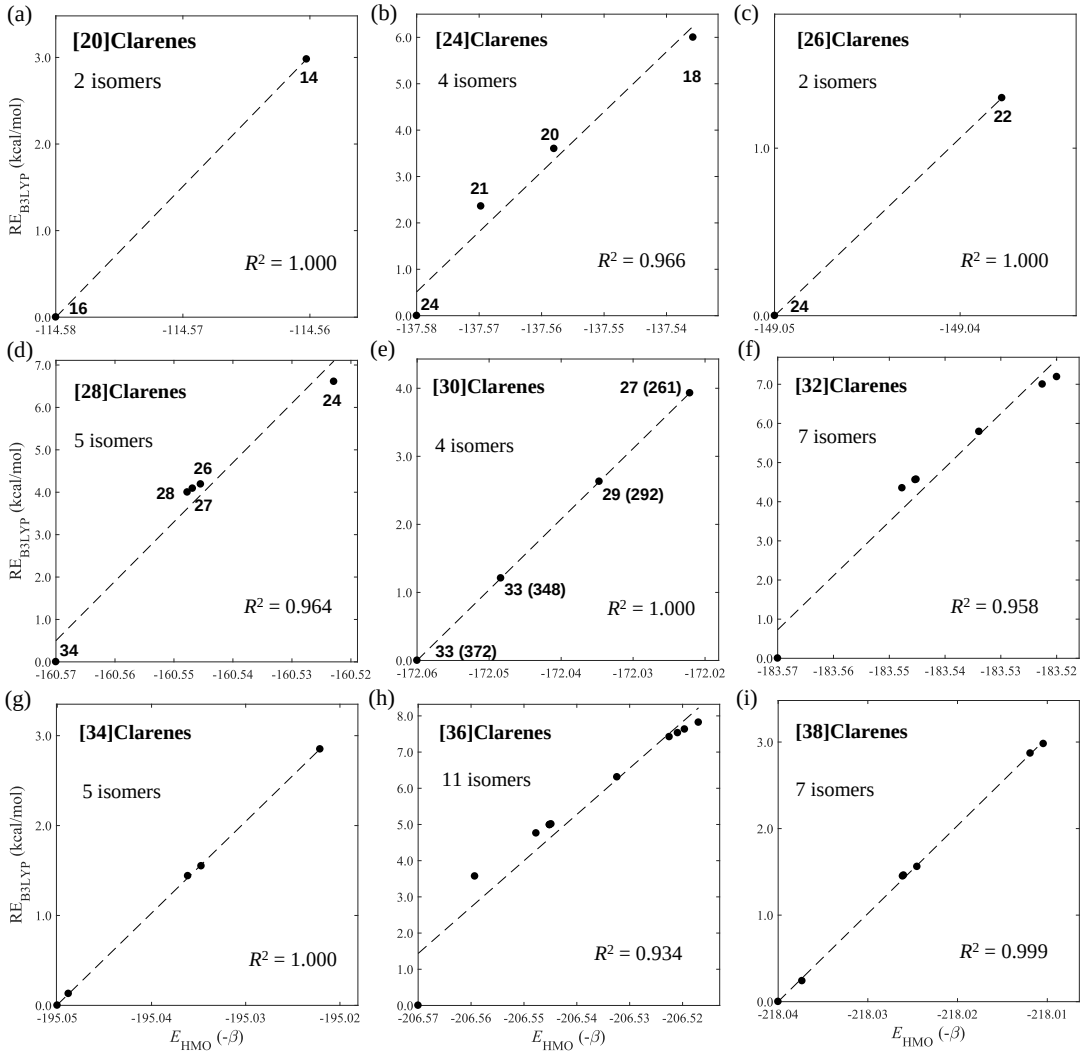


Figure S23. DFT relative energies, $\mathrm{RE_{B3LYP}}$, versus HMO π energies, E_{HMO}, for (a) [20]clarenes, (b)-(i) [24]clarenes to [38]clarenes. In (a)–(e), the number of Clar resonators with the second largest number of sextets are represented by black bold numbers. In (e), the numbers in brackets indicate the number of Clar resonators with the third largest number of sextets.

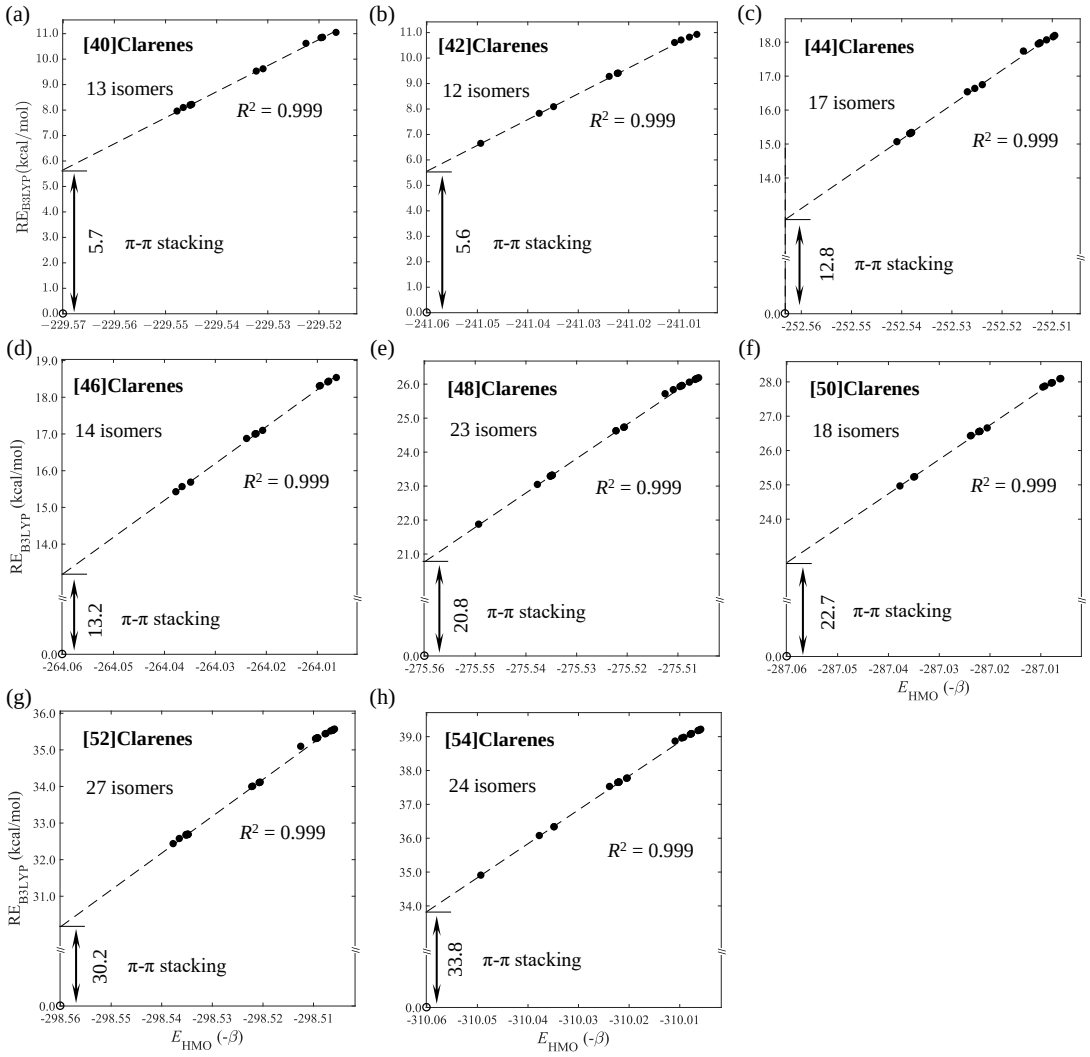


Figure S24. Idem Fig. S23 for clarenes of 40 to 54 rings. Structures with $\pi-\pi$ stacking are indicated by hollow symbols. The intercept of the y axis in (c)–(h) represents $\pi-\pi$ stacking effect. Squared correlation coefficients (R^2) are only for filled symbols.

8 IRI maps for $\pi-\pi$ stacking in equiangular hexagonal clarenes

Fig. S25-S26 shows IRI[15] maps for the lowest-energy isomers of [48] and [60]clarenes. As we can see, the region between the two longest opposite sides of clarenes is dominated by the IRI isosurface with green color, indicating clearly the existence of $\pi-\pi$ stacking in the clarenes.

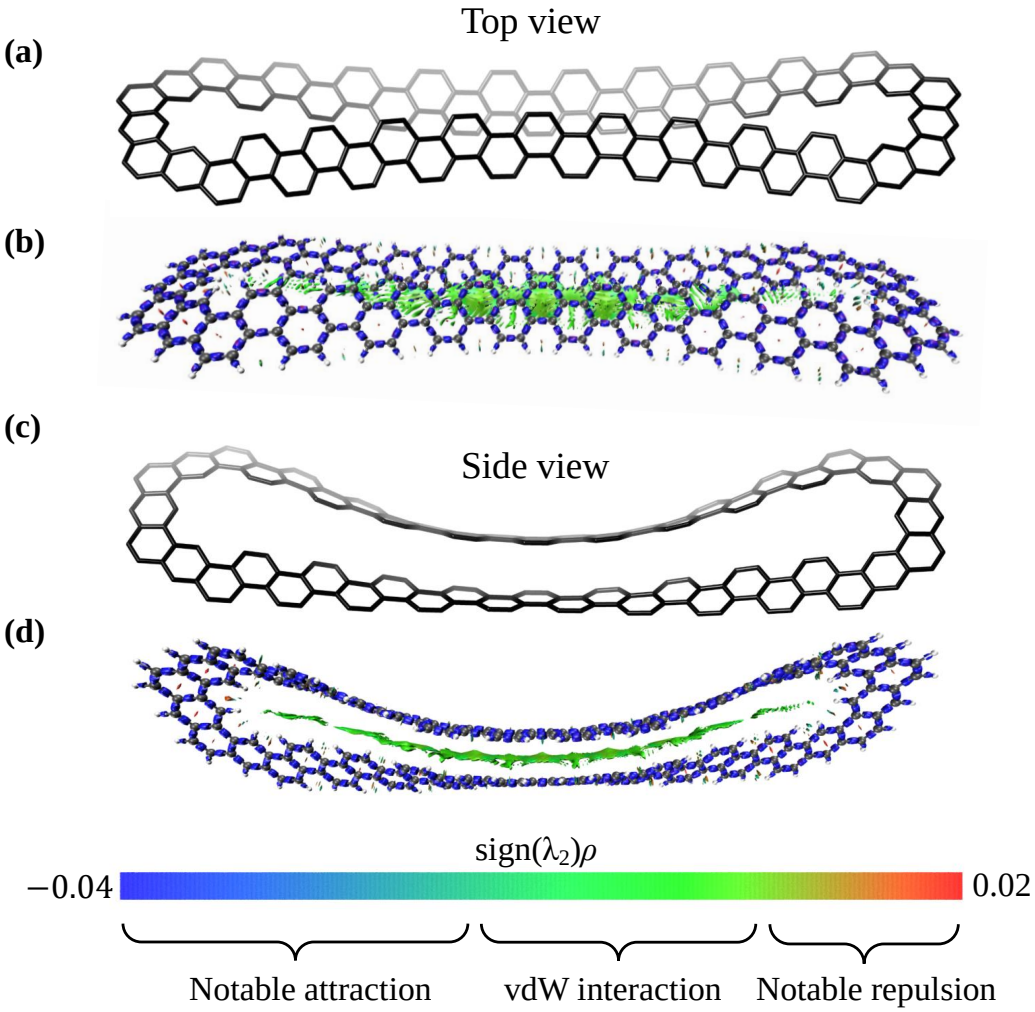


Figure S25. (a) Top view and (c) side view of the optimized structure calculated at the ωB97XD/cc-pVDZ level for the lowest-energy isomer of [48]clarene <2,2,20,2,2,20>. (b) Top view and (d) side view of the sign(λ_2)ρ mapped isosurface of IRI = 1.0 for the same molecule. The color bar below denotes the different types of noncovalent interactions, as represented by the colors of the isosurface.

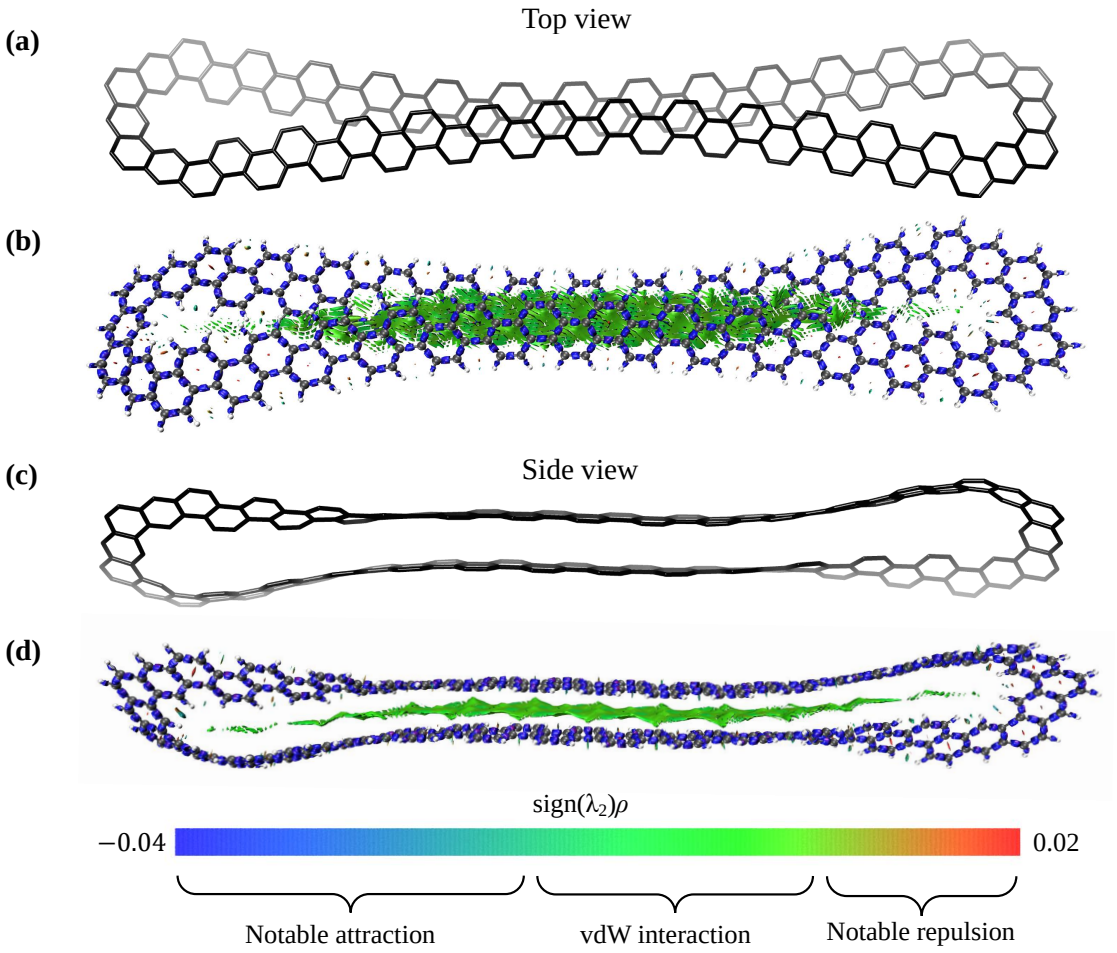


Figure S26. Idem Fig. S25 for the lowest-energy isomer of [60]clarene <2,2,26,2,2,26>.

9 Demonstration of construction of nonequiangular hexagons

For [42], [46], [50], [54], and [58]clarenes, we additionally construct nonequiangular hexagonal clarenes with distorted structures based on stadium-type clarenes ($N_{\mathrm{ring}} = 44$, 48, 52, 56, 60) with distorted structures to obtain more stable isomers at the same ring sizes. Fig. S27(a) shows the construction diagram of the nonequiangular stadium-type hexagons, and we only need to deduct two rings from either long side of clarenes. For stadium-type structure of [60]clarene, <2,2,26,2,2,26>, we also considered the nonequiangular stadium-type structures of [60]clarene, <2,2,24,2,2,28> and <2,2,22,2,2,30>, as shown in Fig. S27(b).

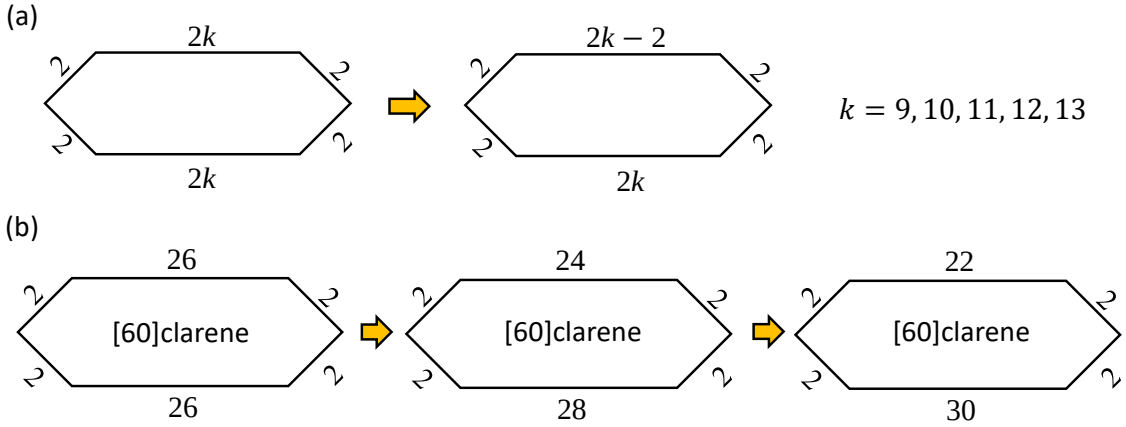


Figure S27. Construction method of nonequiangular hexagons. Side lengths represent the valid number of benzene rings as mentioned in Section 3.1 in main text.

10 Simple HMO model for predicting relative energies of kekulenes

Fig. S28-S29 show the correlation between π energy predicted by HMO, E_{HMO} and the DFT relative energies of kekulene isomers, $\mathrm{RE_{B3LYP}}$. The relative energies of isomers are good correlation with π energy predicted by HMO with squared correlation coefficient (R^2) higher than 0.9.

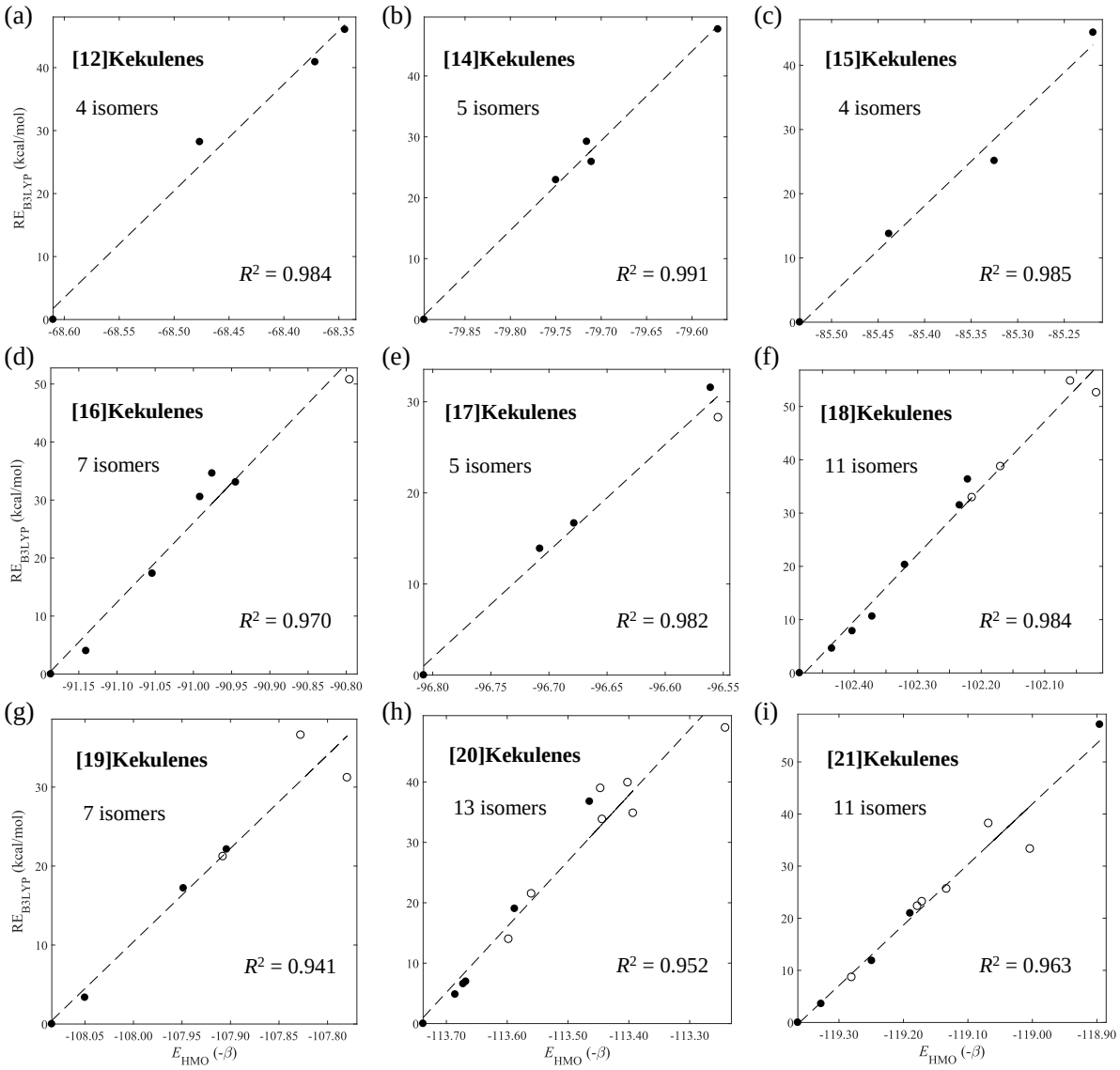


Figure S28. DFT relative energies, $\mathrm{RE_{B3LYP}}$, versus HMO π energies, E_{HMO}, for kekulenes of 12 to 21 rings. Closed shell structures and open-shell singlet structures are represented by black filled circle and black hollow circle, respectively. Squared correlation coefficients (R^2) are provided in each plot.

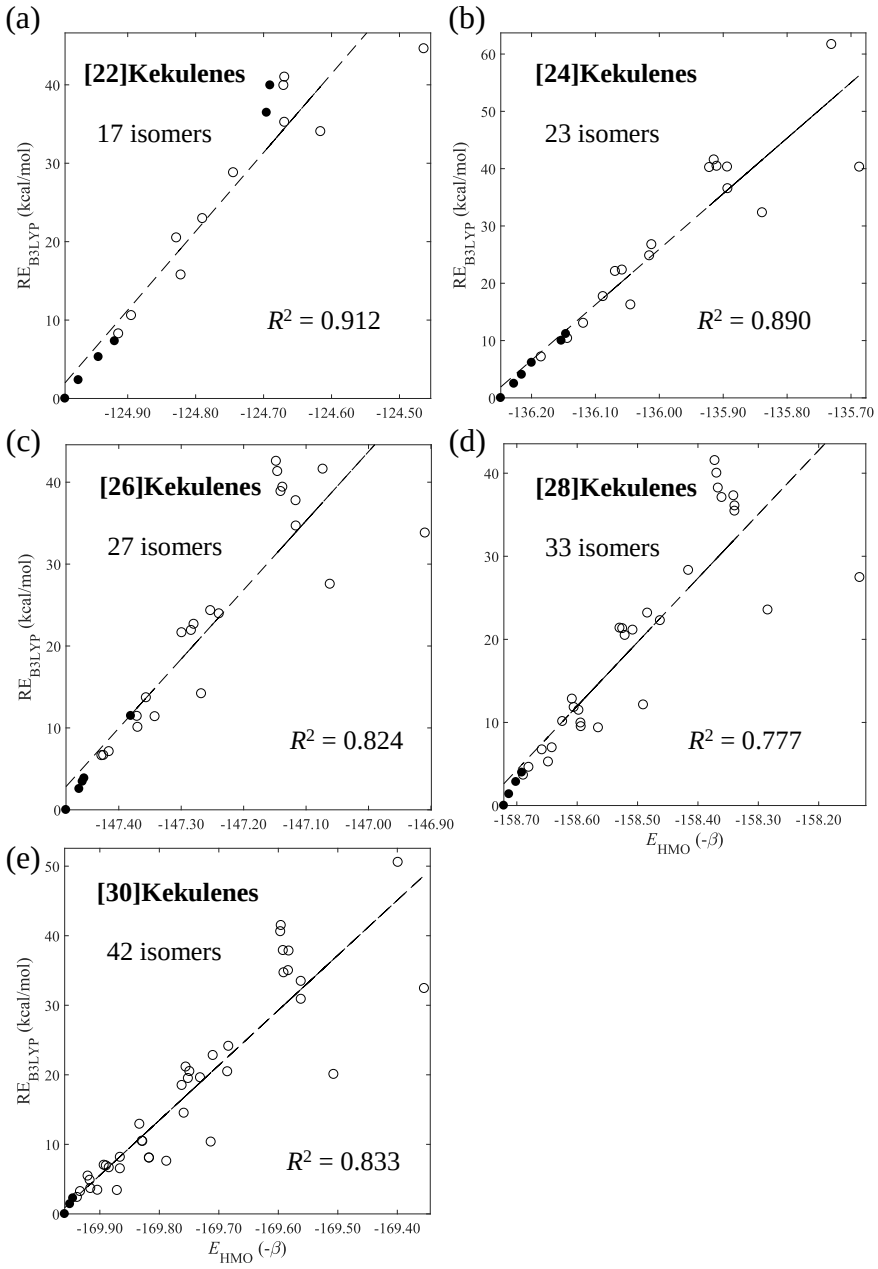


Figure S29. Idem Fig. S28 for kekulenes of 22 to 30 rings.

11 Lowest-energy kekulene and clarene isomers

Tables S1 and S2 list the relative energies of lowest-energy kekulenes and clarenes relative to the lowest-energy isomer of cycloarenes of same molecular size, and corresponding structures are shown in Fig. S30-S34.

Table S1. Lowest-energy isomers of kekulenes with the number of rings (N_{ring}) from 8 to 60. We also present the ωB97XD/cc-pVDZ relative energies (RE) of these isomers relative to lowest-energy isomer of cycloarenes.

N_{ring}	Kekulene	RE(kcal/mol)	N_{ring}	Kekulene	RE(kcal/mol)
8	[1,1,2,1,1,2]	0.00	21	[3,4,3,4,3,4]	0.00
9	[1,2,1,2,1,2]	0.00	22	[3,4,4,3,4,4]	45.63
10	[1,2,2,1,2,2]	0.00	24	[4,4,4,4,4,4]	61.32
11	[1,2,2,2,1,3]	0.00	26	[4,4,5,4,4,5]	72.70
12	[2,2,2,2,2,2]	0.00	28	[4,5,5,4,5,5]	91.59
13	[1,3,2,2,2,3]	0.00	30	[5,5,5,5,5,5]	103.77
14	[2,2,3,2,2,3]	0.00	32	[4,4,8,4,4,8]	116.40
15	[2,3,2,3,2,3]	0.00	34	[4,4,9,4,4,9]	123.46
16	[2,3,3,2,3,3]	15.68	36	[4,4,10,4,4,10]	139.82
17	[2,3,3,3,2,4]	0.00	42	[2,2,17,2,2,17]	173.87
18	[3,3,3,3,3,3]	21.96	48	[1,2,21,1,2,21]	208.90
19	[2,4,3,3,3,4]	0.00	54	[2,2,23,2,2,23]	245.62
20	[3,3,4,3,3,4]	36.28	60	[1,2,27,1,2,27]	280.44

Table S2. Idem Table S1 for Clarenes with the number of rings (N_{ring}) from 16 to 60.

N_{ring}	Clarene	RE(kcal/mol)	N_{ring}	Clarene	RE(kcal/mol)
16	<2, 2, 4, 2, 2, 4>	0.00	42	<2, 2, 16, 2, 2, 18>[a]	0.00
18	<2, 4, 2, 4, 2, 4>	0.00	44	<2, 2, 18, 2, 2, 18>	0.00
20	<2, 2, 6, 2, 2, 6>	0.00	46	<2, 4, 16, 4, 2, 18>	12.56
22	<2, 4, 4, 4, 2, 6>	0.00	46	<2, 2, 18, 2, 2, 20>[a]	0.00
24	<2, 2, 8, 2, 2, 8>	0.00	48	<2, 2, 20, 2, 2, 20>	0.00
26	<2, 4, 6, 4, 2, 8>	0.00	50	<2, 4, 18, 4, 2, 20>	22.66
28	<2, 2, 10, 2, 2, 10>	0.00	50	<2, 2, 20, 2, 2, 22>[a]	0.00
30	<2, 8, 2, 8, 2, 8>	0.00	52	<2, 2, 22, 2, 2, 22>	0.00
32	<2, 2, 12, 2, 2, 12>	0.00	54	<2, 16, 2, 16, 2, 16>	32.34
34	<2, 4, 10, 4, 2, 12>	0.00	54	<2, 2, 22, 2, 2, 24>[a]	0.00
36	<2, 2, 14, 2, 2, 14>	0.00	56	<2, 2, 24, 2, 2, 24>	0.00
38	<2, 4, 12, 4, 2, 14>	0.00	58	<2, 4, 22, 4, 2, 24>	44.51
40	<2, 2, 16, 2, 2, 16>	0.00	58	<2, 2, 24, 2, 2, 26>[a]	0.00
42	<2, 12, 2, 12, 2, 12>	3.92	60	<2, 2, 26, 2, 2, 26>	0.00

[a] represent nonequiangular hexagonal clarenes.

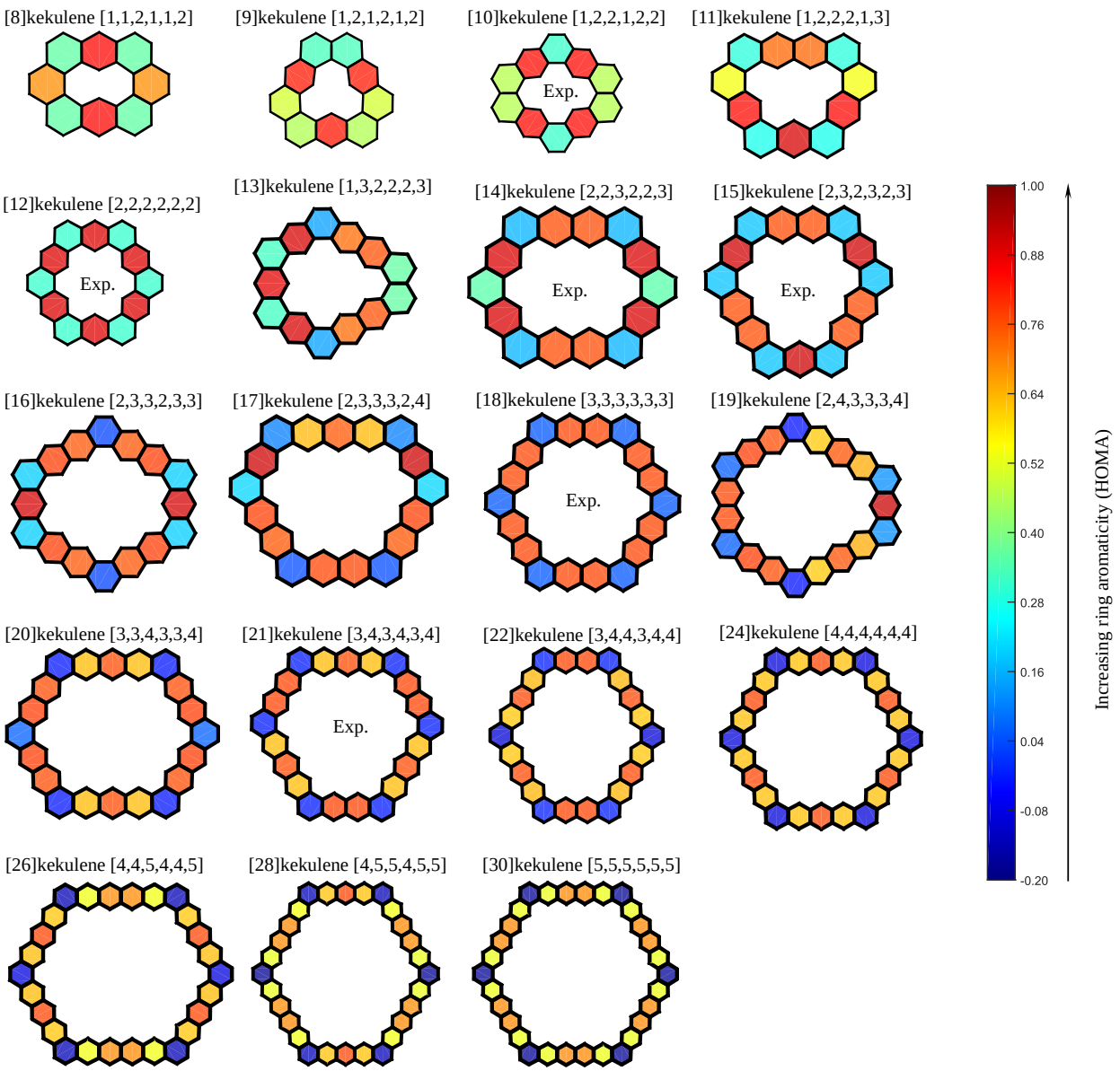


Figure S30. Structures of the most stable isomers of kekulenes of 8 to 30 rings. The rings are colorized according to the ωB97XD/cc-pVDZ computed HOMA[16] values.

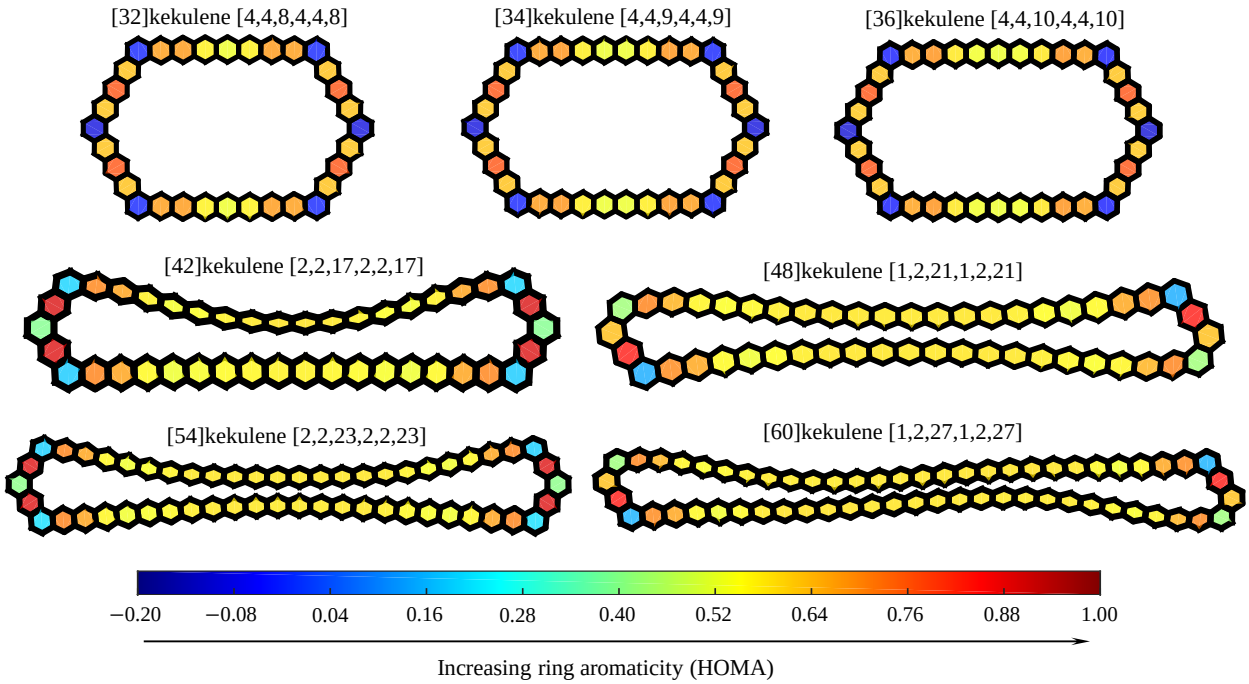


Figure S31. Idem Fig. S30 for the lowest-energy isomers of kekulenes of 32 to 60 rings.

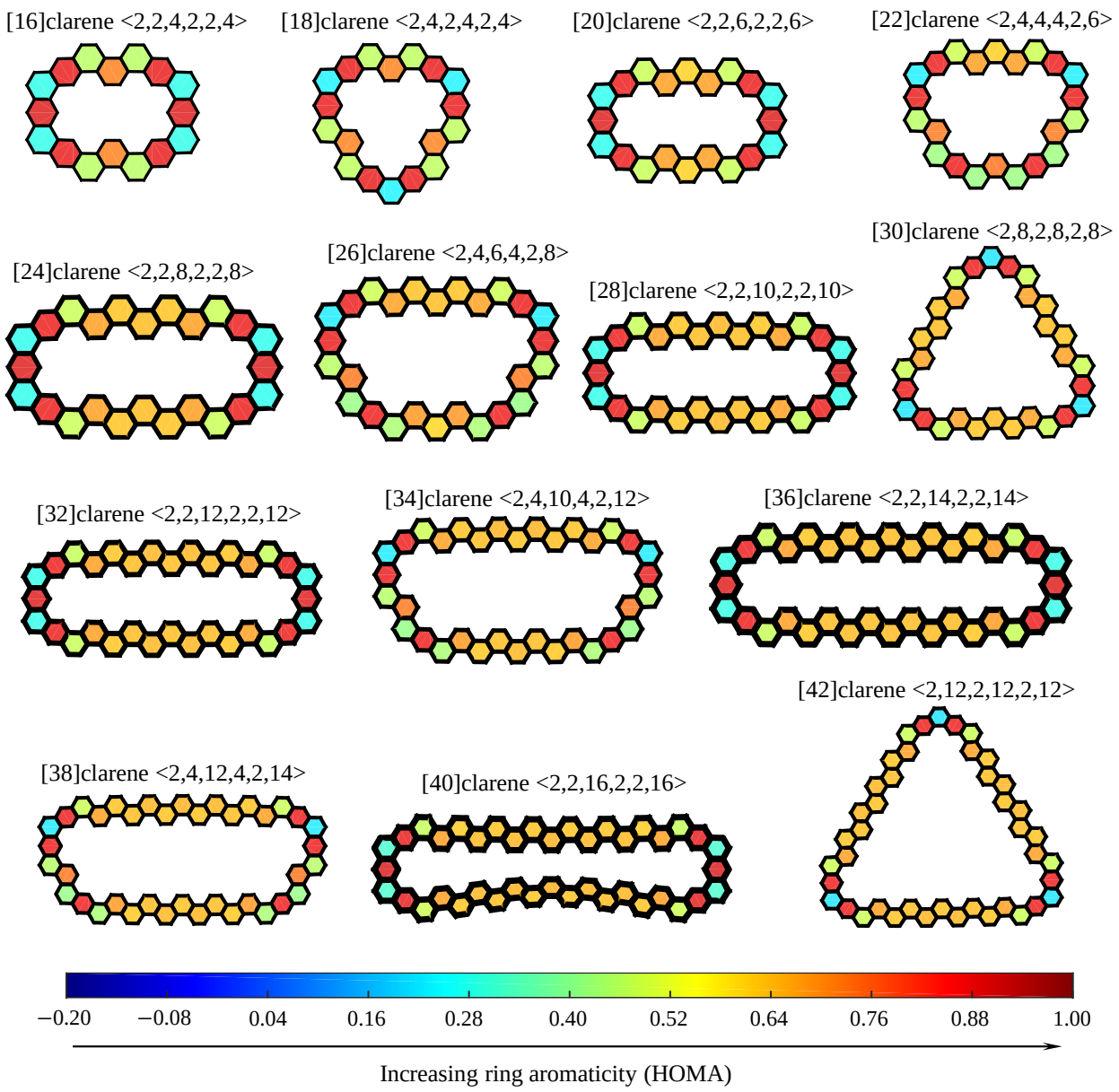


Figure S32. Idem Fig. S30 for the lowest-energy isomers of clarenes of 16 to 42 rings.

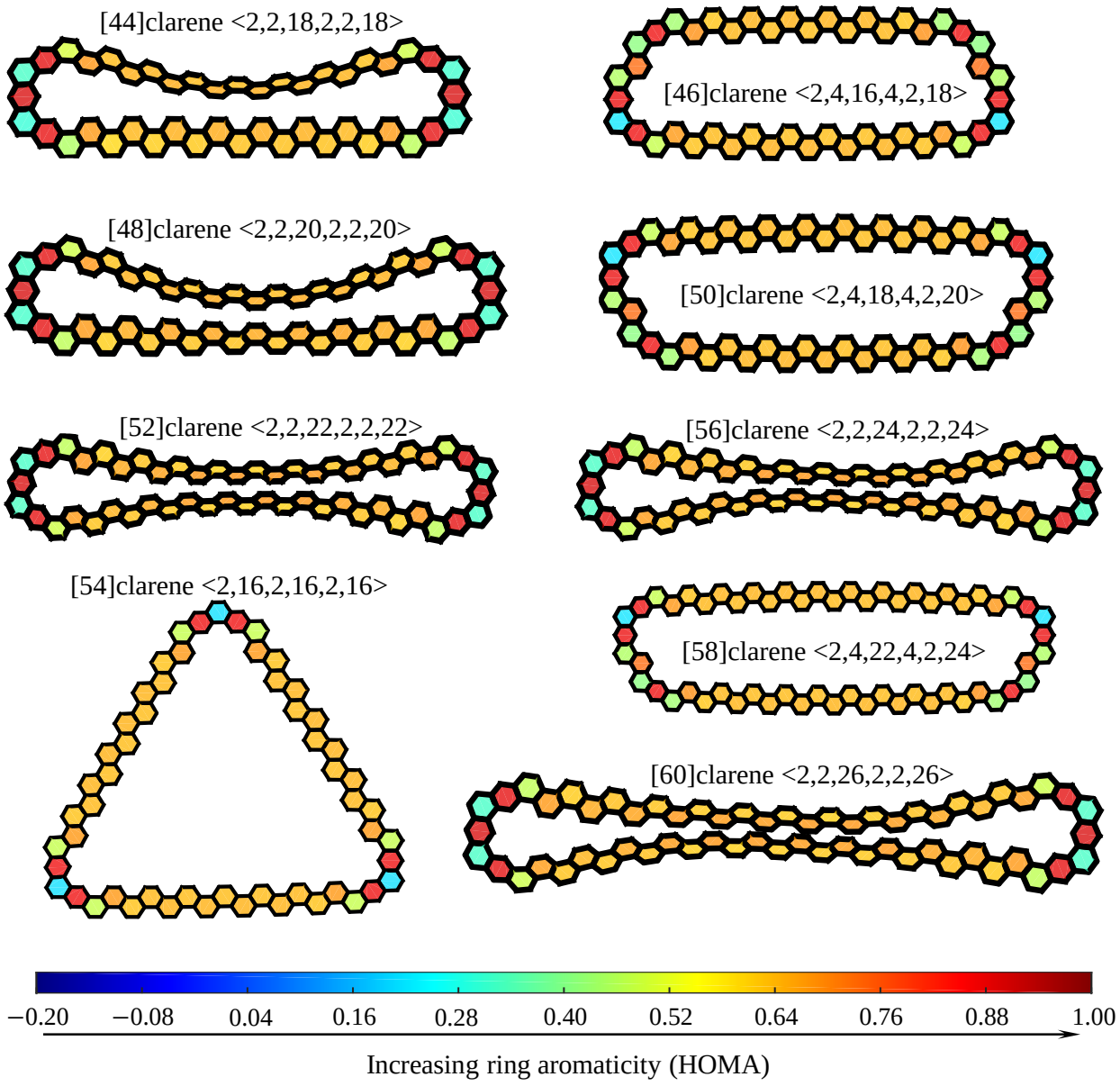


Figure S33. Idem Fig. S30 for the lowest-energy isomers of clarenes of 44 to 60 rings.

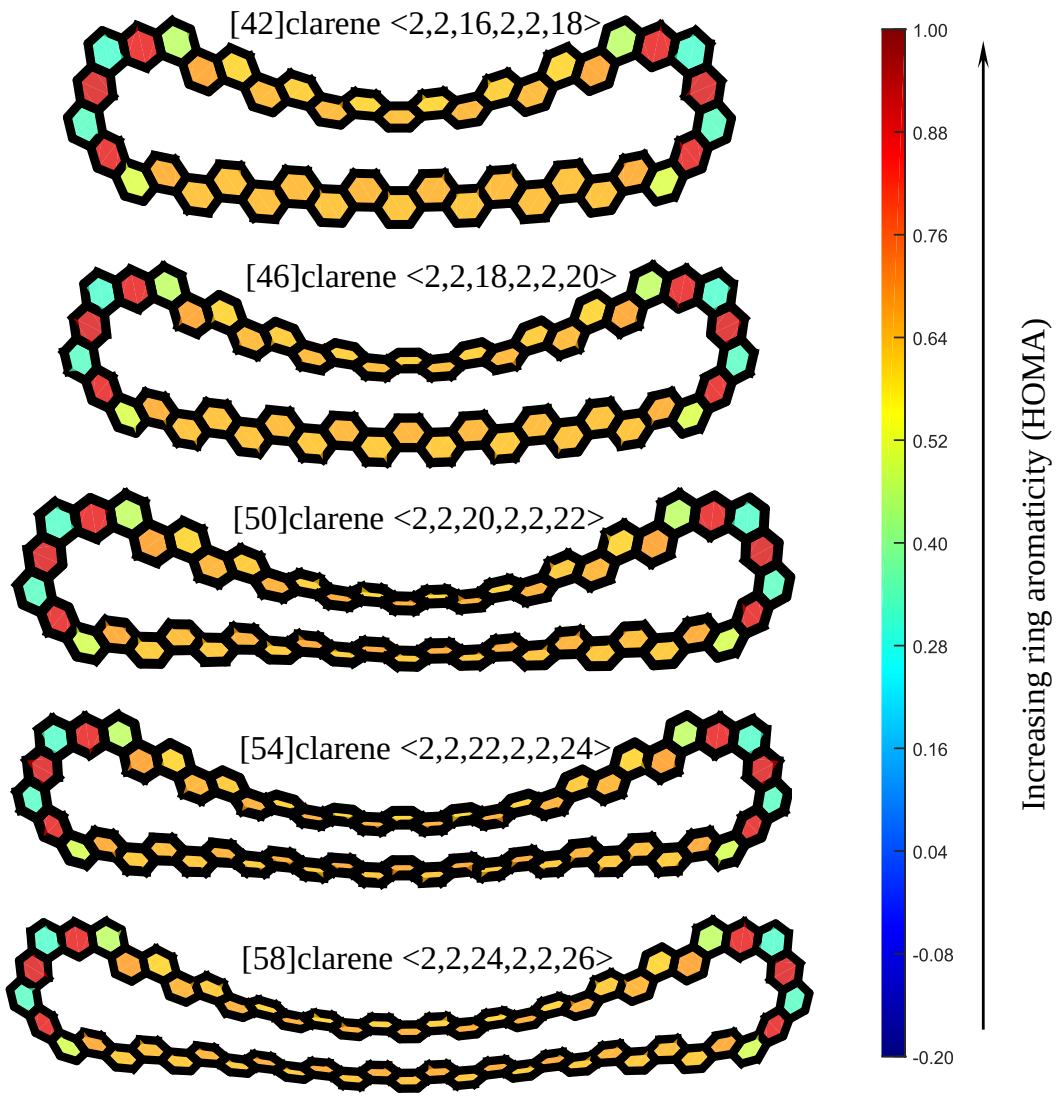


Figure S34. Idem Fig. S30 for the lowest-energy nonequiangular hexagonal clarene structures from 42 to 58 rings.

12 Clar resonance structures for [30]clarene <2,8,2,8,2,8>

In Fig. S35, we show some representative Clar resonators[17] with different number of sextets for [30]clarene <2,8,2,8,2,8>.

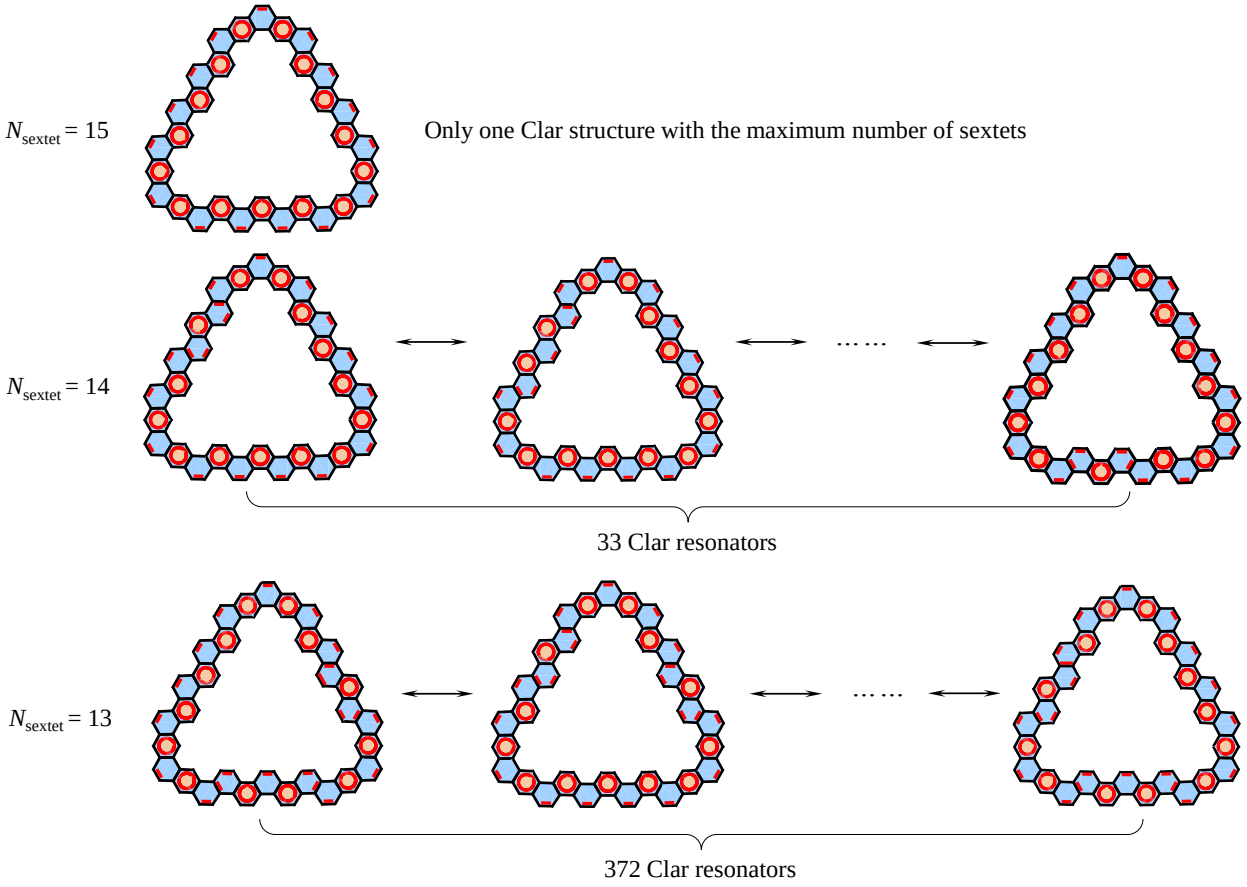


Figure S35. Clar resonators for [30]clarene <2,8,2,8,2,8> with the number of sextets, N_{sextet} = 13, 14, 15. Clar sextets are represented by red circles.

13 IRI maps for $\pi-\pi$ stacking in nonequiangular hexagonal clarenes

Fig. S36-S37 shows the IRI[15] maps for the lowest-energy isomers of [50] and [54]clarenes. As we can see, the region between the longest opposite sides of clarenes is dominated by the IRI isosurface with green color, indicating clearly the existence of $\pi-\pi$ stacking in the clarenes.

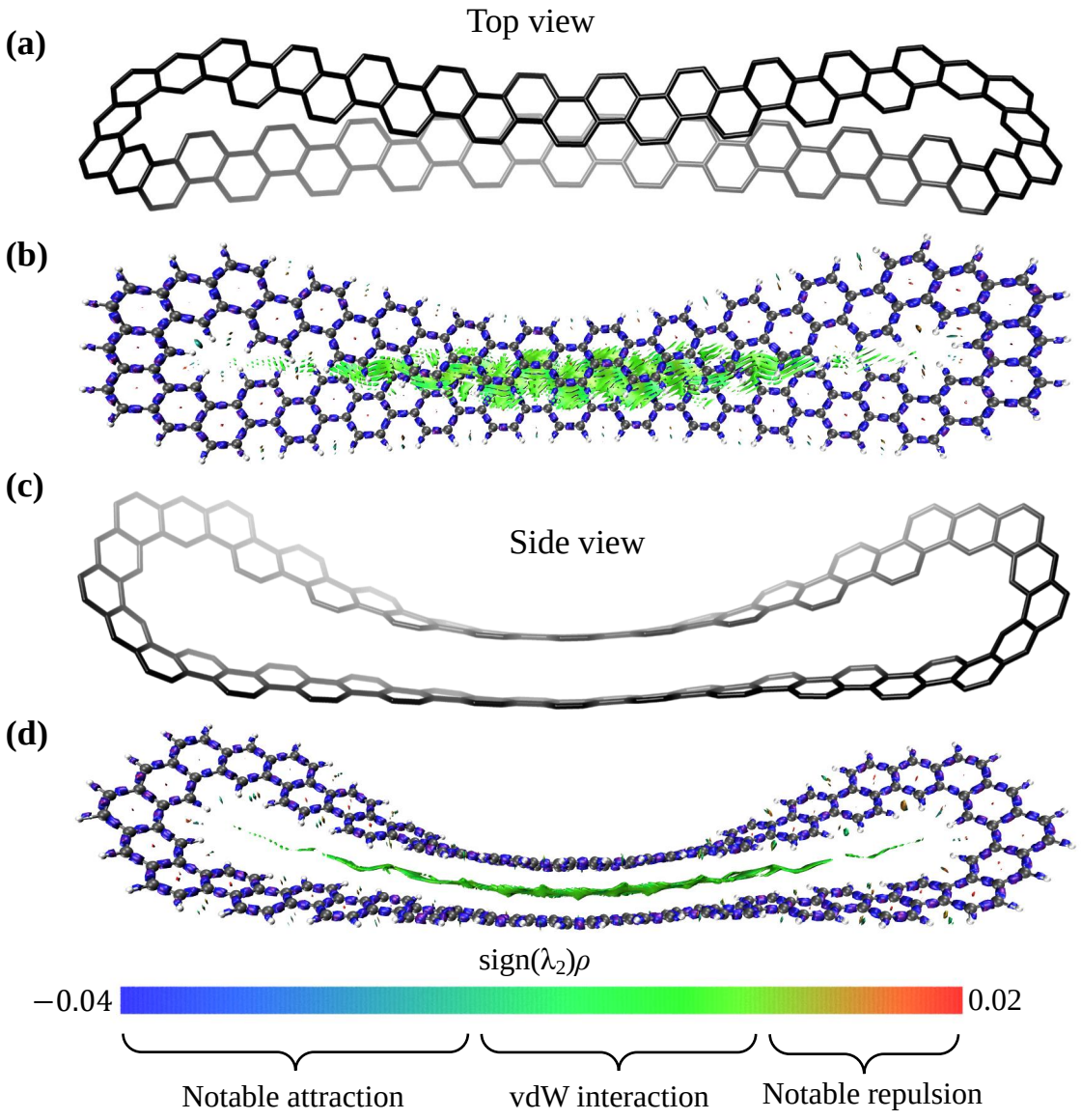


Figure S36. Idem Fig. S25 for the lowest-energy isomer of [50]clarene <2,2,20,2,2,22>.

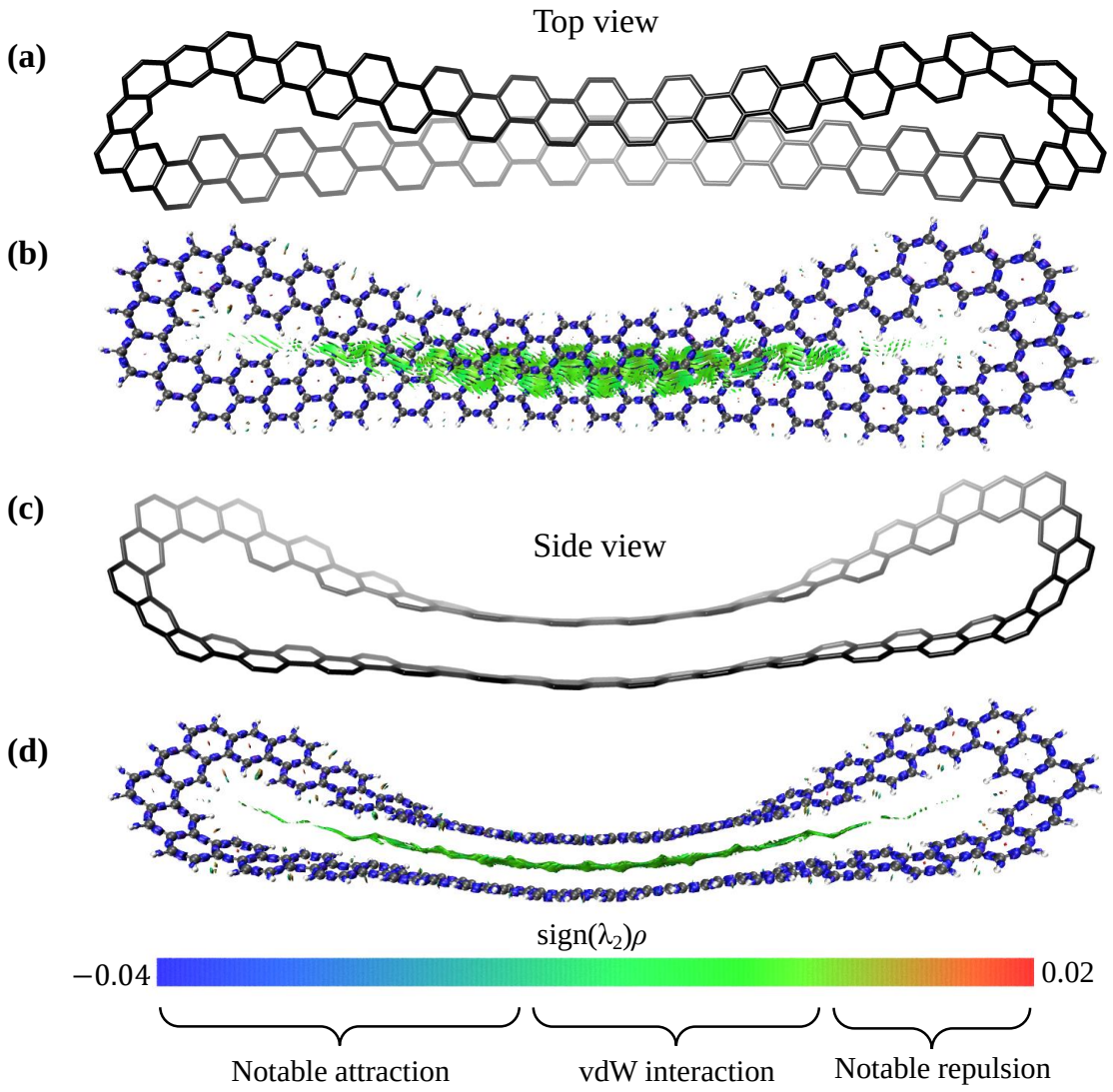


Figure S37. Idem Fig. S25 for the lowest-energy isomer of [54]clarene <2,2,22,2,2,24>.

14 Relative stability of $\pi-\pi$ stacking conformers

We consider three isomers of [60]clarenes (<2,2,26,2,2,26>, <2,2,24,2,2,28> and <2,2,22,2,2,30>) and search all possible conformers for each isomer, 37 in total, as shown in Table S3. Different conformers of each isomer can be converted into each other. Obviously, for [60]clarene <2,2,22,2,2,30> (see Fig. S38(c) and (d)), the relative shift between the longest opposite sides of clarene can cause the existence of different conformers.

Table S3. Different conformers of each isomer and corresponding relative energies with respect to lowest-energy conformers. Labels represent different conformers.

<2,2,26,2,2,26>		<2,2,24,2,2,28>		<2,2,22,2,2,30>	
Labels	RE(kcal/mol)	Labels	RE(kcal/mol)	Labels	RE(kcal/mol)
1	0.97	1	0.00	1	2.73
2	0.83	2	0.02	2	2.73
3	0.97	3	0.01	3	2.74
4	0.97	4	0.02	4	0.03
5	0.97	5	0.02	5	0.00
6	0.97	6	0.01	6	0.03
7	0.97	7	0.01	7	0.02
8	0.00	8	0.01	8	0.02
9	0.00	9	0.01	9	0.01
10	0.00	10	0.01	10	0.02
11	0.00	11	0.01	11	0.00
12	0.00	12	0.01	-	-
13	0.00	13	0.01	-	-

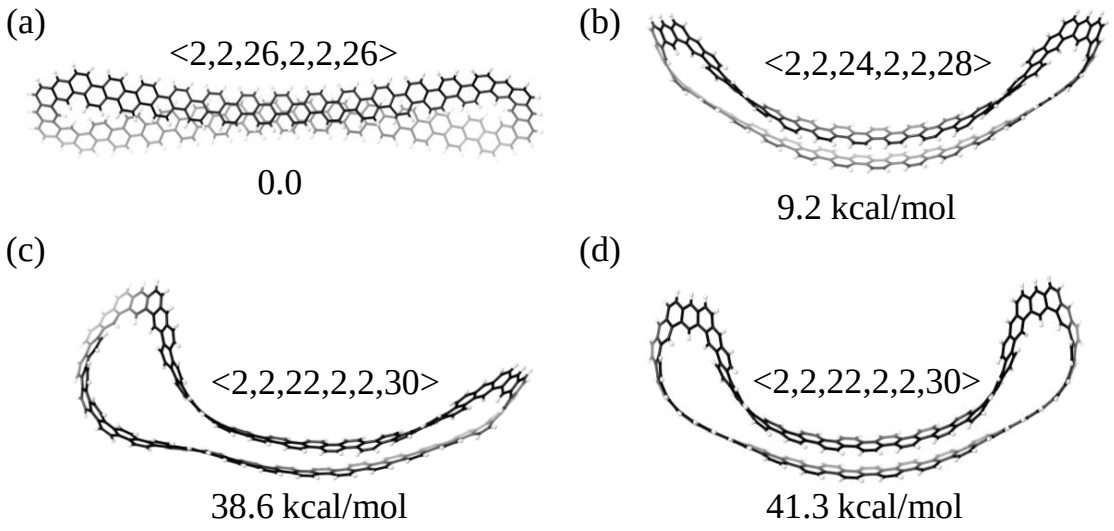


Figure S38. (a)-(c) Structures of lowest-energy $\pi-\pi$ stacking conformers for [60]clarenes, <2,2,26,2,2,26>, <2,2,24,2,2,28> and <2,2,22,2,2,30>, respectively. (d) The most unstable $\pi-\pi$ stacking conformers of [60]clarenes <2,2,22,2,2,30>. Relative energies computed at the B3LYP-D3(BJ)/6-31G* level are given below each conformer structure in kcal/mol.

15 Cartesian coordinates and absolute energies for lowest-energy kekulene and clarene isomers

In the following, we provide the Cartesian coordinates of the lowest-energy isomers of kekulene and clarene isomers, optimized at the wB97XD/cc-pVDZ level. For each molecule, we provide the absolute energies. All energies are given in Hartree and the atomic coordinates are in Å.

1. **[8]kekulene [1,1,2,1,1,2]**

```
E(wB97XD/cc-pVDZ) = -1228.73389954
No imaginary frequency (B3LYP/6-31G*)

6    -0.84157700 -0.28430300 0.42460100
6    0.51560700 -0.17520800 0.28782000
6    0.28089500 2.14064500 -0.47960400
6    1.10172200 1.03398600 -0.16962600
6    2.53559900 1.14844800 -0.28271600
1    3.13822600 0.27734000 -0.01615600
6    3.13752700 2.31543200 -0.62601300
6    2.35069400 3.44851800 -1.03334800
6    0.93647300 3.27885600 -1.13337600
1    -1.29498500 -1.23701600 0.70640400
1    1.16366300 -1.02904700 0.49661900
1    4.22593700 2.40370300 -0.61903400
6    -4.24024800 4.17325000 -0.43157700
6    -3.42780400 3.06669300 -0.14715900
6    -2.01550900 3.25422900 -0.05203400
6    -1.54374800 4.56629700 -0.05231900
6    -3.95106000 1.75171000 0.10973400
6    -1.11287600 2.09800800 -0.08331500
6    -1.67986200 0.84731000 0.24655000
6    -3.11191200 0.71579500 0.36425600
1    -5.03335000 1.60663500 0.11818900
1    -5.32692100 4.05764700 -0.42681100
1    -3.51441700 -0.27135200 0.60208500
6    2.91108200 4.68474600 -1.38437400
6    2.09863900 5.79130400 -1.66877900
6    0.68634000 5.60377400 -1.76387900
6    0.21456800 4.29171100 -1.76357800
6    2.62189500 7.10628700 -1.92567900
6    -0.21628600 6.76000100 -1.73258100
6    0.35069900 8.01069600 -2.06246100
6    1.78275000 8.14220500 -2.18018800
1    3.70418700 7.25135600 -1.93415000
1    3.99775500 4.80034300 -1.38915500
1    2.18525400 9.12935000 -2.41802800
6    -3.67986000 5.40947900 -0.78259000
6    -2.26564200 5.57914700 -0.68253700
6    -1.61005400 6.71736700 -1.33628900
6    -2.43088200 7.82402400 -1.64627400
6    -3.86476100 7.70955700 -1.53320000
6    -4.46669100 6.54256900 -1.18992300
6    -0.48758400 9.14231000 -2.24050800
6    -1.84476800 9.03321600 -2.10372100
1    -4.46738700 8.58066600 -1.79976300
1    -5.55510100 6.45429400 -1.19691700
1    -0.03417700 10.09502000 -2.52232300
1    -2.49282500 9.88705400 -2.31252700
1    -0.52583500 4.76026900 0.25934000
1    -0.80336400 4.09774900 -2.07519100
```

2. **[9]kekulene [1,2,1,2,1,2]**

```
E(wB97XD/cc-pVDZ) = -1382.34916085
No imaginary frequency (B3LYP/6-31G*)

6    -0.00817800 4.21006300 -0.22489300
6    -0.00549100 2.83019600 -0.45677500
6    -1.30461300 2.13831100 -0.41243500
6    -2.48780400 2.84189300 -0.00660400
6    -2.42738200 4.27229100 0.10783900
6    -1.24538100 4.92238100 -0.03241600
6    -1.46761900 0.76604900 -0.61101100
6    -3.67695700 2.13529000 0.24179100
6    -3.73079600 0.73413000 0.23061700
6    -2.54901700 0.02913400 -0.13245200
6    -2.48552000 -1.41868200 -0.02391300
6    -3.67669400 -2.12614200 0.12753200
6    -4.89707100 -1.39828800 0.37186900
6    -4.91736300 -0.04057000 0.48263500
1    -0.74439200 0.20431200 -1.16483900
1    -3.34234200 4.82329200 0.33522400
1    -1.19976200 6.00777500 0.08080300
1    -4.58274200 2.70133100 0.47422000
1    -5.81680700 -1.96967100 0.51713300
1    -5.84519900 0.47875100 0.73170600
6    2.41076800 4.28171700 0.10789000
6    2.47677000 2.85156400 -0.00657500
6    1.29632200 2.14339000 -0.41241200
6    1.22623900 4.92718700 -0.03238000
1    3.32356300 4.83628400 0.33530800
1    1.17638500 6.01239400 0.08085200
6    3.66864800 2.14955900 0.24180900
6    3.72791900 0.74861600 0.23061700
6    2.54888600 0.03904100 -0.13244300
6    1.46463700 0.77177700 -0.61097600
1    5.84329700 0.50144600 0.73169700
1    4.57223500 2.71909800 0.47425600
6    4.91748500 -0.02147500 0.48263000
6    2.49101200 -1.40901500 -0.02390800
1    0.74352900 0.20729300 -1.16477500
6    3.68491900 -2.11185300 0.12753800
6    4.90246100 -1.37926500 0.37187400
1    5.82440900 -1.94706700 0.51714300
6    3.66412000 -3.54992300 0.04678700
6    2.50908100 -4.24130700 -0.15884500
6    1.23656900 -3.56792200 -0.18326800
```

```
6    1.23452300 -2.14690300 -0.03145700
1    4.61329800 -4.08546400 0.12243400
1    2.53007900 -5.32826900 -0.26307400
6    0.00824500 -4.24654100 -0.23522600
6    -1.22271000 -3.57269600 -0.18326500
6    -1.22617200 -2.15168700 -0.03145600
6    0.00295900 -1.52303100 0.17552300
1    -2.50937200 -5.33804700 -0.26307500
1    0.01037100 -5.33848900 -0.28623800
6    -2.49260100 -4.25101100 -0.15884500
1    0.00097500 -0.50761700 0.54571500
6    -3.65031900 -3.56411700 0.04678100
1    -4.59740600 -4.10334600 0.12242100
```

3. [10]kekulene [1,2,2,1,2,2]

```
E(wB97XD/cc-pVDZ) = -1535.96866297
No imaginary frequency (B3LYP/6-31G*)

6    -0.00054500 4.88211100 0.03138900
6    -1.23723100 5.59713900 0.18217400
6    -2.42856700 4.95404300 0.31913800
6    -2.50441000 3.52410200 0.23755500
6    -1.28944500 2.79565100 0.03227500
6    0.00001900 3.48012400 0.02497900
6    2.42742600 4.95862600 -0.25555600
6    1.23556400 5.59948400 -0.11282500
6    1.29003400 2.79675800 0.01149400
6    2.50443000 3.52806100 -0.18699600
6    5.06197900 0.68318500 -0.08693900
6    3.82949400 1.45648100 -0.14220000
6    2.61863900 0.73635100 0.01266200
6    2.61920400 -0.71669100 0.01068800
6    3.83038900 -1.43585000 0.16751600
6    5.06234500 -0.66156400 0.11431500
6    2.50695300 -3.50851000 0.21003700
6    1.29229700 -2.77819500 0.00951800
6    0.00288000 -3.46262400 -0.00626400
6    0.00346800 -4.86461100 -0.01265400
6    1.23991400 -5.58097400 0.13367600
6    2.43100700 -4.93914000 0.27843200
6    -1.28711000 -2.77918500 -0.01586400
6    -2.50114200 -3.50863500 -0.22312600
6    -2.42400200 -4.93851900 -0.30451500
6    -1.23237600 -5.58064500 -0.16552900
6    -2.61626800 0.73420000 0.01256900
6    -3.82771500 1.45189700 0.17408300
6    -5.05956300 0.67811400 0.11184500
6    -5.05883100 -0.66474200 -0.10168800
6    -3.82624300 -1.43750900 -0.16192300
6    -2.61564400 -0.71880900 0.00148600
6    3.74434500 2.84716600 -0.22460900
6    1.43246900 1.41919700 0.22307800
6    1.43391900 -1.40049100 -0.20168600
6    3.74624200 -2.82660400 0.24976100
6    -1.42986000 -1.40358600 0.20788400
6    -3.74097900 -2.82739500 -0.25673600
6    -3.74374800 2.84185000 0.26907700
6    -1.43074000 1.41997100 -0.19190000
1    -1.19983200 6.68849800 0.20904400
1    -3.34890800 5.52331000 0.46636600
1    3.34731500 5.52995900 -0.39751300
1    1.19728400 6.69101300 -0.12973700
1    6.01151700 1.21750800 -0.16696300
1    6.01217600 -1.19512800 0.19591300
1    1.20249900 -6.67253400 0.15051900
1    3.35112100 -5.50971900 0.42195100
1    -3.34363100 -5.50853800 -0.45327200
1    -1.19404700 -6.67197400 -0.19230100
1    -6.00954000 1.21089800 0.19677900
1    -6.00822700 -1.19831700 -0.18813700
1    4.65977400 3.43955500 -0.30447500
1    0.60585900 0.85410100 0.62536400
1    0.60744600 -0.83609700 -0.60526300
1    4.66202100 -3.41824600 0.33113600
1    -0.60388600 -0.84236000 0.61686300
1    -4.65628200 -3.41900900 -0.34350900
1    -4.65967500 3.43270900 0.35438800
1    -0.60370300 0.85946600 -0.59967800
```

4. [11]kekulene [1,2,2,2,1,3]

```
E(wB97XD/cc-pVDZ) = -1689.57832875
No imaginary frequency (B3LYP/6-31G*)

6    0.57561900 5.29088600 0.07154900
6    -0.66134900 6.01555600 -0.11211300
6    -1.84585400 5.37433900 -0.26066000
6    -1.94217600 3.94376000 -0.09088500
6    -0.73843100 3.22337900 0.25536800
6    0.55550600 3.89752000 0.14460900
6    3.01068700 5.32487700 0.23693600
6    1.82638500 5.98981200 0.13842600
6    1.81616900 3.18290400 0.05215600
6    3.05065000 3.89415700 0.16474900
6    5.53663900 1.03313700 -0.01400600
6    4.30160200 1.79245300 -0.01156100
6    3.07571600 1.09298400 -0.20272900
6    3.08079400 -0.36761000 -0.30421500
6    4.31082600 -1.07465100 -0.25501100
6    5.54129100 -0.31541800 -0.14081600
6    3.08517100 -3.19699700 -0.25398700
6    1.85799600 -2.48503800 -0.30316300
6    0.59045900 -3.21061200 -0.20051100
6    0.59735200 -4.62185900 -0.00830600
6    1.87232700 -5.31207200 -0.01098100
6    3.04261400 -4.64213200 -0.13879400
6    -1.84904500 -3.16395700 0.05575600
6    -3.09792800 -2.42895700 0.14826200
6    -4.29478200 -3.14276400 0.07638300
6    -4.27513200 -4.57534600 0.14438100
6    -3.10735600 -5.26889300 0.24284800
6    -1.84813600 -4.58858800 0.16945900
6    -3.16053000 -0.97116500 0.25775700
6    -4.38630400 -0.28898900 -0.08865200
6    -5.57737500 -1.08747100 -0.25718000
6    -5.54077900 -2.43373200 -0.10732900
6    4.26303400 3.17899900 0.13347400
6    1.88939800 1.81094300 -0.22746500
6    1.89340500 -1.09370400 -0.33844100
6    4.28675400 -2.47582100 -0.25117700
6    -0.62431000 -2.54198900 -0.22511600
6    -0.62279700 -5.28128800 0.13793700
6    -2.08923600 1.20696600 0.52998300
6    -3.24670600 1.87506000 0.02127400
6    -4.40832600 1.09734700 -0.19610600
6    -2.10547700 -0.19182500 0.70528500
6    -3.15392400 3.26972700 -0.19722000
```

```
6    -0.88573700 1.92039300 0.70394800
1    -0.61200200 7.10372400 -0.19278500
1    -2.75744000 5.93524000 -0.47717000
1    3.94976200 5.87511500 0.32539500
1    1.80971800 7.08193900 0.12904700
1    6.47732700 1.57712100 0.09663000
1    6.48614500 -0.86344100 -0.13028000
1    1.87138500 -6.39866700 0.10031200
1    3.98949600 -5.18664700 -0.12838700
1    -5.22944600 -5.10668100 0.13588900
1    -3.11469000 -6.35721600 0.33211200
1    -6.51886200 -0.57833100 -0.47365400
1    -6.45869100 -3.02037800 -0.18692800
1    5.20147800 3.73321400 0.21851200
1    0.97618400 1.29723400 -0.49836200
1    0.95369500 -0.55075800 -0.32668600
1    5.23251100 -3.02199000 -0.19994600
1    -0.63635000 -1.49454200 -0.49702700
1    -0.63377400 -6.37105900 0.22374700
1    -5.34135400 1.59474000 -0.47298700
1    -1.22712000 -0.65277300 1.15226600
1    -4.05122900 3.82899800 -0.47411300
1    -0.04679700 1.39046800 1.15029900
```

5. [12]kekulene [2,2,2,2,2,2]

```
E(wB97XD/cc-pVDZ) = -1843.21554423
No imaginary frequency (B3LYP/6-31G*)

6    -2.74773600 -1.75906700 0.63146800
6    -1.40003400 -1.65137900 0.53128500
6    -0.76041800 -0.40113700 0.17709600
6    -1.58128800 0.73237600 -0.06871500
6    -3.03532400 0.61610700 0.03918100
6    -3.62178800 -0.62981700 0.38954700
6    0.63049000 -0.26581200 0.06804200
6    -0.97072300 1.93564200 -0.40888600
6    0.40865500 2.08196000 -0.51973100
6    1.23435400 0.95174500 -0.27521500
6    2.66941700 1.10868200 -0.39201900
1    3.30105800 0.23771300 -0.20352100
6    3.23165700 2.29645800 -0.72527300
6    2.42805800 3.47360100 -0.98254400
6    1.01524000 3.36343700 -0.87899300
1    1.26390500 -1.13673600 0.25658600
1    -3.20203200 -2.71517800 0.90090600
1    -0.76586900 -2.52057200 0.71950800
1    -1.59858700 2.79907000 -0.59620600
1    4.31737700 2.38476500 -0.80593200
6    -8.30943600 3.80822500 -0.49245800
6    -7.51762100 2.67804200 -0.24639900
6    -6.10536900 2.79401400 -0.35136600
6    -5.56202500 4.02821300 -0.69475300
6    -8.07864600 1.39176300 0.11198600
6    -5.25789600 1.62884300 -0.09965400
6    -5.84976500 0.38531600 0.24993600
6    -7.29305200 0.31192300 0.34600000
6    -5.01736100 -0.71727000 0.48701100
1    -5.47061200 -1.67506800 0.75624700
6    -3.87157700 1.70366200 -0.19382700
1    -9.16466900 1.30633400 0.19173200
1    -9.39632100 3.72127900 -0.41235600
1    -4.48434500 4.11436500 -0.77372600
1    -7.74455600 -0.64568200 0.61481700
1    -3.42243100 2.65326800 -0.46128300
6    2.98673000 4.71182700 -1.32828500
6    2.19489300 5.84208700 -1.57406300
6    0.78267400 5.72619500 -1.46872900
6    0.23933700 4.49205000 -1.12508900
6    2.75593000 7.12835400 -1.93243600
6    -0.06480500 6.89141200 -1.72023500
6    0.52708100 8.13495400 -2.06980600
6    1.97034000 8.20827300 -2.16612100
6    -0.30533300 9.23757500 -2.30681700
1    0.14790500 10.19539300 -2.57602300
6    -1.45113400 6.81661000 -1.62610900
1    3.84193200 7.21371200 -2.01247900
1    4.07356800 4.79868800 -1.40887800
1    -0.83829200 4.40607600 -1.04548400
1    2.42183700 9.16589800 -2.43488000
1    -1.90029800 5.86692000 -1.35901700
6    -7.75078000 5.04649900 -0.83809100
6    -6.33792000 5.15675400 -0.94126600
6    -5.73133500 6.43825100 -1.30056100
6    -6.55706000 7.56844300 -1.54518500
6    -7.99213600 7.41144600 -1.42861400
6    -8.55439000 6.22362100 -1.09558400
6    -4.35197100 6.58457800 -1.41144800
6    -5.95321400 8.78599900 -1.88843700
6    -4.56230200 8.92138900 -1.99735200
6    -3.74141900 7.78790100 -1.75152200
6    -2.28739300 7.90417900 -1.85925600
6    -1.70094500 9.15012000 -2.20954200
6    -2.57495400 10.27940300 -2.45135900
6    -3.92267500 10.17167400 -2.35133800
1    -3.72404200 5.72115100 -1.22431700
1    -8.62376300 8.28241300 -1.61720200
1    -9.64012800 6.13527200 -1.01514500
1    -6.58663300 9.65689800 -2.07711300
1    -2.12062400 11.23560300 -2.72037700
1    -4.55683300 11.04088200 -2.53953200
```

6. [13]kekulene [1,3,2,2,2,3]

```
E(wB97XD/cc-pVDZ) = -1996.78772008
No imaginary frequency (B3LYP/6-31G*)

6    -0.00000000 6.34942400 0.00000000
6    -1.24353800 7.06774800 0.12413000
6    -2.43055400 6.42212700 0.24496400
6    -2.50628600 4.98876400 0.12617600
6    -1.27969400 4.26033800 -0.09618000
6    0.00000000 4.95657700 0.00000000
6    2.43055400 6.42212700 -0.24496300
6    1.24353800 7.06774800 -0.12413000
6    1.27969400 4.26033800 0.09618000
6    2.50628600 4.98876400 -0.12617600
6    6.21758700 -0.00929900 -0.08825600
6    5.00154600 0.77781800 0.02688600
6    3.76464200 0.08016500 0.27401400
6    3.74458400 -1.38724700 0.22712400
6    4.96388000 -2.10561400 0.10819800
6    6.20387500 -1.35924600 -0.01981800
6    3.71425000 -4.21123900 0.09416800
6    2.49350200 -3.48806600 0.13612300
6    1.22262800 -4.20922400 0.06521500
6    1.22382000 -5.63138400 0.04005800
```

```
6    2.49176200 -6.32787700 0.04606100
6    3.66838800 -5.65659200 0.05630600
6    -1.22262800 -4.20922400 -0.06521500
6    -2.49350200 -3.48806600 -0.13612300
6    -3.71425000 -4.21123900 -0.09416800
6    -3.66838800 -5.65659200 -0.05630600
6    -2.49176200 -6.32787700 -0.04606100
6    -1.22382000 -5.63138400 -0.04005800
6    -3.76464200 0.08016500 -0.27401400
6    -5.00154600 0.77781800 -0.02688600
6    -6.21758700 -0.00929900 0.08825600
6    -6.20387500 -1.35924600 0.01981800
6    -4.96388000 -2.10561400 -0.10819800
6    -3.74458400 -1.38724700 -0.22712400
6    3.72720900 4.31562300 -0.15959000
6    1.39401800 2.92282000 0.45097200
6    2.60829500 2.22469800 0.36016100
6    3.81059800 2.91916300 0.02129100
6    5.00529000 2.15880400 -0.08938700
6    2.62745300 0.81986800 0.50633500
6    2.54832000 -2.09576000 0.22593200
6    4.92470200 -3.50137400 0.07250900
6    0.00000000 -3.54314200 0.00000000
6    0.00000000 -6.30997800 -0.00000000
6    -2.54832000 -2.09576000 -0.22593200
6    -4.92470200 -3.50137400 -0.07250900
6    -2.60829500 2.22469800 -0.36016100
6    -3.81059800 2.91916300 -0.02129100
6    -5.00529000 2.15880400 0.08938800
6    -2.62745300 0.81986800 -0.50633500
6    -3.72720900 4.31562300 0.15959000
6    -1.39401800 2.92282000 -0.45097200
1    -1.20578700 8.15872900 0.16143300
1    -3.35496400 6.98354700 0.39560800
1    3.35496400 6.98354700 -0.39560800
1    1.20578700 8.15872900 -0.16143200
1    7.16088700 0.52359800 -0.22694400
1    7.13659300 -1.92210300 -0.09908800
1    2.48139200 -7.41986000 0.02612900
1    4.61374600 -6.20342300 0.04103600
1    -4.61374600 -6.20342300 -0.04103600
1    -2.48139200 -7.41986000 -0.02612900
1    -7.16088700 0.52359800 0.22694400
1    -7.13659300 -1.92210300 0.09908800
1    4.64206200 4.88805000 -0.33311600
1    0.52717500 2.36788500 0.79868700
1    5.94659900 2.67572700 -0.29330300
1    1.68493800 0.33255700 0.75740300
1    1.61798600 -1.53737500 0.26802400
1    5.86303300 -4.05817200 0.00384800
1    0.00000000 -2.45784400 0.00000000
1    0.00000000 -7.40322100 -0.00000000
1    -1.61798600 -1.53737500 -0.26802400
1    -5.86303300 -4.05817200 -0.00384800
1    -5.94659900 2.67572700 0.29330400
1    -1.68493800 0.33255700 -0.75740300
1    -4.64206200 4.88805000 0.33311600
1    -0.52717500 2.36788500 -0.79868700
```

7. [14]kekulene [2,2,3,2,2,3]

E(wB97XD/cc-pVDZ) = -2150.40684392
No imaginary frequency (B3LYP/6-31G*)

```
6    -0.61424500 6.05836400 -0.00156400
6    -1.88841600 6.75486000 0.00246300
6    -3.06544500 6.08879600 0.00431800
6    -3.12774400 4.63763900 0.00243300
6    -1.88891900 3.90685400 -0.00154300
6    -0.61578300 4.63766100 -0.00358500
6    4.28255500 6.06150000 -0.01338500
6    3.10827300 6.73957500 -0.00955900
6    1.83616700 6.05140400 -0.00743800
6    1.83069400 4.63189500 -0.00942600
6    3.09595000 3.90130700 -0.01344400
6    4.32254600 4.61576100 -0.01547200
6    6.79381400 1.74182600 -0.02539700
6    5.55361900 2.49709700 -0.02133300
6    4.32399200 1.78540600 -0.01925500
6    4.32766400 0.31739400 -0.02126100
6    5.57999200 -0.39010800 -0.02530100
6    6.80552900 0.38945400 -0.02724500
6    3.12774400 -4.63763900 -0.02527800
6    1.88891900 -3.90685300 -0.02122800
6    0.61578300 -4.63766100 -0.01919900
6    0.61424500 -6.05836400 -0.02129000
6    1.88841500 -6.75486000 -0.02536400
6    3.06544500 -6.08879500 -0.02721800
6    -1.83069400 -4.63189500 -0.01336700
6    -3.09595000 -3.90130700 -0.00935000
6    -4.32254600 -4.61576100 -0.00743500
6    -4.28255500 -6.06150000 -0.00958700
6    -3.10827400 -6.73957500 -0.01338900
6    -1.83616700 -6.05140400 -0.01543300
6    -4.32766300 -0.31739400 -0.00151100
6    -5.57999200 0.39010800 0.00244200
6    -6.80552900 -0.38945400 0.00430100
6    -6.79381400 -1.74182600 0.00242700
6    -5.55361900 -2.49709700 -0.00157100
6    -4.32399200 -1.78540600 -0.00353000
6    0.60951600 6.73390400 -0.00354600
6    0.60252700 3.97016500 -0.00748200
6    5.52694700 3.89468900 -0.01937700
6    3.13675100 2.50679600 -0.01535300
6    3.15990500 -0.41510100 -0.01942200
6    3.15676900 -1.82272900 -0.02136900
6    4.39320200 -2.53656200 -0.02537900
6    5.59146400 -1.77927600 -0.02724900
6    1.93933100 -2.52931900 -0.01940700
6    4.33654500 -3.95295800 -0.02724000
6    -0.60252700 -3.97016500 -0.01527100
6    -0.60951600 -6.73390400 -0.01934800
6    -3.13675100 -2.50679600 -0.00735700
6    -5.52694800 -3.89468900 -0.00357400
6    -3.15676900 1.82272900 -0.00136800
6    -4.39320200 2.53656200 0.00255500
6    -5.59146300 1.77927600 0.00437200
6    -3.15990500 0.41510100 -0.00328700
6    -4.33654500 3.95295800 0.00437400
6    -1.93933100 2.52931900 -0.00329800
1    -1.87735800 7.84712300 0.00398400
1    -4.00737000 6.64185500 0.00733200
1    5.22984500 6.60528100 -0.01494400
1    3.10563400 7.83184900 -0.00801800
1    7.73421400 2.29751800 -0.02695200
1    7.75544800 -0.14976400 -0.03029400
1    1.87735800 -7.84712300 -0.02692800
1    4.00737000 -6.64185500 -0.03027400
1    -5.22984600 -6.60528000 -0.00809700
1    -3.10563400 -7.83184900 -0.01497700
1    -7.75544900 0.14976400 0.00730000
1    -7.73421400 -2.29751800 0.00390900
```

```
1    0.61235700 7.82721600 -0.00202300
1    0.59759200 2.88548700 -0.00913300
1    6.47236400 4.44377000 -0.02093100
1    2.19971900 1.96032800 -0.01368200
1    2.18874700 0.07852300 -0.01638100
1    6.55060000 -2.30374900 -0.03032200
1    1.02623700 -1.93509100 -0.01637500
1    5.27029200 -4.52138900 -0.03031100
1    -0.59759300 -2.88548700 -0.01358500
1    -0.61235700 -7.82721600 -0.02093100
1    -2.19971800 -1.96032900 -0.00890000
1    -6.47236400 -4.44376900 -0.00209900
1    -6.55060000 2.30374900 0.00737600
1    -2.18874600 -0.07852300 -0.00627700
1    -5.27029200 4.52138900 0.00738700
1    -1.02623700 1.93509100 -0.00626100
```

8. [15]kekulene [2,3,2,3,2,3]

```
E(wB97XD/cc-pVDZ) = -2304.00175841
No imaginary frequency (B3LYP/6-31G*)

6    7.40138900 1.38885800 0.00763500
6    6.16174000 2.14346700 0.00610800
6    4.93257700 1.43565700 0.00552100
6    4.93360000 -0.03172100 0.00648300
6    6.18574600 -0.74041400 0.00794400
6    7.41208700 0.03635500 0.00848300
6    4.90362700 5.71580200 0.00295000
6    3.73769600 6.40134100 0.00164700
6    2.45179000 5.72767700 0.00077600
6    2.43948100 4.28897600 0.00130700
6    3.70974300 3.55442200 0.00300200
6    4.93725400 4.26493900 0.00371400
6    6.13759300 3.54364500 0.00522800
6    3.74504700 2.16256000 0.00400900
6    3.73422000 -4.98719700 0.00838400
6    2.49442100 -4.25724600 0.00692900
6    1.22320300 -4.99015800 0.00619900
6    1.22479800 -6.40850200 0.00696200
6    2.49817600 -7.10475900 0.00846700
6    3.67477100 -6.43766300 0.00913000
6    3.76485800 -0.76367900 0.00599900
6    3.76090600 -2.17155500 0.00683400
6    4.99769700 -2.88555400 0.00825700
6    6.19618000 -2.12953000 0.00879400
6    2.54376100 -2.87910200 0.00622100
6    4.94239100 -4.30151900 0.00901600
6    -4.93257700 1.43566700 -0.00348300
6    -6.16174300 2.14347400 -0.00470500
6    -7.40138900 1.38886000 -0.00510300
6    -7.41208400 0.03635700 -0.00426200
6    -6.18574200 -0.74041000 -0.00294200
6    -4.93359700 -0.03171200 -0.00261700
6    -2.45179900 5.72769000 -0.00357200
6    -3.73770400 6.40135400 -0.00484500
6    -4.90363700 5.71581500 -0.00550700
6    -4.93726500 4.26495200 -0.00492100
6    -3.70975400 3.55443700 -0.00372000
6    -2.43949300 4.28898900 -0.00310500
6    -6.13760000 3.54365300 -0.00541000
6    -3.74504900 2.16257600 -0.00303600
6    -1.22319000 -4.99015100 0.00391600
6    -2.49441000 -4.25723600 0.00224200
6    -3.73421100 -4.98718700 0.00184000
6    -3.67476400 -6.43765300 0.00286900
6    -2.49817100 -7.10474900 0.00418300
6    -1.22479100 -6.40849600 0.00478300
6    -3.76485400 -0.76367000 -0.00142300
6    -6.19617400 -2.12952500 -0.00198800
6    -4.99769000 -2.88554700 -0.00065300
6    -3.76090100 -2.17154600 -0.00038500
6    -2.54375500 -2.87909100 0.00101300
6    -4.94238200 -4.30151100 0.00043200
6    1.25392500 6.43112700 -0.00060900
6    -0.00000400 5.77106100 -0.00153400
6    -0.00000700 4.34294300 -0.00115700
6    1.22132100 3.64262700 0.00019500
6    -1.25393000 6.43113400 -0.00281000
6    -1.22134000 3.64263200 -0.00201200
6    0.00000900 -4.32512700 0.00473200
6    0.00000200 -7.08743600 0.00627300
1    8.34180700 1.94446500 0.00808200
1    8.36108900 -0.50441100 0.00961200
1    5.85498900 6.25246200 0.00352000
1    3.74394500 7.49358900 0.00118000
1    7.08445900 4.09018000 0.00575800
1    2.80496700 1.62063000 0.00365900
1    2.48730600 -8.19699500 0.00905900
1    4.61759800 -6.98912200 0.01025600
1    2.79421800 -0.26904200 0.00492100
1    7.15480200 -2.65487800 0.00989700
1    1.62999500 -2.28594900 0.00512200
1    5.87670900 -4.86895200 0.01011400
1    -8.34180900 1.94446200 -0.00608400
1    -8.36108500 -0.50441000 -0.00455900
1    -3.74395300 7.49360200 -0.00526500
1    -5.85499800 6.25247600 -0.00646800
1    -7.08446800 4.09018500 -0.00632700
1    -2.80496400 1.62065400 -0.00203000
1    -4.61759200 -6.98911200 0.00251800
1    -2.48730300 -8.19698600 0.00488200
1    -2.79421400 -0.26903300 -0.00118800
1    -7.15479500 -2.65487500 -0.00224600
1    -1.62999300 -2.28593300 0.00109300
1    -5.87669900 -4.86894600 0.00015000
1    1.27817900 7.52399500 -0.00099000
1    1.16465600 2.55469600 0.00034800
1    -1.27817900 7.52400300 -0.00317400
1    -1.16468600 2.55470000 -0.00170900
1    0.00001500 -3.24012700 0.00425800
1    -0.00000100 -8.18072800 0.00693500
```

9. [16]kekulene [2,3,3,2,3,3]

```
E(wB97XD/cc-pVDZ) = -2457.59860591
No imaginary frequency (B3LYP/6-31G*)

6    -1.22443300 7.10656500 0.01807100
6    -2.49641500 7.80414600 0.02239600
6    -3.67334500 7.13765300 0.02486800
6    -3.73254700 5.68770200 0.02334400
6    -2.49511200 4.95650100 0.01906300
6    -1.22327300 5.68774200 0.01640100
6    3.67351500 7.13758500 0.00469700
6    2.49660100 7.80410000 0.00869400
6    1.22460200 7.10654300 0.01135000
```

```
6    1.22340700 5.68771900 0.00967400
6    2.49522900 4.95645500 0.00532600
6    3.73268200 5.68763300 0.00282700
6    7.42634000 0.67501700 -0.01307300
6    6.19386600 1.44845100 -0.00880200
6    4.94388100 0.73608400 -0.00622600
6    4.94386400 -0.73617400 -0.00788400
6    6.19383200 -1.44856300 -0.01215100
6    7.42632400 -0.67515000 -0.01464700
6    3.73254700 -5.68770200 -0.01021800
6    2.49511300 -4.95650200 -0.00594100
6    1.22327300 -5.68774200 -0.00327700
6    1.22443300 -7.10656600 -0.00493100
6    2.49641500 -7.80414600 -0.00925100
6    3.67334500 -7.13765300 -0.01173200
6    -1.22340700 -5.68771800 0.00345400
6    -2.49522900 -4.95645500 0.00780700
6    -3.73268200 -5.68763300 0.01028600
6    -3.67351500 -7.13758500 0.00841600
6    -2.49660100 -7.80409900 0.00443700
6    -1.22460200 -7.10654200 0.00178800
6    -4.94386500 0.73617400 0.02101200
6    -6.19383200 1.44856300 0.02527000
6    -7.42632500 0.67515000 0.02775300
6    -7.42634100 -0.67501700 0.02616900
6    -6.19386600 -1.44845100 0.02191000
6    -4.94388200 -0.73608400 0.01935900
6    0.00009300 7.78536800 0.01550700
6    0.00005900 5.02243600 0.01224700
6    4.94269700 5.00298000 -0.00126100
6    2.54713100 3.57678600 0.00354500
6    3.76477100 2.87280700 -0.00057800
6    4.99909800 3.58923400 -0.00307500
6    6.20135700 2.83447900 -0.00721400
6    3.77447500 1.46200600 -0.00224500
6    3.77444000 -1.46207500 -0.00544600
6    3.76470300 -2.87287600 -0.00704100
6    4.99901300 -3.58932500 -0.01129700
6    6.20129000 -2.83459100 -0.01375600
6    2.54704600 -3.57683400 -0.00447400
6    4.94257900 -5.00307000 -0.01277400
6    -0.00005800 -5.02243600 0.00086300
6    -0.00009300 -7.78536800 -0.00236400
6    -2.54713100 -3.57678600 0.00961500
6    -3.76477100 -2.87280700 0.01372600
6    -4.99909800 -3.58923400 0.01619000
6    -4.94269700 -5.00298000 0.01436500
6    -3.77447500 -1.46200600 0.01540500
6    -6.20135800 -2.83447900 0.02031500
6    -3.76470300 2.87287600 0.02016400
6    -4.99901300 3.58932400 0.02441900
6    -6.20129000 2.83459100 0.02687400
6    -3.77444100 1.46207500 0.01857100
6    -4.94257800 5.00307000 0.02589900
6    -2.54704700 3.57683400 0.01759800
1    -2.48463200 8.89637900 0.02363900
1    -4.61599500 7.68942300 0.02810800
1    4.61617900 7.68933800 0.00278100
1    2.48484600 8.89633300 0.01001500
1    8.37182400 1.22203200 -0.01502100
1    8.37179500 -1.22218100 -0.01787200
1    2.48463300 -8.89637900 -0.01048400
1    4.61599500 -7.68942300 -0.01497000
1    -4.61617900 -7.68933800 0.01032000
1    -2.48484600 -8.89633200 0.00312100
1    -8.37179600 1.22218100 0.03097100
1    -8.37182500 -1.22203200 0.02810200
1    0.00010700 8.87868400 0.01679800
1    0.00004400 3.93721600 0.01096400
1    5.87608700 5.57199400 -0.00311700
1    1.63388700 2.98261200 0.00532200
1    7.15842300 3.36271900 -0.00920300
1    2.80632900 0.96186900 -0.00023100
1    2.80630800 -0.96192000 -0.00215300
1    7.15834300 -3.36284700 -0.01699900
1    1.63381600 -2.98264600 -0.00124400
1    5.87595500 -5.57210000 -0.01600900
1    -0.00004300 -3.93721600 0.00211300
1    -0.00010700 -8.87868400 -0.00364900
1    -1.63388700 -2.98261100 0.00787100
1    -5.87608700 -5.57199400 0.01620700
1    -2.80633000 -0.96186800 0.01342200
1    -7.15842300 -3.36271900 0.02228500
1    -7.15834300 3.36284700 0.03011100
1    -2.80630800 0.96192000 0.01527300
1    -5.87595500 5.57210000 0.02913600
1    -1.63381600 2.98264500 0.01437400
```

10. [17]kekulene [2,3,3,3,2,4]

```
E(wB97XD/cc-pVDZ) = -2611.19024584
No imaginary frequency (B3LYP/6-31G*)

6    -0.64715100 7.48585700 -0.00000000
6    -1.91848500 8.19004000 0.00000000
6    -3.09802800 7.53141000 -0.00000000
6    -3.16782100 6.07988800 -0.00000000
6    -1.92630400 5.33777200 -0.00000000
6    -0.64980100 6.06727700 -0.00000000
6    4.24960200 7.50738400 -0.00000000
6    3.07367100 8.17571900 0.00000000
6    1.80150900 7.47948700 -0.00000000
6    1.79713600 6.06190800 -0.00000000
6    3.06707800 5.32800400 -0.00000000
6    4.30563600 6.05774200 -0.00000000
6    7.99651000 1.04603300 -0.00000000
6    6.76344700 1.81769100 -0.00000000
6    5.51333300 1.10500400 -0.00000000
6    5.51480500 -0.36719800 -0.00000000
6    6.76464200 -1.07689200 -0.00000000
6    7.99703900 -0.30403100 -0.00000000
6    4.31523800 -5.32100100 0.00000000
6    3.07570300 -4.59365200 0.00000000
6    1.80011100 -5.32844500 0.00000000
6    1.80789200 -6.76733900 0.00000000
6    3.09275400 -7.44937500 0.00000000
6    4.26219000 -6.77475200 0.00000000
6    -3.08011400 -5.32038300 0.00000000
6    -4.35055800 -4.58730700 0.00000000
6    -5.57606500 -5.29976800 0.00000000
6    -5.54314700 -6.74956200 -0.00000000
6    -4.37653900 -7.43400500 0.00000000
6    -3.09299900 -6.75790900 0.00000000
6    -5.58479200 -1.00040800 0.00000000
6    -6.84835000 -0.29633200 0.00000000
6    -8.07045200 -1.08254300 0.00000000
6    -8.05098800 -2.43335600 -0.00000000
6    -6.80550100 -3.18223000 0.00000000
6    -5.57823100 -2.47066200 0.00000000
6    0.57714600 8.16131000 -0.00000000
6    0.57054000 5.39932100 -0.00000000
6    5.51461700 5.37157000 -0.00000000
```

```
6    3.11713900 3.94789400 -0.00000000
6    4.33406100 3.24224600 -0.00000000
6    5.56902000 3.95807600 -0.00000000
6    6.77096600 3.20356700 -0.00000000
6    4.34365100 1.83116300 -0.00000000
6    4.34536600 -1.09619900 -0.00000000
6    4.33901500 -2.50575000 0.00000000
6    5.57412600 -3.21866800 0.00000000
6    6.77393300 -2.46398900 -0.00000000
6    3.12174000 -3.21643200 0.00000000
6    5.52096500 -4.63513700 0.00000000
6    0.58667200 -4.67816400 0.00000100
6    -0.64032300 -5.37504700 0.00000100
6    -0.64297100 -6.80250300 0.00000000
6    0.61129400 -7.46651000 0.00000000
6    -1.85979100 -4.67383900 0.00000100
6    -1.89438400 -7.46195700 0.00000000
6    -4.38963200 -3.19370200 0.00000100
6    -6.77865100 -4.58022900 0.00000000
6    -4.42571400 1.15193100 0.00000000
6    -5.67683800 1.86280900 0.00000000
6    -6.87183900 1.08537800 0.00000000
6    -4.42574000 -0.26481500 0.00000000
6    -3.21031400 3.25758700 0.00000000
6    -4.45160000 3.98547600 0.00000000
6    -5.65829200 3.26705800 0.00000000
6    -3.22680600 1.86350900 0.00000000
6    -4.37608600 5.40915400 0.00000000
6    -1.98355000 3.96620700 -0.00000000
1    -1.90028000 9.28220200 0.00000000
1    -4.03755100 8.08848800 0.00000000
1    5.19333400 8.05728800 0.00000000
1    3.06319600 9.26796000 0.00000000
1    8.94144100 1.59397500 0.00000000
1    8.94247000 -0.85112500 0.00000000
1    3.09075600 -8.54169000 -0.00000000
1    5.20869000 -7.31999800 -0.00000000
1    -6.49436200 -7.28647900 -0.00000000
1    -4.38108300 -8.52625900 -0.00000000
1    -9.02264700 -0.54740600 0.00000000
1    -8.98768400 -2.99525600 -0.00000000
1    0.57985300 9.25463000 0.00000000
1    0.56788100 4.31393600 -0.00000100
1    6.44882300 5.93923300 0.00000000
1    2.20288100 3.35518600 -0.00000100
1    7.72801600 3.73182200 0.00000000
1    3.37557500 1.33074900 -0.00000100
1    3.37648900 -0.59736000 -0.00000000
1    7.73181600 -2.99076000 0.00000000
1    2.20474100 -2.62754700 0.00000000
1    6.45625900 -5.20103100 -0.00000000
1    0.53679200 -3.58949700 0.00000100
1    0.63210000 -8.55947500 -0.00000000
1    -1.80353700 -3.58573200 0.00000100
1    -1.91902700 -8.55484100 -0.00000000
1    -3.45057400 -2.64926200 0.00000100
1    -7.72422100 -5.12905900 -0.00000000
1    -7.83517200 1.60204300 0.00000000
1    -3.45134800 -0.75225100 0.00000000
1    -6.60495300 3.81352000 0.00000000
1    -2.28020300 1.31710000 0.00000000
1    -5.30527600 5.98495000 0.00000000
1    -1.07388300 3.36652900 0.00000000
```

11. [18]kekulene [3,3,3,3,3,3]

```
E(wB97XD/cc-pVDZ) = -2764.79161826
No imaginary frequency (B3LYP/6-31G*)

6    8.63687500 0.67507200 -0.00871600
6    7.40409100 1.44630400 -0.00732700
6    6.15433200 0.73594100 -0.00640600
6    6.15432900 -0.73592000 -0.00691100
6    7.40408600 -1.44628600 -0.00835400
6    8.63687200 -0.67505900 -0.00920000
6    4.90345700 7.14322500 -0.00398500
6    3.73424500 7.81836100 -0.00308900
6    2.44987700 7.13639600 -0.00194500
6    2.44022400 5.69895800 -0.00167100
6    3.71481100 4.96301100 -0.00299600
6    4.95489100 5.68996000 -0.00406500
6    7.41275700 2.83341700 -0.00692300
6    6.21284600 3.58737400 -0.00562600
6    4.97756800 2.87434000 -0.00469200
6    4.98439100 1.46473000 -0.00511500
6    6.16033100 5.00356000 -0.00529500
6    3.76047500 3.58543900 -0.00340800
6    4.95486800 -5.68993400 -0.00802400
6    3.71478700 -4.96298500 -0.00649900
6    2.44019600 -5.69893700 -0.00575300
6    2.44985500 -7.13637700 -0.00675300
6    3.73422400 -7.81833600 -0.00826900
6    4.90343400 -7.14319800 -0.00882400
6    4.98438600 -1.46470600 -0.00607800
6    4.97755700 -2.87431600 -0.00666300
6    6.21283200 -3.58735200 -0.00813700
6    7.41274600 -2.83340000 -0.00892400
6    3.76046100 -3.58541200 -0.00587200
6    6.16031100 -5.00353800 -0.00877600
6    -6.15433300 0.73591900 0.00328800
6    -7.40408900 1.44628700 0.00335100
6    -8.63687600 0.67505900 0.00316700
6    -8.63687900 -0.67507100 0.00271700
6    -7.40409500 -1.44630300 0.00236500
6    -6.15433600 -0.73594000 0.00276400
6    -2.44985300 7.13637300 0.00167800
6    -3.73422400 7.81833300 0.00208300
6    -4.90343300 7.14319500 0.00266900
6    -4.95486600 5.68993000 0.00299200
6    -3.71478500 4.96298100 0.00289600
6    -2.44019300 5.69893400 0.00215900
6    -4.97755700 2.87431300 0.00353300
6    -6.21283200 3.58735000 0.00349500
6    -7.41274800 2.83340000 0.00350000
6    -4.98438800 1.46470200 0.00351100
6    -6.16031000 5.00353600 0.00332400
6    -3.76046000 3.58540600 0.00331400
6    -2.44022100 -5.69895500 -0.00195500
6    -3.71480900 -4.96300700 -0.00065700
6    -4.95488900 -5.68995600 -0.00093000
6    -4.90345600 -7.14322000 -0.00208000
6    -3.73424500 -7.81835600 -0.00304200
6    -2.44987600 -7.13639300 -0.00313100
6    -4.98439400 -1.46472700 0.00241300
6    -7.41276000 -2.83341600 0.00156000
6    -6.21284700 -3.58737100 0.00100300
6    -4.97756900 -2.87433800 0.00146200
6    -3.76047400 -3.58543500 0.00070200
6    -6.16033100 -5.00355800 -0.00009000
6    1.25281100 7.83724100 -0.00106200
6    0.00001200 7.17478700 0.00010700
6    0.00001800 5.74846500 0.00060000
6    1.22430700 5.04985500 -0.00022600
6    -1.25279400 7.83722800 0.00073500
```

```
6    -1.22426600 5.04984500 0.00168800
6    1.22427100 -5.04984800 -0.00417600
6    -0.00001300 -5.74846600 -0.00369900
6    -0.00001000 -7.17478700 -0.00480000
6    1.25279400 -7.83723000 -0.00626200
6    -1.22430100 -5.04985500 -0.00227600
6    -1.25281100 -7.83723900 -0.00445900
1    9.58171100 1.22312400 -0.00938500
1    9.58170700 -1.22311400 -0.01026300
1    5.85049600 7.68746600 -0.00476800
1    3.73213600 8.91064700 -0.00316200
1    8.37028000 3.36076200 -0.00765400
1    4.01574500 0.96550300 -0.00439800
1    7.09593800 5.56886200 -0.00609700
1    2.84330400 2.99690500 -0.00283600
1    3.73212000 -8.91062200 -0.00895600
1    5.85047400 -7.68743800 -0.00995400
1    4.01574200 -0.96547600 -0.00495400
1    8.37026600 -3.36074800 -0.01003600
1    2.84329800 -2.99687000 -0.00479900
1    7.09591500 -5.56884300 -0.00993900
1    -9.58171100 1.22311600 0.00336400
1    -9.58171600 -1.22312400 0.00255200
1    -3.73211900 8.91061900 0.00183300
1    -5.85047400 7.68743300 0.00288900
1    -8.37026800 3.36075000 0.00352500
1    -4.01574400 0.96546900 0.00352300
1    -7.09591400 5.56884100 0.00336800
1    -2.84329700 2.99686300 0.00334600
1    -5.85049600 -7.68746000 -0.00213500
1    -3.73213800 -8.91064200 -0.00386400
1    -4.01574800 -0.96549800 0.00270500
1    -8.37028200 -3.36076200 0.00125500
1    -2.84330500 -2.99689900 0.00113900
1    -7.09593700 -5.56886000 -0.00032900
1    1.27469500 8.93015800 -0.00130500
1    1.17303200 3.96130400 0.00027600
1    -1.27468700 8.93014500 0.00037300
1    -1.17297400 3.96129700 0.00198800
1    1.17298200 -3.96129900 -0.00327800
1    1.27468500 -8.93014700 -0.00705900
1    -1.17302400 -3.96130500 -0.00155700
1    -1.27469700 -8.93015600 -0.00534900
```

12. [19]kekulene [2,4,3,3,3,4]

```
E(wB97XD/cc-pVDZ) = -2918.37919837
No imaginary frequency (B3LYP/6-31G*)

6    -1.22400300 8.55182900 0.00000100
6    -2.49461300 9.25561600 0.00000100
6    -3.67339900 8.59563400 0.00000100
6    -3.73997100 7.14468000 0.00000000
6    -2.49889200 6.40314000 -0.00000100
6    -1.22374500 7.13423100 -0.00000000
6    3.67339900 8.59563400 0.00000100
6    2.49461300 9.25561600 0.00000100
6    1.22400300 8.55182900 0.00000100
6    1.22374500 7.13423100 -0.00000000
6    2.49889200 6.40314000 -0.00000100
6    3.73997100 7.14468000 0.00000000
6    8.65811200 -0.00344000 0.00000100
6    7.42990300 0.77740500 0.00000000
6    6.16845600 0.06865100 -0.00000100
6    6.16450300 -1.40565700 -0.00000000
6    7.41254100 -2.11961600 0.00000000
6    8.65005500 -1.35244700 0.00000000
6    4.95437500 -6.35685400 0.00000000
6    3.71611800 -5.62830700 0.00000000
6    2.44057700 -6.36264400 0.00000000
6    2.44937500 -7.80021100 0.00000000
6    3.73258300 -8.48391400 0.00000000
6    4.90230800 -7.80991100 0.00000000
6    -2.44057700 -6.36264400 0.00000000
6    -3.71611800 -5.62830700 0.00000000
6    -4.95437500 -6.35685400 0.00000000
6    -4.90230800 -7.80991100 0.00000000
6    -3.73258300 -8.48391400 0.00000000
6    -2.44937500 -7.80021100 0.00000000
6    -6.16845600 0.06865100 -0.00000100
6    -7.42990300 0.77740500 0.00000000
6    -8.65811200 -0.00344000 0.00000100
6    -8.65005500 -1.35244700 0.00000000
6    -7.41254100 -2.11961600 0.00000000
6    -6.16450300 -1.40565700 -0.00000000
6    0.00000000 9.23018800 0.00000100
6    0.00000000 6.46883500 -0.00000100
6    4.94834700 6.47315100 0.00000000
6    2.55618000 5.03028600 -0.00000100
6    3.78265300 4.32229900 -0.00000100
6    5.02258600 5.05105200 -0.00000000
6    6.23120400 4.33350800 0.00000000
6    3.80223000 2.92612400 -0.00000200
6    5.00163600 2.21789900 -0.00000100
6    6.25084000 2.93168200 -0.00000000
6    7.44958100 2.15645400 0.00000000
6    5.00799600 0.79830900 -0.00000100
6    4.99362900 -2.13057100 -0.00000000
6    4.98232000 -3.54176200 -0.00000000
6    6.21558200 -4.25719100 0.00000000
6    7.41815800 -3.50502400 0.00000000
6    3.76426200 -4.24997500 -0.00000000
6    6.16132300 -5.67209400 0.00000000
6    1.22486600 -5.71272100 0.00000000
6    0.00000000 -6.41080800 0.00000000
6    0.00000000 -7.83732300 0.00000000
6    1.25215900 -8.50036100 0.00000000
6    -1.22486600 -5.71272100 0.00000000
6    -1.25215900 -8.50036100 0.00000000
6    -3.76426200 -4.24997500 -0.00000000
6    -4.98232000 -3.54176200 -0.00000000
6    -6.21558200 -4.25719100 0.00000000
6    -6.16132300 -5.67209400 0.00000000
6    -4.99362900 -2.13057100 -0.00000000
6    -7.41815800 -3.50502400 0.00000000
6    -5.00163600 2.21789900 -0.00000100
6    -6.25084000 2.93168200 -0.00000000
6    -7.44958100 2.15645400 0.00000000
6    -5.00799600 0.79830900 -0.00000100
6    -3.78265300 4.32229900 -0.00000100
6    -5.02258600 5.05105200 -0.00000000
6    -6.23120400 4.33350800 0.00000000
6    -3.80223000 2.92612400 -0.00000200
6    -4.94834700 6.47315100 0.00000000
6    -2.55618000 5.03028600 -0.00000100
1    -2.47690500 10.34777000 0.00000200
1    -4.61392800 9.15097900 0.00000200
1    4.61392800 9.15097900 0.00000200
1    2.47690500 10.34777000 0.00000200
1    9.60627900 0.53888200 0.00000100
1    9.59196700 -1.90559600 0.00000100
1    3.72929700 -9.57621100 0.00000000
```

```
1    5.84892100 -8.35492400 0.00000000
1    -5.84892100 -8.35492400 0.00000000
1    -3.72929700 -9.57621100 0.00000000
1    -9.60627900 0.53888200 0.00000100
1    -9.59196700 -1.90559600 0.00000100
1    0.00000000 10.32351000 0.00000200
1    0.00000000 5.38320100 -0.00000200
1    5.87778200 7.04854400 0.00000100
1    1.64601400 4.43119800 -0.00000200
1    7.17698600 4.88148900 0.00000100
1    2.85655400 2.37810800 -0.00000200
1    8.41104800 2.67658600 0.00000100
1    4.03634000 0.30478100 -0.00000200
1    4.02633400 -1.62833100 -0.00000000
1    8.37439800 -4.03476500 0.00000000
1    2.84778100 -3.66015900 -0.00000000
1    7.09593100 -6.23911000 0.00000000
1    1.17462100 -4.62400500 0.00000000
1    1.27358200 -9.59331600 0.00000000
1    -1.17462100 -4.62400500 0.00000000
1    -1.27358200 -9.59331600 0.00000000
1    -2.84778100 -3.66015900 -0.00000000
1    -7.09593100 -6.23911000 0.00000000
1    -4.02633400 -1.62833100 -0.00000000
1    -8.37439800 -4.03476500 0.00000000
1    -8.41104800 2.67658600 0.00000100
1    -4.03634000 0.30478100 -0.00000200
1    -7.17698600 4.88148900 0.00000100
1    -2.85655400 2.37810800 -0.00000200
1    -5.87778200 7.04854400 0.00000100
1    -1.64601400 4.43119800 -0.00000200
```

13. [20]kekulene [3,3,4,3,3,4]

```
E(wB97XD/cc-pVDZ) = -3071.97647329
No imaginary frequency (B3LYP/6-31G*)

6    -1.83980200 8.19588800 -0.00000800
6    -3.12231800 8.88467600 -0.00000400
6    -4.29463100 8.21727700 0.00000100
6    -4.35629500 6.76336500 0.00000300
6    -3.11313800 6.02484200 0.00000000
6    -1.83411600 6.75797500 -0.00000600
6    5.51075700 8.19505200 -0.00003300
6    4.34165700 8.87013300 -0.00003100
6    3.05828900 8.18726000 -0.00002500
6    3.04747300 6.75046300 -0.00002300
6    4.32194500 6.01457300 -0.00002600
6    5.56089300 6.74219900 -0.00003100
6    9.25449800 1.73802100 -0.00003500
6    8.01676000 2.50428100 -0.00003200
6    6.76856000 1.79027300 -0.00002700
6    6.77314900 0.31602000 -0.00002400
6    8.03441400 -0.39127400 -0.00002700
6    9.26268000 0.38907100 -0.00003300
6    4.35629500 -6.76336500 -0.00000300
6    3.11313800 -6.02484200 -0.00000000
6    1.83411600 -6.75797500 0.00000500
6    1.83980200 -8.19588800 0.00000800
6    3.12231800 -8.88467600 0.00000500
6    4.29463100 -8.21727700 -0.00000000
6    -3.04747300 -6.75046300 0.00002200
6    -4.32194500 -6.01457300 0.00002600
6    -5.56089300 -6.74219900 0.00003100
6    -5.51075700 -8.19505200 0.00003400
6    -4.34165700 -8.87013300 0.00003100
6    -3.05828900 -8.18726000 0.00002500
6    -6.77314900 -0.31602000 0.00002400
6    -8.03441400 0.39127400 0.00002700
6    -9.26268000 -0.38907100 0.00003300
6    -9.25449800 -1.73802100 0.00003500
6    -8.01676000 -2.50428100 0.00003200
6    -6.76856000 -1.79027300 0.00002700
6    0.60959000 8.22791500 -0.00001700
6    -0.64283200 8.89333100 -0.00001300
6    -0.62080900 6.10623000 -0.00000900
6    0.60710000 6.80199300 -0.00001400
6    1.86138900 8.88920700 -0.00002200
6    1.83001200 6.10204300 -0.00001700
6    6.76720700 6.05649000 -0.00003400
6    4.36897100 4.63600900 -0.00002400
6    5.58653500 3.92676700 -0.00002700
6    6.82022900 4.64174800 -0.00003200
6    8.02253100 3.88961100 -0.00003500
6    5.59763000 2.51544900 -0.00002400
6    5.61264400 -0.41522500 -0.00001900
6    5.60796800 -1.83412100 -0.00001700
6    6.85731600 -2.54572100 -0.00002000
6    8.05484500 -1.77083900 -0.00002500
6    4.40847300 -2.54582000 -0.00001100
6    4.39216200 -3.94046500 -0.00000900
6    5.63318900 -4.66645700 -0.00001200
6    6.83933900 -3.94901200 -0.00001700
6    3.16587300 -4.65420200 -0.00000300
6    5.56116500 -6.09104800 -0.00000900
6    0.62080900 -6.10623000 0.00000800
6    -0.60710000 -6.80199300 0.00001400
6    -0.60959000 -8.22791500 0.00001700
6    0.64283200 -8.89333100 0.00001400
6    -1.83001200 -6.10204300 0.00001700
6    -1.86138900 -8.88920700 0.00002200
6    -4.36897100 -4.63600900 0.00002300
6    -5.58653500 -3.92676700 0.00002600
6    -6.82022900 -4.64174800 0.00003200
6    -6.76720700 -6.05649000 0.00003400
6    -5.59763000 -2.51544900 0.00002400
6    -8.02253100 -3.88961100 0.00003500
6    -5.60796800 1.83412100 0.00001600
6    -6.85731600 2.54572100 0.00002000
6    -8.05484500 1.77083900 0.00002500
6    -5.61264400 0.41522500 0.00001900
6    -4.39216200 3.94046500 0.00000800
6    -5.63318900 4.66645700 0.00001200
6    -6.83933900 3.94901200 0.00001700
6    -4.40847300 2.54582000 0.00001100
6    -5.56116500 6.09104800 0.00000900
6    -3.16587300 4.65420200 0.00000300
1    -3.11379400 9.97696700 -0.00000600
1    -5.23843500 8.76714300 0.00000300
1    6.45801000 8.73893600 -0.00003800
1    4.33915000 9.96242700 -0.00003200
1    10.19615500 2.29158500 -0.00003900
1    10.21074200 -0.15342300 -0.00003500
1    3.11379400 -9.97696700 0.00000700
1    5.23843500 -8.76714300 -0.00000300
1    -6.45801000 -8.73893600 0.00003800
1    -4.33915000 -9.96242700 0.00003300
1    -10.21074200 0.15342300 0.00003500
1    -10.19615500 -2.29158500 0.00003900
1    -0.66210600 9.98633100 -0.00001500
1    -0.57279200 5.01731500 -0.00000700
1    1.88430500 9.98213300 -0.00002400
```

```
1    1.77839200 5.01336200 -0.00001600
1    7.70230900 6.62268200 -0.00003800
1    3.45189600 4.04707100 -0.00001900
1    8.97881700 4.41925900 -0.00003900
1    4.63032700 2.01315200 -0.00002000
1    4.64067200 0.07777700 -0.00001700
1    9.01664000 -2.29037000 -0.00002700
1    3.46187300 -1.99940700 -0.00000900
1    7.78600300 -4.49548000 -0.00001900
1    2.25265700 -4.05936400 -0.00000100
1    6.49207400 -6.66406800 -0.00001100
1    0.57279200 -5.01731500 0.00000600
1    0.66210600 -9.98633100 0.00001600
1    -1.77839200 -5.01336200 0.00001500
1    -1.88430500 -9.98213300 0.00002400
1    -3.45189600 -4.04707100 0.00001900
1    -7.70230900 -6.62268200 0.00003800
1    -4.63032700 -2.01315200 0.00002000
1    -8.97881700 -4.41925900 0.00003900
1    -9.01664000 2.29037000 0.00002700
1    -4.64067200 -0.07777700 0.00001600
1    -7.78600300 4.49548000 0.00001900
1    -3.46187300 1.99940700 0.00000900
1    -6.49207400 6.66406800 0.00001100
1    -2.25265700 4.05936400 0.00000100
```

14. [21]kekulene [3,4,3,4,3,4]

```
E(wB97XD/cc-pVDZ) = -3225.56881307
No imaginary frequency (B3LYP/6-31G*)

6    9.86237500 1.38603200 0.00563000
6    8.62517200 2.15261400 0.00448400
6    7.37665900 1.44064800 0.00392300
6    7.37962300 -0.03355100 0.00407300
6    8.64064100 -0.74166300 0.00555600
6    9.86954100 0.03709300 0.00627500
6    6.13196300 7.84922000 0.00252800
6    4.96738800 8.53000100 0.00226200
6    3.67843100 7.85522500 0.00128400
6    3.66117500 6.40915500 0.00050800
6    4.93627100 5.66943000 0.00162100
6    6.17713400 6.39446100 0.00231900
6    8.63252800 3.53860700 0.00416900
6    7.43188800 4.29126800 0.00335200
6    6.19752000 3.57878900 0.00299200
6    6.20609400 2.16818100 0.00338100
6    7.38092300 5.70744000 0.00309300
6    4.98046800 4.29194900 0.00221500
6    4.96303200 -7.11335100 0.00541000
6    3.71926700 -6.37551100 0.00382700
6    2.44115300 -7.11004400 0.00350800
6    2.44878500 -8.54720100 0.00443400
6    3.73133300 -9.23533600 0.00577800
6    4.90311400 -8.56702400 0.00629400
6    6.21858900 -0.76444300 0.00281200
6    6.21320700 -2.18344700 0.00339900
6    7.46245900 -2.89528400 0.00518300
6    8.66025500 -2.12122100 0.00607800
6    5.01363300 -2.89531400 0.00245300
6    4.99730500 -4.29011900 0.00336200
6    6.23853700 -5.01583200 0.00513300
6    7.44459700 -4.29845900 0.00595000
6    3.77132300 -5.00459700 0.00273000
6    6.16744900 -6.44025200 0.00601600
6    -7.37665300 1.44062300 -0.00349100
6    -8.62516200 2.15259300 -0.00283000
6    -9.86236900 1.38601600 -0.00215800
6    -9.86954100 0.03707800 -0.00187100
6    -8.64064300 -0.74168200 -0.00229800
6    -7.37962200 -0.03357700 -0.00333400
6    -3.67840600 7.85520000 -0.00193600
6    -4.96736600 8.52997300 -0.00151800
6    -6.13193800 7.84919000 -0.00189700
6    -6.17710800 6.39443100 -0.00266000
6    -4.93624400 5.66940000 -0.00331300
6    -3.66114500 6.40913000 -0.00306100
6    -6.19750400 3.57876000 -0.00376000
6    -7.43187000 4.29124300 -0.00307300
6    -8.63251200 3.53858600 -0.00269600
6    -6.20608400 2.16815200 -0.00401000
6    -7.38089900 5.70741400 -0.00260900
6    -4.98044900 4.29191700 -0.00391200
6    -2.44118900 -7.11007200 0.00097500
6    -3.71929700 -6.37554500 -0.00008700
6    -4.96306200 -7.11338600 0.00075200
6    -4.90314400 -8.56705900 0.00190000
6    -3.73136000 -9.23536900 0.00234500
6    -2.44881400 -8.54722700 0.00203100
6    -6.21859000 -0.76447300 -0.00393800
6    -8.66026300 -2.12124000 -0.00169300
6    -7.46247000 -2.89530900 -0.00197100
6    -6.21321400 -2.18347700 -0.00321500
6    -5.01364300 -2.89534800 -0.00339800
6    -7.44461500 -4.29848300 -0.00095400
6    -6.23855800 -5.01586300 -0.00093100
6    -4.99732300 -4.29015300 -0.00215600
6    -3.77134200 -5.00463400 -0.00179000
6    -6.16747700 -6.44028300 0.00032400
6    2.49339300 8.56181300 0.00085400
6    1.22421800 7.91124600 -0.00040100
6    1.21619300 6.47343000 -0.00167100
6    2.44788000 5.76884100 -0.00127500
6    0.00001000 8.59718600 -0.00043200
6    -1.22419200 7.91123700 -0.00151900
6    -1.21615700 6.47342200 -0.00283900
6    0.00002000 5.79031400 -0.00300000
6    -2.49337300 8.56179600 -0.00124800
6    -2.44784100 5.76882600 -0.00366000
6    1.22600900 -6.45977000 0.00246900
6    -0.00002000 -7.15735500 0.00222400
6    -0.00001400 -8.58260800 0.00308500
6    1.25202600 -9.24634500 0.00417900
6    -1.22605500 -6.45978300 0.00122000
6    -1.25204800 -9.24635900 0.00298700
1    10.80416800 1.93930000 0.00608700
1    10.81688500 -0.50658800 0.00728200
1    7.08201100 8.38819900 0.00310700
1    4.97037500 9.62227300 0.00265700
1    9.58937700 4.06716300 0.00463100
1    5.23812800 1.66726700 0.00329000
1    8.31726500 6.27151500 0.00361400
1    4.06214300 3.70489900 0.00219000
1    3.72315700 -10.32759500 0.00645100
1    5.84760900 -9.11564000 0.00739100
1    5.24683700 -0.27110000 0.00131200
1    9.62156000 -2.64157700 0.00720800
1    4.06704400 -2.34894700 0.00111500
1    8.39124300 -4.84487300 0.00729600
1    2.85786800 -4.41018600 0.00138900
1    7.09886100 -7.01238000 0.00724500
1    -10.80415900 1.93928900 -0.00180600
```

```
1    -10.81688500 -0.50660300 -0.00128200
1    -4.97035400 9.62224400 -0.00085400
1    -7.08198800 8.38816600 -0.00155000
1    -9.58935900 4.06714600 -0.00217200
1    -5.23812100 1.66723400 -0.00447200
1    -8.31723900 6.27149100 -0.00208300
1    -4.06213000 3.70485900 -0.00435500
1    -5.84763900 -9.11567400 0.00233300
1    -3.72318000 -10.32762800 0.00311800
1    -5.24683500 -0.27113300 -0.00484400
1    -9.62157000 -2.64159300 -0.00088100
1    -4.06705000 -2.34898700 -0.00431600
1    -8.39126600 -4.84489200 -0.00002400
1    -2.85788100 -4.41022900 -0.00283500
1    -7.09889200 -7.01240800 0.00099900
1    2.52324700 9.65450900 0.00148800
1    2.38995000 4.68053100 -0.00241300
1    0.00000500 9.69022300 0.00054800
1    0.00002400 4.69735400 -0.00397100
1    -2.52323300 9.65449000 -0.00037400
1    -2.38989900 4.68051800 -0.00464500
1    1.17653100 -5.37096000 0.00186400
1    1.27252000 -10.33928400 0.00491300
1    -1.17659600 -5.37097000 0.00077900
1    -1.27253300 -10.33929800 0.00379800
```

15. [22]kekulene [3,4,4,3,4,4]

```
E(wB97XD/cc-pVDZ) = -3379.16164989
No imaginary frequency (B3LYP/6-31G*)

6    -2.44839500 9.24596900 -0.00000700
6    -3.73024300 9.93520800 -0.00000300
6    -4.90231500 9.26760800 0.00000200
6    -4.96258900 7.81401000 0.00000400
6    -3.72001900 7.07518300 0.00000000
6    -2.44129700 7.80873700 -0.00000500
6    4.90241200 9.26755700 -0.00003200
6    3.73034700 9.93516900 -0.00002900
6    2.44849200 9.24594400 -0.00002400
6    2.44137900 7.80871100 -0.00002200
6    3.72009400 7.07514400 -0.00002600
6    4.96267000 7.81395800 -0.00003000
6    9.88284100 0.67401800 -0.00003400
6    8.65005500 1.44932300 -0.00003200
6    7.39031600 0.73806300 -0.00002800
6    7.39030800 -0.73814000 -0.00002500
6    8.65004000 -1.44941400 -0.00002700
6    9.88283400 -0.67412100 -0.00003200
6    4.96258900 -7.81401000 -0.00000300
6    3.72001900 -7.07518300 -0.00000100
6    2.44129700 -7.80873700 0.00000500
6    2.44839500 -9.24596900 0.00000800
6    3.73024300 -9.93520800 0.00000600
6    4.90231500 -9.26760800 0.00000000
6    -2.44137900 -7.80871100 0.00002200
6    -3.72009400 -7.07514400 0.00002500
6    -4.96267000 -7.81395800 0.00003200
6    -4.90241200 -9.26755700 0.00003500
6    -3.73034700 -9.93516900 0.00003200
6    -2.44849200 -9.24594400 0.00002500
6    -7.39030800 0.73814000 0.00002400
6    -8.65004000 1.44941400 0.00002800
6    -9.88283400 0.67412100 0.00003500
6    -9.88284100 -0.67401800 0.00003700
6    -8.65005500 -1.44932300 0.00003300
6    -7.39031600 -0.73806300 0.00002600
6    0.00004900 9.28060400 -0.00001600
6    -1.25158900 9.94469500 -0.00001200
6    -1.22633400 7.15796000 -0.00000900
6    0.00004100 7.85522400 -0.00001400
6    1.25169300 9.94468200 -0.00002100
6    1.22640900 7.15794700 -0.00001800
6    6.16791900 7.14190000 -0.00003300
6    3.77360500 5.70383500 -0.00002500
6    5.00017900 4.99106200 -0.00002700
6    6.24001500 5.71826200 -0.00003200
6    7.44769100 5.00218300 -0.00003400
6    5.01913800 3.59527900 -0.00002600
6    6.21943500 2.88620100 -0.00002800
6    7.46717700 3.60027300 -0.00003200
6    8.66719300 2.82747800 -0.00003400
6    6.22863500 1.46581500 -0.00002600
6    6.22861900 -1.46588000 -0.00002100
6    6.21940500 -2.88626600 -0.00001800
6    7.46713900 -3.60035100 -0.00002000
6    8.66716300 -2.82756900 -0.00002500
6    5.01910100 -3.59533200 -0.00001400
6    5.00012700 -4.99111400 -0.00001000
6    6.23995500 -5.71832700 -0.00001200
6    7.44763900 -5.00226100 -0.00001700
6    3.77354500 -5.70387400 -0.00000500
6    6.16784500 -7.14196500 -0.00000800
6    1.22633400 -7.15796000 0.00000700
6    -0.00004100 -7.85522400 0.00001300
6    -0.00004900 -9.28060400 0.00001700
6    1.25158900 -9.94469500 0.00001400
6    -1.22640900 -7.15794700 0.00001600
6    -1.25169300 -9.94468200 0.00002300
6    -3.77360500 -5.70383500 0.00002100
6    -5.00017900 -4.99106100 0.00002500
6    -6.24001500 -5.71826200 0.00003200
6    -6.16791900 -7.14190000 0.00003500
6    -5.01913800 -3.59527900 0.00002200
6    -6.21943500 -2.88620100 0.00002500
6    -7.46717700 -3.60027300 0.00003200
6    -7.44769100 -5.00218300 0.00003500
6    -6.22863500 -1.46581500 0.00002200
6    -8.66719300 -2.82747800 0.00003600
6    -6.21940500 2.88626600 0.00001500
6    -7.46713900 3.60035100 0.00002000
6    -8.66716300 2.82756900 0.00002600
6    -6.22861900 1.46588000 0.00001700
6    -5.00012700 4.99111400 0.00000700
6    -6.23995500 5.71832700 0.00001200
6    -7.44763900 5.00226100 0.00001800
6    -5.01910100 3.59533200 0.00000900
6    -6.16784500 7.14196500 0.00001000
6    -3.77354500 5.70387400 0.00000200
1    -3.72141600 11.02748600 -0.00000400
1    -5.84651300 9.81677600 0.00000500
1    5.84661500 9.81671500 -0.00003500
1    3.72153200 11.02744700 -0.00003000
1    10.82773100 1.22205200 -0.00003700
1    10.82771800 -1.22216500 -0.00003300
1    3.72141600 -11.02748600 0.00000800
1    5.84651300 -9.81677600 -0.00000100
1    -5.84661500 -9.81671500 0.00004000
1    -3.72153200 -11.02744700 0.00003400
1    -10.82771800 1.22216500 0.00003800
1    -10.82773100 -1.22205200 0.00004200
1    -1.27188500 11.03767500 -0.00001300
```

```
1    -1.17751900 6.06901500 -0.00000800
1    1.27200000 11.03766100 -0.00002200
1    1.17758300 6.06900300 -0.00001600
1    7.09865200 7.71519900 -0.00003600
1    2.86045600 5.10879700 -0.00002200
1    8.39349800 5.55012900 -0.00003700
1    4.07339700 3.04735000 -0.00002300
1    9.62757300 3.34962000 -0.00003800
1    5.25799800 0.96989400 -0.00002300
1    5.25798800 -0.96994900 -0.00002000
1    9.62753800 -3.34972100 -0.00002600
1    4.07336600 -3.04739300 -0.00001200
1    8.39344000 -5.55021700 -0.00001800
1    2.86040300 -5.10882600 -0.00000400
1    7.09857200 -7.71527300 -0.00001000
1    1.17751900 -6.06901500 0.00000500
1    1.27188500 -11.03767500 0.00001600
1    -1.17758300 -6.06900300 0.00001300
1    -1.27200000 -11.03766100 0.00002500
1    -2.86045600 -5.10879700 0.00001600
1    -7.09865200 -7.71519900 0.00004000
1    -4.07339700 -3.04735000 0.00001600
1    -8.39349800 -5.55012900 0.00004100
1    -5.25799800 -0.96989400 0.00001700
1    -9.62757300 -3.34962000 0.00004100
1    -9.62753800 3.34972100 0.00002900
1    -5.25798800 0.96994900 0.00001400
1    -8.39344000 5.55021700 0.00002100
1    -4.07336600 3.04739300 0.00000600
1    -7.09857200 7.71527300 0.00001300
1    -2.86040300 5.10882600 -0.00000100
```

16. [16]clarene <2,2,4,2,2,4>

```
E(wB97XD/cc-pVDZ) = -2457.62359521
No imaginary frequency (B3LYP/6-31G*)

6    0.33267800 5.56643200 0.00996900
6    -0.36595100 6.80798600 0.01497600
6    -1.76256900 6.79810400 0.01983600
6    -2.49623300 5.60114400 0.01993300
6    -1.79996100 4.36253300 0.01491100
6    -0.40279300 4.38738900 0.01004700
6    4.62857900 5.56694200 -0.00491500
6    3.90707700 6.76716000 0.00000400
6    2.50691900 6.79182800 0.00493100
6    1.79749000 5.56090700 0.00490200
6    2.52524300 4.37368800 0.00002200
6    3.91728300 4.33712400 -0.00487500
6    6.76884600 1.87272400 -0.01984400
6    6.07909900 3.08717500 -0.01498700
6    4.65457500 3.07136400 -0.00996200
6    4.00133600 1.84485600 -0.01004100
6    4.67838300 0.62246900 -0.01491000
6    6.09916300 0.63882700 -0.01993300
6    2.49623300 -5.60114400 -0.01993300
6    1.79996100 -4.36253300 -0.01491100
6    0.40279300 -4.38738900 -0.01004800
6    -0.33267800 -5.56643200 -0.00996900
6    0.36595100 -6.80798600 -0.01497600
6    1.76256900 -6.79810400 -0.01983600
6    -1.79749000 -5.56090700 -0.00490200
6    -2.52524300 -4.37368800 -0.00002200
6    -3.91728300 -4.33712400 0.00487500
6    -4.62857900 -5.56694200 0.00491500
6    -3.90707700 -6.76716000 -0.00000400
6    -2.50691900 -6.79182800 -0.00493100
6    -4.00133600 -1.84485600 0.01004100
6    -4.67838300 -0.62246900 0.01491000
6    -6.09916300 -0.63882700 0.01993300
6    -6.76884600 -1.87272400 0.01984400
6    -6.07909900 -3.08717500 0.01498700
6    -4.65457500 -3.07136400 0.00996200
6    4.67672100 -1.86553400 -0.01993100
6    3.96675000 -0.64809200 -0.01495400
6    2.54991900 -0.68531400 -0.01002900
6    1.86853900 -1.86518100 -0.01002400
6    2.54450800 -3.11097500 -0.01495000
6    3.95394300 -3.11723700 -0.01993700
6    -1.86853900 1.86518100 0.01002400
6    -2.54450800 3.11097500 0.01495000
6    -3.95394300 3.11723700 0.01993700
6    -4.67672100 1.86553400 0.01993100
6    -3.96675000 0.64809200 0.01495400
6    -2.54991900 0.68531400 0.01002900
6    -3.93362600 5.57029700 0.02492300
6    -4.62045800 4.39771500 0.02492200
6    1.75438900 8.02953200 0.01007900
6    0.40048400 8.03719800 0.01482500
6    6.76039600 4.36556800 -0.01484000
6    6.07672200 5.53418100 -0.01007100
6    4.62045800 -4.39771500 -0.02492200
6    3.93362600 -5.57029700 -0.02492300
6    -1.75438900 -8.02953200 -0.01007900
6    -0.40048400 -8.03719800 -0.01482500
6    -6.76039600 -4.36556800 0.01484000
6    -6.07672200 -5.53418100 0.01007100
6    6.79107700 -0.62149600 -0.02490900
6    6.11889400 -1.80255600 -0.02489700
6    -6.11889400 1.80255600 0.02489700
6    -6.79107700 0.62149600 0.02490900
1    -2.30165000 7.74911800 0.02367600
1    0.13199800 3.44436500 0.00615000
1    4.45370400 7.71393700 0.00000100
1    1.98285200 3.43437100 0.00002700
1    7.86199800 1.88146400 -0.02370300
1    2.91729400 1.83632500 -0.00612100
1    -0.13199800 -3.44436500 -0.00615000
1    2.30165000 -7.74911800 -0.02367600
1    -1.98285200 -3.43437100 -0.00002700
1    -4.45370400 -7.71393700 -0.00000100
1    -2.91729400 -1.83632500 0.00612100
1    -7.86199800 -1.88146400 0.02370200
1    1.97381300 0.23721800 -0.00613800
1    0.78163200 -1.82682700 -0.00611400
1    -0.78163200 1.82682700 0.00611300
1    -1.97381300 -0.23721800 0.00613700
1    -4.47575400 6.51834300 0.02878300
1    -5.70884800 4.43662600 0.02884800
1    2.30907700 8.97044400 0.01006300
1    -0.14382600 8.98411200 0.01866200
1    7.85260700 4.36773400 -0.01870200
1    6.61420500 6.48502900 -0.01005700
1    5.70884800 -4.43662600 -0.02884800
1    4.47575400 -6.51834300 -0.02878300
1    -2.30907700 -8.97044400 -0.01006300
1    0.14382600 -8.98411200 -0.01866200
1    -7.85260700 -4.36773500 0.01870200
1    -6.61420500 -6.48502900 0.01005700
1    7.88317700 -0.61703400 -0.02877000
1    6.69681700 -2.72564000 -0.02878100
1    -6.69681700 2.72564000 0.02878100
```

```
1    -7.88317700 0.61703400 0.02877000
```

17. [18]clarene <2,4,2,4,2,4>

```
E(wB97XD/cc-pVDZ) = -2764.82661608
No imaginary frequency (B3LYP/6-31G*)

6    7.83617400 1.25431800 -0.00499800
6    7.14943600 2.46914300 -0.00472100
6    5.72466200 2.45785800 -0.00482500
6    5.06878700 1.23317400 -0.00524000
6    5.74362700 0.00807700 -0.00556400
6    7.16398200 0.02153200 -0.00539800
6    5.71300800 4.95676600 -0.00403000
6    5.00423600 6.15889000 -0.00368200
6    3.60050300 6.19292600 -0.00372200
6    2.87870400 4.96952300 -0.00414000
6    3.60232500 3.77255600 -0.00452800
6    4.99091500 3.72850200 -0.00446800
6    3.56327000 -6.21457400 -0.00681700
6    2.86472700 -4.97778100 -0.00677100
6    1.46631500 -5.00579200 -0.00683100
6    0.73364000 -6.18616200 -0.00694200
6    1.43630800 -7.42569600 -0.00702400
6    2.83174800 -7.41310800 -0.00696100
6    5.74072400 -2.47979200 -0.00610500
6    5.03116200 -1.26190700 -0.00600800
6    3.61408100 -1.29954400 -0.00636500
6    2.93261900 -2.47959700 -0.00665700
6    3.60837000 -3.72580100 -0.00660800
6    5.01797000 -3.73148600 -0.00639400
6    -5.06878700 1.23317400 -0.00524000
6    -5.72466200 2.45785800 -0.00482500
6    -7.14943600 2.46914300 -0.00472100
6    -7.83617400 1.25431800 -0.00499800
6    -7.16398200 0.02153200 -0.00539800
6    -5.74362700 0.00807700 -0.00556400
6    -2.87870400 4.96952400 -0.00414000
6    -3.60050300 6.19292600 -0.00372200
6    -5.00423600 6.15889000 -0.00368200
6    -5.71300800 4.95676600 -0.00403000
6    -4.99091500 3.72850200 -0.00446800
6    -3.60232500 3.77255600 -0.00452800
6    -0.73364000 -6.18616200 -0.00694200
6    -1.46631500 -5.00579200 -0.00683100
6    -2.86472700 -4.97778100 -0.00677100
6    -3.56327000 -6.21457400 -0.00681700
6    -2.83174800 -7.41310800 -0.00696100
6    -1.43630800 -7.42569600 -0.00702400
6    -2.93261900 -2.47959700 -0.00665700
6    -3.61408100 -1.29954400 -0.00636500
6    -5.03116200 -1.26190700 -0.00600900
6    -5.74072400 -2.47979200 -0.00610500
6    -5.01797000 -3.73148600 -0.00639400
6    -3.60837000 -3.72580100 -0.00660800
6    1.42263900 4.98750000 -0.00414300
6    0.72268200 6.21102800 -0.00377600
6    -0.72268200 6.21102800 -0.00377600
6    -1.42263900 4.98750000 -0.00414300
6    -0.68135700 3.77919300 -0.00447900
6    0.68135600 3.77919300 -0.00447900
6    7.85545100 -1.23842100 -0.00560200
6    7.18249000 -2.41890700 -0.00590200
6    7.83833600 3.74448100 -0.00429100
6    7.16191700 4.91584700 -0.00396600
6    -0.67632800 -8.65996500 -0.00714000
6    0.67632800 -8.65996500 -0.00714000
6    5.68608500 -5.01057700 -0.00645300
6    5.00012500 -6.18354400 -0.00667300
6    -7.16191700 4.91584700 -0.00396600
6    -7.83833600 3.74448100 -0.00429100
6    -1.49628200 7.42918400 -0.00339300
6    -2.85508900 7.42170400 -0.00335700
6    -5.68608500 -5.01057700 -0.00645300
6    -5.00012500 -6.18354400 -0.00667300
6    -7.85545100 -1.23842100 -0.00560200
6    -7.18249000 -2.41890700 -0.00590200
6    2.85508900 7.42170400 -0.00335700
6    1.49628200 7.42918400 -0.00339300
1    8.92935000 1.26075700 -0.00487900
1    3.98444600 1.22705600 -0.00525900
1    5.55630100 7.10243000 -0.00336000
1    3.05508800 2.83631200 -0.00489600
1    0.92953700 -4.06356700 -0.00674700
1    3.37275300 -8.36303600 -0.00700200
1    3.03806900 -0.37686000 -0.00645000
1    1.84562300 -2.44150900 -0.00694900
1    -3.98444600 1.22705600 -0.00525900
1    -8.92935000 1.26075600 -0.00487900
1    -5.55630100 7.10243000 -0.00336000
1    -3.05508800 2.83631200 -0.00489700
1    -0.92953700 -4.06356700 -0.00674700
1    -3.37275300 -8.36303600 -0.00700200
1    -1.84562300 -2.44150900 -0.00694900
1    -3.03806900 -0.37686000 -0.00645000
1    -1.19224700 2.81896300 -0.00472000
1    1.19224700 2.81896300 -0.00472000
1    8.94755500 -1.23422100 -0.00548100
1    7.75957700 -3.34244900 -0.00600800
1    8.93054900 3.73970700 -0.00422700
1    7.70378600 5.86417300 -0.00363800
1    -1.22664200 -9.60341400 -0.00721900
1    1.22664200 -9.60341400 -0.00721900
1    6.77446200 -5.04848700 -0.00631800
1    5.54247100 -7.13146800 -0.00671400
1    -7.70378600 5.86417300 -0.00363800
1    -8.93054900 3.73970700 -0.00422700
1    -0.98493900 8.39069600 -0.00311100
1    -3.40482200 8.36536100 -0.00304400
1    -6.77446200 -5.04848700 -0.00631800
1    -5.54247100 -7.13146800 -0.00671400
1    -8.94755500 -1.23422100 -0.00548100
1    -7.75957700 -3.34244900 -0.00600800
1    3.40482200 8.36536100 -0.00304400
1    0.98493900 8.39069600 -0.00311100
```

18. [20]clarene <2,2,6,2,2,6>

```
E(wB97XD/cc-pVDZ) = -3072.03428393
No imaginary frequency (B3LYP/6-31G*)

6    1.40777500 7.42583600 0.01301100
6    0.71502700 8.67136800 0.03060500
6    -0.68042400 8.66953800 0.04221500
6    -1.42073500 7.47724000 0.03433300
6    -0.73236900 6.23369200 0.00967500
6    0.66589000 6.25039500 0.00112400
6    5.70404600 7.42201200 -0.00964900
```

```
6    4.98337700 8.62181000 0.00003100
6    3.58400400 8.64686800 0.01021100
6    2.87309200 7.41646700 0.00756800
6    3.60051400 6.22844800 0.00103800
6    4.99303100 6.19175000 -0.00595600
6    7.85284800 3.73854900 -0.04074200
6    7.15786300 4.94861300 -0.02942300
6    5.73286100 4.92694700 -0.01095200
6    5.08473900 3.69737400 0.00216600
6    5.76818500 2.47740200 -0.00615500
6    7.18932900 2.50184200 -0.03176200
6    1.42273300 -7.47723400 -0.02842800
6    0.73437000 -6.23369100 -0.00338400
6    -0.66389000 -6.25039400 0.00517400
6    -1.40577600 -7.42583200 -0.00706300
6    -0.71302900 -8.67136100 -0.02493500
6    0.68242100 -8.66953000 -0.03656700
6    -2.87109300 -7.41646500 -0.00173800
6    -3.59851500 -6.22844600 0.00486900
6    -4.99103300 -6.19174900 0.01173900
6    -5.70204900 -7.42201100 0.01519100
6    -4.98137900 -8.62180800 0.00541700
6    -3.58200600 -8.64686500 -0.00463400
6    -5.08274000 -3.69737300 0.00397700
6    -5.76618800 -2.47740200 0.01226200
6    -7.18733700 -2.50184300 0.03754300
6    -7.85085800 -3.73855100 0.04629300
6    -7.15587100 -4.94861400 0.03500100
6    -5.73086500 -4.92694700 0.01679900
6    5.78742200 -0.00628800 -0.01517900
6    5.06706700 1.20165000 0.00777000
6    3.64746200 1.14778000 0.04549700
6    2.97651200 -0.03652100 0.05362700
6    3.66440400 -1.28092300 0.02280000
6    5.07544200 -1.26672700 -0.00998100
6    3.63248700 -3.76408800 -0.00914000
6    2.94009600 -2.53454400 0.02317900
6    1.51845600 -2.55984000 0.05433600
6    0.82737100 -3.73248800 0.04701700
6    1.48964400 -4.98932000 0.00975600
6    2.89598700 -5.01036900 -0.01354900
6    -2.97449600 0.03651500 -0.04672500
6    -3.66239500 1.28091800 -0.01611800
6    -5.07344100 1.26672600 0.01628300
6    -5.78542400 0.00628800 0.02135300
6    -5.06506500 -1.20165100 -0.00142400
6    -3.64545000 -1.14778500 -0.03877100
6    -0.82535300 3.73247400 -0.03986700
6    -1.48763800 4.98931600 -0.00317500
6    -2.89398600 5.01037000 0.01983700
6    -3.63048500 3.76408800 0.01550900
6    -2.93808500 2.53453800 -0.01640900
6    -1.51643400 2.55982500 -0.04709000
6    -2.85702500 7.46006700 0.05144700
6    -3.55258700 6.29283500 0.04682600
6    2.83675400 9.88730400 0.02419900
6    1.48361500 9.89886300 0.03567800
6    7.83762800 6.22746800 -0.03557800
6    7.15189300 7.39403600 -0.02430500
6    3.55458400 -6.29282900 -0.04092800
6    2.85902200 -7.46005900 -0.04569300
6    -2.83475500 -9.88729800 -0.01880400
6    -1.48161600 -9.89885500 -0.03026600
6    -7.83563600 -6.22747000 0.04091900
6    -7.14989800 -7.39403700 0.02965000
6    7.89151500 1.24874900 -0.04866400
6    7.22738500 0.06335000 -0.04303300
6    5.74481000 -2.53146900 -0.03940800
6    5.06248800 -3.71236900 -0.03897300
6    -7.22539300 -0.06335100 0.04888900
6    -7.88952500 -1.24874900 0.05435100
6    -5.06049300 3.71237200 0.04498700
6    -5.74281500 2.53147200 0.04541200
1    -1.21410700 9.62346300 0.05841200
1    1.19499800 5.30375300 -0.01422200
1    5.53030400 9.56841800 -0.00039200
1    3.05790300 5.28880500 0.00134500
1    8.94582100 3.75235900 -0.05765400
1    4.00040100 3.68355000 0.01840700
1    -1.19299700 -5.30375700 0.02077300
1    1.21610400 -9.62345000 -0.05301500
1    -3.05590300 -5.28880400 0.00466400
1    -5.52830600 -9.56841600 0.00563200
1    -3.99839800 -3.68354700 -0.01200700
1    -8.94383500 -3.75236200 0.06298500
1    3.06361700 2.06541500 0.07152900
1    1.88994600 -0.00741700 0.08479100
1    0.95102400 -1.63267000 0.08502300
1    -0.25921100 -3.68490700 0.07341400
1    -1.88792200 0.00740700 -0.07762300
1    -3.06160000 -2.06542100 -0.06465100
1    0.26123900 3.68488600 -0.06585700
1    -0.94899100 1.63264600 -0.07730100
1    -3.39068400 8.41268500 0.07017000
1    -4.64057200 6.33868600 0.06235200
1    3.39509700 10.82602800 0.02681000
1    0.94118200 10.84676100 0.04792000
1    8.92974900 6.23087700 -0.04846800
1    7.68641700 8.34652900 -0.02769500
1    4.64256600 -6.33867600 -0.05662600
1    3.39267600 -8.41267300 -0.06469100
1    -3.39309900 -10.82602200 -0.02159600
1    -0.93918300 -10.84675000 -0.04268400
1    -8.92775900 -6.23088200 0.05363000
1    -7.68442300 -8.34653000 0.03286700
1    8.98333600 1.26195900 -0.06810100
1    7.81029600 -0.85644400 -0.05836700
1    6.83284600 -2.56908900 -0.06489700
1    5.63863500 -4.63608900 -0.06402900
1    -7.80830700 0.85644300 0.06412800
1    -8.98135000 -1.26195900 0.07355900
1    -5.63664700 4.63609600 0.06976000
1    -6.83085800 2.56909600 0.07061300
```

19. [22]clarene <2,4,4,4,2,6>

```
E(wB97XD/cc-pVDZ) = -3379.23436325
No imaginary frequency (B3LYP/6-31G*)

6    0.24081000 8.09825600 0.00617200
6    -0.45416900 9.34295600 0.00690000
6    -1.84871900 9.34069600 0.00616700
6    -2.58899400 8.14784700 0.00474800
6    -1.89983500 6.90517100 0.00402700
6    -0.50023500 6.92284100 0.00474900
6    4.53820600 8.11336000 0.00852000
6    3.80996500 9.31305200 0.00915100
6    2.41515500 9.32889400 0.00839800
6    1.70865100 8.09126300 0.00694700
6    2.43875100 6.90849100 0.00632600
6    3.83764900 6.87755600 0.00706100
6    8.83643700 0.67006300 0.00464700
```

```
6    8.15468300 1.89172200 0.00525600
6    6.73072100 1.89382200 0.00448300
6    6.06505100 0.66718900 0.00314300
6    6.73316900 -0.55785300 0.00248900
6    8.15716200 -0.55276600 0.00328100
6    4.55839000 -6.78651400 -0.00379100
6    3.85065800 -5.55085800 -0.00322200
6    2.45564900 -5.58461600 -0.00403500
6    1.72621200 -6.77447000 -0.00539400
6    2.44020000 -8.00655500 -0.00593800
6    3.83907000 -7.98622300 -0.00513000
6    -4.03652600 -6.76187100 -0.00847400
6    -4.76321500 -5.56612200 -0.00792600
6    -6.15259800 -5.52579300 -0.00859300
6    -6.87097200 -6.75648900 -0.00990200
6    -6.15945000 -7.95628500 -0.01044100
6    -4.75634500 -7.98661300 -0.00974500
6    -6.24544600 -3.02880100 -0.00666100
6    -6.92987100 -1.80785400 -0.00602200
6    -8.35063300 -1.83246800 -0.00678600
6    -9.01350400 -3.07003400 -0.00812100
6    -8.31820800 -4.27889400 -0.00871900
6    -6.89280900 -4.25826200 -0.00797400
6    6.71673900 4.38355600 0.00654100
6    5.99204300 5.63257400 0.00720400
6    4.58193700 5.62518700 0.00638500
6    3.91003400 4.37745600 0.00489100
6    4.59516500 3.19815900 0.00428200
6    6.01183500 3.16354300 0.00511200
6    6.72449000 -3.04816600 0.00046100
6    6.01675900 -1.82930600 0.00102600
6    4.60091200 -1.86767000 0.00011900
6    3.91868700 -3.04938100 -0.00124200
6    4.59346200 -4.29468500 -0.00180300
6    6.00295800 -4.29805100 -0.00097000
6    0.26715000 -6.78703500 -0.00624100
6    -0.47145300 -5.57765800 -0.00582400
6    -1.83533700 -5.57422900 -0.00655600
6    -2.57976500 -6.78005700 -0.00776100
6    -1.88088200 -8.00482100 -0.00826800
6    -0.43683400 -8.00768300 -0.00750600
6    -4.14056900 0.70858400 -0.00240300
6    -4.82997100 1.95252900 -0.00175000
6    -6.24129800 1.93767000 -0.00254700
6    -6.95226300 0.67637300 -0.00398900
6    -6.23041500 -0.53139500 -0.00459600
6    -4.81046800 -0.47626600 -0.00376700
6    -1.99308200 4.40394600 0.00188800
6    -2.65546800 5.66117500 0.00257200
6    -4.06244500 5.68239600 0.00182700
6    -4.79915600 4.43596200 0.00035900
6    -4.10618800 3.20643400 -0.00029500
6    -2.68420200 3.23137300 0.00051600
6    -4.02500000 8.13161200 0.00397700
6    -4.72114600 6.96457800 0.00258400
6    1.66253100 10.56731400 0.00907000
6    0.31048500 10.57397200 0.00837000
6    8.83940400 3.15674300 0.00666400
6    8.16030400 4.33157400 0.00728100
6    6.67695100 -5.57605300 -0.00159900
6    5.99652600 -6.74993000 -0.00293500
6    -4.01199700 -9.21569000 -0.01025500
6    -2.65388400 -9.22337900 -0.00954600
6    -9.00181100 -5.55673000 -0.01007100
6    -8.31979900 -6.72416800 -0.01062300
6    6.66071600 6.91137700 0.00870100
6    5.97480900 8.08357800 0.00931600
6    8.84460900 -1.81651500 0.00265800
6    8.16823200 -2.99273100 0.00134300
6    0.33022900 -9.23170300 -0.00800300
6    1.68721200 -9.23211100 -0.00728100
6    -8.39199600 0.60568600 -0.00482900
6    -9.05461800 -0.58071900 -0.00614900
6    -6.22946700 4.38370400 -0.00048600
6    -6.91138800 3.20239400 -0.00186400
1    -2.38274500 10.29453400 0.00671100
1    0.02964100 5.97637100 0.00415800
1    4.35322400 10.26166000 0.01027200
1    1.89990300 5.96703500 0.00524200
1    9.92954800 0.67115500 0.00526400
1    4.98082300 0.66595400 0.00261800
1    1.91500900 -4.64471000 -0.00355300
1    4.38466600 -8.93342400 -0.00554400
1    -4.21830000 -4.62814300 -0.00692100
1    -6.70903400 -8.90124000 -0.01142700
1    -5.16088200 -3.01465300 -0.00610100
1    -10.10657100 -3.08451500 -0.00870300
1    2.82293300 4.33699200 0.00418100
1    4.02147200 2.27383700 0.00310900
1    4.02449300 -0.94501900 0.00047400
1    2.83148300 -3.01140300 -0.00190700
1    0.04198900 -4.61859100 -0.00492200
1    -2.34428900 -4.61274500 -0.00620200
1    -3.05365800 0.68017600 -0.00181200
1    -4.22546000 -1.39344400 -0.00420300
1    -0.90627900 4.35600300 0.00247400
1    -2.11646900 2.30400900 0.00005300
1    -4.55796100 9.08479500 0.00452800
1    -5.80921000 7.01055800 0.00204600
1    2.21843000 11.50744600 0.01017200
1    -0.23618600 11.51949700 0.00890400
1    9.93147200 3.15766700 0.00724200
1    8.73145100 5.25859200 0.00834800
1    7.76526900 -5.60957700 -0.00099200
1    6.54131200 -7.69640500 -0.00337200
1    -4.56257700 -10.15882400 -0.01122100
1    -2.14288500 -10.18486000 -0.00996400
1    -10.09400100 -5.55628500 -0.01063500
1    -8.85590400 -7.67573100 -0.01163500
1    7.74891300 6.94944600 0.00938200
1    6.51616500 9.03203900 0.01045200
1    9.93667900 -1.81502800 0.00327900
1    8.74165500 -3.91830300 0.00094300
1    -0.18667700 -10.19001300 -0.00900000
1    2.23264000 -10.17821500 -0.00770500
1    -8.97587200 1.52496100 -0.00439700
1    -10.14658000 -0.59580900 -0.00674600
1    -6.80623100 5.30737600 -0.00003800
1    -7.99973100 3.23967800 -0.00244500
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20. [24]clarene <2,2,8,2,2,8>

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E(wB97XD/cc-pVDZ) = -3686.44493678
No imaginary frequency (B3LYP/6-31G*)

6    2.47814900 9.28881700 0.00815000
6    1.78857700 10.53511600 0.06449400
6    0.39386700 10.53604200 0.09081300
6    -0.34902600 9.34658200 0.05122400
6    0.33462100 8.10276000 -0.03529100
6    1.73327000 8.11592600 -0.04842200
6    6.77396100 9.28457600 -0.01973400
```

```
6    6.05349100 10.48388800 0.00136100
6    4.65463600 10.50845300 0.02274800
6    3.94341500 9.27806800 0.00894900
6    4.67084900 8.08979300 0.00188300
6    6.06363500 8.05373500 -0.00540500
6    8.92700100 5.60773100 -0.08684500
6    8.22932200 6.81541100 -0.06094000
6    6.80522800 6.78995100 -0.00431000
6    6.16149700 5.55867800 0.05283300
6    6.84890800 4.34055700 0.03995600
6    8.26787400 4.36987100 -0.04669400
6    0.34694300 -9.34325000 -0.04621300
6    -0.33670400 -8.09942700 0.04029200
6    -1.73535400 -8.11259300 0.05342500
6    -2.48023200 -9.28548400 -0.00313800
6    -1.79066000 -10.53178400 -0.05947200
6    -0.39595000 -10.53271000 -0.08579200
6    -3.94549800 -9.27473500 -0.00393400
6    -4.67293100 -8.08646000 0.00311700
6    -6.06571700 -8.05040100 0.01041700
6    -6.77604300 -9.28124200 0.02476600
6    -6.05557400 -10.48055500 0.00368100
6    -4.65671900 -10.50512000 -0.01771300
6    -6.16358000 -5.55534400 -0.04783200
6    -6.85099100 -4.33722300 -0.03496300
6    -8.26995700 -4.36653700 0.05169300
6    -8.92908300 -5.60439600 0.09185400
6    -8.23140400 -6.81207600 0.06595300
6    -6.80731000 -6.78661700 0.00931700
6    6.88073900 1.85812200 0.03412000
6    6.15603400 3.06139000 0.10294600
6    4.74213100 2.99719500 0.23892300
6    4.08013000 1.80802800 0.28580400
6    4.77102100 0.56778300 0.19075000
6    6.17765600 0.59344800 0.06616200
6    4.75806500 -1.90994900 0.09938200
6    4.05868500 -0.69198700 0.21365000
6    2.63973700 -0.73809900 0.34662200
6    1.95939800 -1.91597600 0.34659500
6    2.62848900 -3.16812900 0.21357400
6    4.03300000 -3.16529200 0.09926100
6    2.57383300 -5.64586500 0.06581700
6    1.89323600 -4.41462600 0.19061700
6    0.47373700 -4.43570000 0.28587200
6    -0.22567200 -5.60324300 0.23905200
6    0.42516400 -6.86012000 0.10298400
6    1.82961000 -6.88675000 0.03384200
6    -4.08221600 -1.80469500 -0.28084600
6    -4.77310500 -0.56444900 -0.18577900
6    -6.17973900 -0.59011500 -0.06117700
6    -6.88282200 -1.85478800 -0.02913200
6    -6.15811800 -3.05805600 -0.09796300
6    -4.74421700 -2.99386200 -0.23396000
6    -1.96148300 1.91931000 -0.34163100
6    -2.63057300 3.17146300 -0.20859900
6    -4.03508300 3.16862500 -0.09427600
6    -4.76014800 1.91328200 -0.09439900
6    -4.06077000 0.69532000 -0.20867800
6    -2.64182200 0.74143300 -0.34166000
6    0.22358800 5.60657700 -0.23407800
6    -0.42724800 6.86345300 -0.09799300
6    -1.83169300 6.89008300 -0.02884500
6    -2.57591600 5.64919800 -0.06082500
6    -1.89531900 4.41795900 -0.18563900
6    -0.47582200 4.43903500 -0.28090400
6    -1.78416100 9.33534700 0.09813700
6    -2.48431600 8.17180700 0.06932900
6    3.91000300 11.74952300 0.06245300
6    2.55744600 11.76181800 0.09060600
6    8.90765100 8.09442200 -0.08764500
6    8.22105400 9.25981100 -0.05968500
6    2.48223300 -8.16847500 -0.06432100
6    1.78207800 -9.33201500 -0.09312300
6    -3.91208600 -11.74619000 -0.05740800
6    -2.55953000 -11.75848700 -0.08556900
6    -8.90973300 -8.09108800 0.09267200
6    -8.22313600 -9.25647700 0.06472400
6    8.97518700 3.12104900 -0.09313300
6    8.31708500 1.93320400 -0.06390300
6    6.85413500 -0.66231900 -0.03310700
6    6.18106400 -1.84830300 -0.02017500
6    4.69061000 -4.42872500 -0.02063700
6    3.99957400 -5.60433400 -0.03366800
6    -8.31916800 -1.92987000 0.06889900
6    -8.97727000 -3.11771500 0.09813300
6    -6.18314600 1.85163600 0.02517000
6    -6.85621700 0.66565200 0.03810200
6    -4.00165700 5.60766600 0.03866800
6    -4.69269300 4.43205800 0.02563300
1    -0.13732500 11.48989000 0.14509000
1    2.25991500 7.16894100 -0.10159400
1    6.60019800 11.43056700 0.00115000
1    4.12833200 7.14991800 0.00206000
1    10.01865200 5.62420300 -0.14131200
1    5.07811000 5.54160600 0.10642200
1    -2.26199800 -7.16560900 0.10659700
1    0.13524100 -11.48655900 -0.14006100
1    -4.13041500 -7.14658500 0.00291400
1    -6.60228100 -11.42723300 0.00390500
1    -5.08019200 -5.53827100 -0.10141500
1    -10.02073400 -5.62086900 0.14632800
1    4.15711800 3.91117500 0.31986100
1    2.99836400 1.82893700 0.39722800
1    2.06834100 0.18117000 0.45494600
1    0.87760700 -1.88034200 0.45480200
1    -0.08449400 -3.50883900 0.39743500
1    -1.30968700 -5.55319000 0.32012400
1    -3.00045200 -1.82560300 -0.39228700
1    -4.15920600 -3.90784200 -0.31491200
1    -0.87969300 1.88367700 -0.44984500
1    -2.07042700 -0.17783600 -0.44999200
1    1.30760200 5.55652600 -0.31516100
1    0.08240900 3.51217500 -0.39248100
1    -2.31208100 10.28900400 0.16422500
1    -3.57119000 8.22038000 0.11379200
1    4.47014500 12.68703500 0.07595400
1    2.01522400 12.70911800 0.12837400
1    9.99914000 8.09819400 -0.12574200
1    8.75320700 10.21348900 -0.07362700
1    3.56910700 -8.21704900 -0.10877900
1    2.30999700 -10.28567200 -0.15920300
1    -4.47222900 -12.68370300 -0.07089500
1    -2.01730800 -12.70578700 -0.12333100
1    -10.00122200 -8.09485900 0.13077300
1    -8.75529000 -10.21015500 0.07867900
1    10.06505000 3.14019600 -0.15917500
1    8.90233200 1.01606400 -0.10781200
1    7.93823200 -0.68937600 -0.13020800
1    6.75936400 -2.76685300 -0.10631500
1    5.77524100 -4.47054600 -0.10709600
1    4.56484400 -6.52972200 -0.13103100
1    -8.90441400 -1.01273000 0.11281100
1    -10.06713300 -3.13686200 0.16417900
1    -6.76144500 2.77018600 0.11131800
1    -7.94031300 0.69270900 0.13521300
1    -4.56692600 6.53305300 0.13603900
```

1 -5.77732300 4.47387800 0.11209900

21. [26]clarene <2,4,6,4,2,8>

E(wB97XD/cc-pVDZ) = -3993.64412437
No imaginary frequency (B3LYP/6-31G*)

6 1.25505400 9.99355200 0.00417600
6 0.56607400 11.24191100 0.00300800
6 -0.82797300 11.24715100 0.00206500
6 -1.57438300 10.05869500 0.00221500
6 -0.89256100 8.81172800 0.00331900
6 0.50761700 8.82168400 0.00426300
6 5.55271300 9.99824000 0.00718000
6 4.82706100 11.19889900 0.00591600
6 3.43273800 11.21737300 0.00492900
6 2.72320700 9.98120200 0.00522400
6 3.45119600 8.79656600 0.00652300
6 4.85048600 8.76319400 0.00747400
6 9.86462200 2.56899600 0.01500900
6 9.17670400 3.78606100 0.01380100
6 7.75216500 3.78167800 0.01316400
6 7.09246300 2.55173300 0.01405800
6 7.76753400 1.32927700 0.01525500
6 9.19201000 1.34250500 0.01565400
6 3.43017200 -8.63235000 0.01749200
6 2.72994700 -7.39180700 0.01686200
6 1.33369600 -7.41742700 0.01589300
6 0.59770100 -8.60332600 0.01548000
6 1.30566200 -9.83954300 0.01629800
6 2.70364500 -9.82767600 0.01726700
6 -5.16744400 -8.57858500 0.01077900
6 -5.89577400 -7.38330700 0.00963600
6 -7.28570000 -7.34491200 0.00848800
6 -8.00203200 -8.57706900 0.00857800
6 -7.28916300 -9.77553000 0.00974400
6 -5.88653600 -9.80395400 0.01083200
6 -7.38822100 -4.84647000 0.00686700
6 -8.07894100 -3.62850500 0.00565600
6 -9.49975200 -3.66077700 0.00475300
6 -10.15646100 -4.90109800 0.00503000
6 -9.45557900 -6.10616200 0.00620400
6 -8.02997900 -6.07935000 0.00719500
6 7.73155900 6.27150700 0.01122000
6 7.00531900 7.51904300 0.00986000
6 5.59509400 7.51055900 0.00877600
6 4.92539600 6.26154700 0.00892400
6 5.61255000 5.08281700 0.01030300
6 7.02934400 5.04989600 0.01160700
6 7.77803500 -1.15699900 0.01690100
6 7.06118100 0.05310400 0.01598800
6 5.64163900 0.00128300 0.01572200
6 4.96772800 -1.18274100 0.01618500
6 5.65304300 -2.42830200 0.01694600
6 7.06464300 -2.41530800 0.01738600
6 5.62249700 -4.91214300 0.01784500
6 4.92839700 -3.68296200 0.01718500
6 3.50704200 -3.71157700 0.01668900
6 2.81809400 -4.88689500 0.01666400
6 3.48253600 -6.14241100 0.01713500
6 4.88900100 -6.15882700 0.01782300
6 -0.86203700 -8.61090200 0.01423500
6 -1.59845800 -7.40010000 0.01293600
6 -2.96285600 -7.39373300 0.01179700
6 -3.71028300 -8.59782400 0.01190400
6 -3.01305900 -9.82369900 0.01307900
6 -1.56950800 -9.82957600 0.01419500
6 -5.30722900 -1.09016300 0.00577500
6 -6.00628400 0.14903200 0.00473400
6 -7.41804800 0.12209100 0.00391800
6 -8.11874600 -1.14490800 0.00418900
6 -7.38801500 -2.34713000 0.00530800
6 -5.96804100 -2.28033600 0.00606100
6 -3.19030200 2.62858800 0.00516300
6 -3.86585400 3.88379000 0.00404400
6 -5.27505300 3.88507500 0.00318400
6 -6.00040400 2.62918300 0.00342100
6 -5.29515600 1.40921000 0.00450300
6 -3.87032400 1.45126700 0.00538100
6 -1.00592900 6.30963800 0.00448000
6 -1.65747200 7.57312500 0.00345100
6 -3.06405800 7.60568900 0.00254800
6 -3.81160400 6.36576600 0.00274600
6 -3.12962500 5.12941200 0.00380800
6 -1.70692200 5.14270800 0.00463900
6 -3.01008600 10.05359400 0.00127500
6 -3.71429500 8.89184000 0.00144100
6 2.68573500 12.45886200 0.00368000
6 1.33412300 12.47046900 0.00280300
6 9.85790200 5.05282000 0.01323000
6 9.17530500 6.22494800 0.01211100
6 5.55593600 -7.43856000 0.01843300
6 4.86743600 -8.60796900 0.01831700
6 -5.14372400 -11.03359800 0.01205400
6 -3.78606400 -11.04209500 0.01312200
6 -10.13608700 -7.38531600 0.00641400
6 -9.45068400 -8.55030200 0.00750200
6 7.67467000 8.79733000 0.00955600
6 6.98902900 9.96917300 0.00826600
6 9.88890300 0.08523800 0.01671200
6 9.21978700 -1.09537100 0.01726300
6 7.73487700 -3.68029200 0.01825100
6 7.05311800 -4.86061300 0.01846400
6 -0.80771800 -11.05689900 0.01520800
6 0.54867800 -11.06245400 0.01612700
6 -9.55774200 -1.22406200 0.00332500
6 -10.21246200 -2.41443300 0.00357300
6 -7.42859400 2.56657500 0.00259800
6 -8.10026000 1.37905600 0.00284100
6 -5.24128400 6.32866900 0.00190200
6 -5.93439100 5.15352900 0.00210200
1 -1.35687800 12.20381900 0.00118400
1 1.03274500 7.87225800 0.00508900
1 5.37213500 12.14644400 0.00572700
1 2.91046000 7.85591000 0.00688800
1 10.95768900 2.57588800 0.01545500
1 6.00800300 2.54466200 0.01387800
1 0.79861000 -6.47406300 0.01547500
1 3.24363400 -10.77806100 0.01785300
1 -5.35210500 -6.44433800 0.00969400
1 -7.83746000 -10.72121200 0.00983000
1 -6.30348700 -4.82714800 0.00757100
1 -11.24942600 -4.92083100 0.00429400
1 3.83821400 6.21988400 0.00785300
1 5.04044200 4.15737000 0.01023200
1 5.05911600 0.92024400 0.01512500
1 3.88067200 -1.15159600 0.01592600
1 2.93715600 -2.78530500 0.01630500
1 1.73100900 -4.84154900 0.01626800
1 -1.08253800 -6.44221500 0.01271400
1 -3.47010200 -6.43120200 0.01074600
1 -4.21998900 -1.10959500 0.00635200

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1    -5.37634300 -3.19336100 0.00685800
1    -2.10354500 2.58962400 0.00589300
1    -3.29352300 0.52936400 0.00627500
1    0.08059400 6.25319100 0.00515700
1    -1.14744100 4.21020600 0.00542000
1    -3.53566000 11.01084800 0.00042000
1    -4.80191000 8.94529900 0.00069800
1    3.24578200 13.39650200 0.00348700
1    0.79019100 13.41754600 0.00190000
1    10.94994300 5.05655200 0.01376500
1    9.74320000 7.15382400 0.01179500
1    6.64410400 -7.47790700 0.01900500
1    5.40469500 -9.55869200 0.01880500
1    -5.69539700 -11.97607100 0.01213300
1    -3.27570100 -12.00376800 0.01406500
1    -11.22825100 -7.38739600 0.00564200
1    -9.98311500 -9.50390100 0.00761300
1    8.76274400 8.83529900 0.01040400
1    7.52986300 10.91790900 0.00807500
1    10.98089000 0.09478500 0.01701800
1    9.79766400 -2.01822100 0.01799000
1    8.82304500 -3.71801500 0.01876900
1    7.62970200 -5.78420400 0.01913600
1    -1.32821800 -12.01311300 0.01517200
1    1.09109900 -12.01026100 0.01678900
1    -10.14733500 -0.30856900 0.00242200
1    -11.30426600 -2.43730100 0.00287500
1    -8.01243400 3.48585600 0.00176200
1    -9.18879800 1.40626100 0.00219400
1    -5.80891600 7.25786100 0.00107800
1    -7.02242100 5.19995800 0.00141600
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22. [28]clarene <2,2,10,2,2,10>

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No imaginary frequency (B3LYP/6-31G*)

6    3.55514800 11.15329600 -0.02809400
6    2.86688100 12.39919500 -0.10481600
6    1.47274100 12.40021100 -0.14587700
6    0.72924200 11.21163500 -0.09974700
6    1.41085600 9.96843400 0.01106300
6    2.80933400 9.98118800 0.03715000
6    7.85013800 11.15015600 0.03933700
6    7.12990200 12.34910700 0.00332400
6    5.73147200 12.37317200 -0.03304000
6    5.02023900 11.14276000 -0.01703800
6    5.74759300 9.95464400 0.00268400
6    7.14021300 9.91905500 0.02272900
6    10.00291500 7.47549000 0.15061400
6    9.30503400 8.68240500 0.11019400
6    7.88194400 8.65555900 0.03343400
6    7.23973200 7.42366300 -0.03221800
6    7.92781800 6.20610800 -0.00662800
6    9.34524900 6.23733800 0.10397900
6    -0.72888500 -11.21056300 0.10546000
6    -1.41049900 -9.96736300 -0.00535200
6    -2.80897700 -9.98011600 -0.03144100
6    -3.55479100 -11.15222500 0.03380500
6    -2.86652400 -12.39812400 0.11053000
6    -1.47238400 -12.39914000 0.15159200
6    -5.01988200 -11.14168800 0.02275000
6    -5.74723600 -9.95357200 0.00302800
6    -7.13985600 -9.91798400 -0.01701600
6    -7.84978100 -11.14908500 -0.03362300
6    -7.12954500 -12.34803500 0.00239000
6    -5.73111500 -12.37210100 0.03875400
6    -7.23937500 -7.42259200 0.03793200
6    -7.92746100 -6.20503700 0.01234300
6    -9.34489200 -6.23626700 -0.09826400
6    -10.00255800 -7.47441900 -0.14490000
6    -9.30467600 -8.68133400 -0.10448000
6    -7.88158700 -8.65448800 -0.02772100
6    7.96395400 3.72433600 0.00611400
6    7.23803500 4.92558100 -0.08027700
6    5.82724200 4.85667900 -0.24557200
6    5.16957100 3.66521900 -0.30587600
6    5.86158900 2.42689000 -0.19373800
6    7.26501600 2.45811800 -0.03619100
6    5.85813300 -0.04961400 -0.09443800
6    5.15546100 1.16357500 -0.23257400
6    3.74072100 1.10699500 -0.40716700
6    3.06829800 -0.07581000 -0.42749400
6    3.74098900 -1.32396200 -0.27111900
6    5.14157500 -1.30942400 -0.10942700
6    3.70534600 -3.79706500 -0.10889900
6    3.01760800 -2.57696800 -0.27094200
6    1.60034600 -2.61849200 -0.42734100
6    0.91220200 -3.79220600 -0.40662100
6    1.57060500 -5.04562500 -0.23161600
6    2.97263200 -5.04753500 -0.09340300
6    1.50416200 -7.51970500 -0.03442300
6    0.82959200 -6.28873600 -0.19246600
6    -0.58880000 -6.30836800 -0.30483800
6    -1.29197500 -7.47353200 -0.24442400
6    -0.64633600 -8.72980500 -0.07882300
6    0.75694400 -8.75800800 0.00802700
6    -5.16921400 -3.66414700 0.31158900
6    -5.86123200 -2.42581900 0.19945300
6    -7.26465900 -2.45704600 0.04190800
6    -7.96359700 -3.72326500 -0.00039800
6    -7.23767800 -4.92450900 0.08599200
6    -5.82688500 -4.85560700 0.25128500
6    -3.06794100 0.07688100 0.43320900
6    -3.74063200 1.32503300 0.27683500
6    -5.14121800 1.31049500 0.11514400
6    -5.85777600 0.05068500 0.10015600
6    -5.15510400 -1.16250400 0.23829000
6    -3.74036400 -1.10592400 0.41288200
6    -0.91184500 3.79327700 0.41233300
6    -1.57024800 5.04669600 0.23732800
6    -2.97227500 5.04860600 0.09911700
6    -3.70498900 3.79813700 0.11461500
6    -3.01725100 2.57803900 0.27665600
6    -1.59998900 2.61956300 0.43305300
6    1.29233300 7.47460300 0.25013300
6    0.64669300 8.73087600 0.08453300
6    -0.75658700 8.75907900 -0.00231500
6    -1.50380400 7.52077600 0.04013600
6    -0.82923400 6.28980700 0.19817700
6    0.58915800 6.30943900 0.31054600
6    -0.70506600 11.20186600 -0.16317700
6    -1.40669200 10.03973100 -0.12706800
6    4.98774000 13.61393900 -0.09108500
6    3.63569200 13.62575300 -0.13479700
6    9.98284300 9.96151700 0.14079800
6    9.29652700 11.12649300 0.09751200
6    1.40704900 -10.03866000 0.13278300
6    0.70542300 -11.20079500 0.16889300
6    -4.98738300 -13.61286800 0.09680000
6    -3.63533500 -13.62468200 0.14051300
6    -9.98248600 -9.96044500 -0.13508300
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6    -9.29617000 -11.12542100 -0.09179700
6    10.05386200 4.99020200 0.16672000
6    9.39812700 3.80155800 0.13037100
6    7.94458200 1.20641100 0.08543600
6    7.27697100 0.01806000 0.06217800
6    5.80617900 -2.56418200 0.04266900
6    5.12430700 -3.74517600 0.04295900
6    3.62335700 -6.31012000 0.06380400
6    2.92791000 -7.48239500 0.08743800
6    -9.39777000 -3.80048600 -0.12465500
6    -10.05350500 -4.98913100 -0.16100500
6    -7.27661400 -0.01698800 -0.05645800
6    -7.94422500 -1.20534000 -0.07971700
6    -5.12395100 3.74624700 -0.03724200
6    -5.80582200 2.56525400 -0.03695100
6    -2.92755300 7.48346600 -0.08172300
6    -3.62300000 6.31119100 -0.05809000
1    0.94240300 13.35341700 -0.21703300
1    3.33487300 9.03464700 0.10840500
1    7.67644300 13.29587700 0.00354200
1    5.20525000 9.01462800 0.00237900
1    11.09359200 7.49271700 0.22171200
1    6.15725700 7.40554700 -0.10346700
1    -3.33451600 -9.03357600 -0.10269900
1    -0.94204600 -13.35234500 0.22275000
1    -5.20489300 -9.01355700 0.00333200
1    -7.67608600 -13.29480600 0.00217300
1    -6.15690000 -7.40447500 0.10918200
1    -11.09323500 -7.49164500 -0.21599800
1    5.24160200 5.76903100 -0.34042800
1    4.09026500 3.68244100 -0.44087800
1    3.16683300 2.02251900 -0.53414100
1    1.98981600 -0.04824300 -0.56845800
1    1.03724000 -1.69833000 -0.56874400
1    -0.16763100 -3.75315500 -0.53346400
1    -1.14296300 -5.38203000 -0.44010000
1    -2.37493000 -7.42256100 -0.33936200
1    -4.08990800 -3.68137000 0.44659100
1    -5.24124500 -5.76796000 0.34614100
1    -1.98945900 0.04931400 0.57417200
1    -3.16647600 -2.02144700 0.53985500
1    0.16798800 3.75422600 0.53917500
1    -1.03688300 1.69940200 0.57445600
1    2.37528700 7.42363200 0.34506800
1    1.14332100 5.38310100 0.44580600
1    -1.23073900 12.15525400 -0.24816100
1    -2.49283700 10.08889900 -0.18465300
1    5.54818400 14.55123300 -0.10663600
1    3.09367700 14.57245000 -0.18749900
1    11.07370900 9.96550900 0.19367000
1    9.82802600 12.08049700 0.11355500
1    2.49319400 -10.08782700 0.19036900
1    1.23109600 -12.15418200 0.25387800
1    -5.54782700 -14.55016100 0.11235200
1    -3.09332000 -14.57137900 0.19321700
1    -11.07335200 -9.96443800 -0.18795600
1    -9.82766900 -12.07942500 -0.10784000
1    11.14239300 5.01152300 0.25131300
1    9.98390400 2.88557500 0.18725100
1    9.02591400 1.18443300 0.20965100
1    7.85670900 -0.89746700 0.16702900
1    6.88730700 -2.59580500 0.16700000
1    5.69244100 -4.66546700 0.16751400
1    4.70611100 -6.35431500 0.16887000
1    3.48763800 -8.40776200 0.21210500
1    -9.98354700 -2.88450300 -0.18153500
1    -11.14203600 -5.01045200 -0.24559800
1    -7.85635200 0.89853900 -0.16130800
1    -9.02555800 -1.18336100 -0.20393000
1    -5.69208400 4.66653900 -0.16179600
1    -6.88695100 2.59687600 -0.16128100
1    -3.48728100 8.40883300 -0.20639000
1    -4.70575400 6.35538700 -0.16315400
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23. [30]clarene

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No imaginary frequency (B3LYP/6-31G*)

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6    9.37787500 3.71201300 -0.00212000
6    10.06148700 2.48938500 -0.00248100
6    11.48257000 2.51383400 -0.00303000
6    10.02122800 7.43951500 -0.00265200
6    9.32104800 8.64440800 -0.00260400
6    7.91866600 8.68734600 -0.00208000
6    7.18682500 7.46894400 -0.00148200
6    7.90372100 6.26548800 -0.00157300
6    9.29310300 6.21336100 -0.00217600
6    3.56421800 -11.20129200 -0.00347000
6    2.87488200 -9.95833500 -0.00300000
6    1.47422200 -9.97736700 -0.00291400
6    0.73440400 -11.15455500 -0.00330100
6    1.43232600 -12.39819500 -0.00375400
6    2.82584700 -12.39428700 -0.00381800
6    10.09171000 0.00566400 -0.00256700
6    9.36507900 1.21053200 -0.00234700
6    7.94477200 1.14710800 -0.00209800
6    7.28045200 -0.04165700 -0.00195200
6    7.97581100 -1.28312800 -0.00203100
6    9.38764000 -1.25903300 -0.00238800
6    7.96750700 -3.76311400 -0.00221000
6    7.26286100 -2.54277500 -0.00184800
6    5.83788700 -2.58561300 -0.00129400
6    5.15791500 -3.76353200 -0.00130800
6    5.83348900 -5.01890800 -0.00188600
6    7.24269700 -5.01880800 -0.00224500
6    5.78433600 -7.50083200 -0.00256900
6    5.09924400 -6.26619900 -0.00211000
6    3.67643200 -6.28453300 -0.00194600
6    2.97899200 -7.45414700 -0.00221700
6    3.63426000 -8.71589300 -0.00267000
6    5.04109800 -8.74288800 -0.00283800
6    -9.37787500 3.71201300 -0.00233100
6    -10.02747700 4.94128300 -0.00264500
6    -11.45343900 4.95863400 -0.00330700
6    -12.14664400 3.74975200 -0.00357500
6    -11.48257000 2.51383400 -0.00329800
6    -10.06148700 2.48938500 -0.00271200
6    -7.18682500 7.46894400 -0.00165000
6    -7.91866600 8.68734600 -0.00226300
6    -9.32104800 8.64440800 -0.00282200
6    -10.02122800 7.43951500 -0.00288700
6    -9.29310300 6.21336100 -0.00239300
6    -7.90372100 6.26548800 -0.00175900
6    -0.73440400 -11.15455500 -0.00331000
6    -1.47422200 -9.97736700 -0.00292500
6    -2.87488200 -9.95833500 -0.00303300
6    -3.56421800 -11.20129200 -0.00352400
6    -2.82584800 -12.39428700 -0.00386500
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6    -1.43232600 -12.39819500 -0.00377800
6    -7.28045200 -0.04165700 -0.00210700
6    -7.94477200 1.14710800 -0.00228700
6    -9.36507900 1.21053200 -0.00255700
6    -10.09171000 0.00566400 -0.00278300
6    -9.38764100 -1.25903300 -0.00257300
6    -7.97581100 -1.28312800 -0.00217500
6    -5.15791500 -3.76353200 -0.00129700
6    -5.83788700 -2.58561300 -0.00130900
6    -7.26286100 -2.54277500 -0.00194700
6    -7.96750700 -3.76311400 -0.00234000
6    -7.24269700 -5.01880800 -0.00235400
6    -5.83348900 -5.01890800 -0.00193400
6    -2.97899200 -7.45414700 -0.00222300
6    -3.67643200 -6.28453300 -0.00195200
6    -5.09924400 -6.26619900 -0.00215300
6    -5.78433600 -7.50083200 -0.00265000
6    -5.04109800 -8.74288800 -0.00290800
6    -3.63426000 -8.71589300 -0.00270600
6    5.73110400 7.50536800 -0.00089600
6    5.05102800 8.73724600 -0.00119300
6    3.60370500 8.75994900 -0.00085400
6    2.87689100 7.54934000 -0.00003800
6    3.60425200 6.32641200 0.00041700
6    4.96589500 6.30714300 -0.00002600
6    1.42955300 7.56152400 0.00023100
6    0.72491700 8.78189900 -0.00050900
6    -0.72491700 8.78189900 -0.00052600
6    -1.42955300 7.56152400 0.00019700
6    -0.68005800 6.34882300 0.00119700
6    0.68005800 6.34882300 0.00121300
6    -2.87689100 7.54934000 -0.00010500
6    -3.60370500 8.75994900 -0.00093700
6    -5.05102800 8.73724600 -0.00131000
6    -5.73110400 7.50536800 -0.00103000
6    -4.96589500 6.30714300 -0.00014300
6    -3.60425200 6.32641200 0.00033200
6    12.19046600 1.26513200 -0.00330300
6    11.53086500 0.07790700 -0.00305100
6    12.14506800 6.23167400 -0.00339900
6    11.46950700 7.40184000 -0.00323100
6    -0.67559400 -13.63360800 -0.00417400
6    0.67559400 -13.63360800 -0.00416200
6    10.06858500 -2.51652200 -0.00260000
6    9.39562700 -3.70280400 -0.00255100
6    7.90463400 -6.28573100 -0.00267200
6    7.21381100 -7.46170800 -0.00280100
6    5.69805100 -10.02538500 -0.00330900
6    4.99955900 -11.19013800 -0.00359900
6    -11.46950700 7.40184000 -0.00350300
6    -12.14506800 6.23167400 -0.00369100
6    -5.83334000 9.94736500 -0.00196400
6    -7.19130600 9.92479800 -0.00235700
6    -5.69805100 -10.02538500 -0.00339900
6    -4.99955900 -11.19013800 -0.00368100
6    -12.19046600 1.26513200 -0.00358300
6    -11.53086500 0.07790700 -0.00330400
6    -10.06858500 -2.51652200 -0.00279900
6    -9.39562700 -3.70280300 -0.00273000
6    -7.90463400 -6.28573100 -0.00282500
6    -7.21381100 -7.46170800 -0.00293800
6    7.19130600 9.92479800 -0.00219200
6    5.83334000 9.94736500 -0.00183000
6    2.85499800 9.97831800 -0.00140900
6    1.49115400 9.98854300 -0.00128500
6    -1.49115400 9.98854300 -0.00131800
6    -2.85499800 9.97831800 -0.00147400
1    13.23970300 3.76274300 -0.00372000
1    8.29278700 3.69927100 -0.00156700
1    9.87892000 9.58446000 -0.00302600
1    7.35005000 5.33216700 -0.00123900
1    0.94283700 -9.03112400 -0.00254800
1    3.36105200 -13.34743300 -0.00416600
1    7.35574400 2.06201100 -0.00211400
1    6.19313500 -0.01944100 -0.00186200
1    5.26093600 -1.66365000 -0.00079000
1    4.07099600 -3.72508200 -0.00082700
1    3.11402500 -5.35364300 -0.00164900
1    1.89214900 -7.40153300 -0.00210100
1    -8.29278700 3.69927100 -0.00173900
1    -13.23970300 3.76274300 -0.00403700
1    -9.87892000 9.58446000 -0.00325600
1    -7.35005000 5.33216700 -0.00141700
1    -0.94283800 -9.03112400 -0.00254400
1    -3.36105200 -13.34743300 -0.00422600
1    -6.19313500 -0.01944100 -0.00201000
1    -7.35574400 2.06201100 -0.00231800
1    -4.07099700 -3.72508300 -0.00074100
1    -5.26093600 -1.66365000 -0.00074900
1    -1.89214900 -7.40153300 -0.00208100
1    -3.11402500 -5.35364300 -0.00163200
1    3.07951300 5.37383700 0.00106900
1    5.46330400 5.33939700 0.00035100
1    -1.19034600 5.38833400 0.00201700
1    1.19034600 5.38833400 0.00204500
1    -5.46330400 5.33939700 0.00022200
1    -3.07951300 5.37383700 0.00099600
1    13.28233700 1.28392500 -0.00372600
1    12.11649100 -0.84000100 -0.00327700
1    13.23719500 6.22403800 -0.00384500
1    12.00905200 8.35141000 -0.00354200
1    -1.22824300 -14.57560800 -0.00449500
1    1.22824300 -14.57560800 -0.00447200
1    11.15698400 -2.54523800 -0.00281700
1    9.97831700 -4.62270200 -0.00276000
1    8.99266100 -6.33022000 -0.00290600
1    7.78303500 -8.38981700 -0.00311600
1    6.78582100 -10.07351000 -0.00344600
1    5.52915400 -12.14515900 -0.00395800
1    -12.00905200 8.35141000 -0.00382700
1    -13.23719500 6.22403900 -0.00416800
1    -5.33132300 10.91355600 -0.00209900
1    -7.75361400 10.86092700 -0.00279800
1    -6.78582100 -10.07351000 -0.00355600
1    -5.52915400 -12.14515900 -0.00405300
1    -13.28233700 1.28392500 -0.00403500
1    -12.11649100 -0.84000100 -0.00353800
1    -11.15698400 -2.54523800 -0.00304700
1    -9.97831700 -4.62270200 -0.00295600
1    -8.99266100 -6.33022000 -0.00311100
1    -7.78303500 -8.38981700 -0.00329000
1    7.75361400 10.86092700 -0.00262100
1    5.33132300 10.91355600 -0.00197800
1    3.37385800 10.93546800 -0.00202200
1    0.98568600 10.95304900 -0.00180500
1    -0.98568600 10.95304900 -0.00182700
1    -3.37385800 10.93546800 -0.00209800
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24. [32]clarene <2,2,12,2,2,12>

E(wB97XD/cc-pVDZ) = -4915.26574906
No imaginary frequency (B3LYP/6-31G*)

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6    4.63128200 13.02243200 -0.03227600
6    3.94202700 14.26716300 -0.11570000
6    2.54803900 14.26595500 -0.16181400
6    1.80626300 13.07637600 -0.11360600
6    2.48901300 11.83452000 0.00607100
6    3.88715200 11.84945600 0.03654600
6    8.92548500 13.02158200 0.04560200
6    8.20516900 14.22048900 0.00583300
6    6.80674600 14.24414400 -0.03482600
6    6.09603200 13.01352300 -0.01832100
6    6.82333200 11.82576900 0.00406100
6    8.21561600 11.79054800 0.02734600
6    11.07517000 9.34512200 0.16931400
6    10.37879800 10.55275200 0.12439400
6    8.95626800 10.52681000 0.04040100
6    8.31300300 9.29570200 -0.02984300
6    8.99953500 8.07761700 -0.00046200
6    10.41631900 8.10772100 0.11953600
6    -1.80876300 -13.07668900 0.11173400
6    -2.49151300 -11.83483300 -0.00794300
6    -3.88965100 -11.84976900 -0.03841800
6    -4.63378200 -13.02274400 0.03040300
6    -3.94452600 -14.26747500 0.11382800
6    -2.55053900 -14.26626800 0.15994200
6    -6.09853200 -13.01383600 0.01644800
6    -6.82583200 -11.82608100 -0.00593500
6    -8.21811600 -11.79086000 -0.02922000
6    -8.92798500 -13.02189400 -0.04747400
6    -8.20766800 -14.22080100 -0.00770500
6    -6.80924600 -14.24445600 0.03295500
6    -8.31550300 -9.29601400 0.02796800
6    -9.00203600 -8.07792900 -0.00141300
6    -10.41882000 -8.10803300 -0.12141000
6    -11.07767000 -9.34543400 -0.17118800
6    -10.38129800 -10.55306500 -0.12626800
6    -8.95876800 -10.52712200 -0.04227500
6    9.03304900 5.59638500 0.01467200
6    8.30873000 6.79785800 -0.07902400
6    6.89930600 6.72932300 -0.25690400
6    6.24146400 5.53796600 -0.32290300
6    6.93171000 4.29935400 -0.20314800
6    8.33364600 4.33084700 -0.03156800
6    6.92899300 1.82356400 -0.10088500
6    6.22641300 3.03544900 -0.24896700
6    4.81388900 2.97530700 -0.44166700
6    4.14429900 1.79056500 -0.47306500
6    4.81742100 0.54352000 -0.30859600
6    6.21533000 0.56276700 -0.12416500
6    4.79060500 -1.92884900 -0.14740400
6    4.09944300 -0.71303300 -0.32360300
6    2.68567600 -0.76483800 -0.51168200
6    2.00530300 -1.94388400 -0.51204800
6    2.66787200 -3.19393300 -0.32442100
6    4.06637700 -3.18399400 -0.14779900
6    2.62205300 -5.66430900 -0.12601700
6    1.93928200 -4.44435700 -0.31027900
6    0.52285800 -4.48547900 -0.47546400
6    -0.16788300 -5.65802500 -0.44477700
6    0.48680100 -6.91113400 -0.25220700
6    1.88758900 -6.91310500 -0.10345100
6    0.41945900 -9.38379500 -0.03574000
6    -0.25460400 -8.15417100 -0.20722100
6    -1.67229600 -8.17602700 -0.32775000
6    -2.37480700 -9.34164400 -0.26272700
6    -1.72904900 -10.59638400 -0.08518700
6    -0.32640100 -10.62252200 0.00949000
6    -6.24396500 -5.53827800 0.32102500
6    -6.93421100 -4.29966700 0.20127100
6    -8.33614700 -4.33115900 0.02969100
6    -9.03555000 -5.59669700 -0.01654800
6    -8.31123100 -6.79817100 0.07714800
6    -6.90180600 -6.72963600 0.25502700
6    -4.14679900 -1.79087800 0.47118500
6    -4.81992100 -0.54383200 0.30671700
6    -6.21783000 -0.56307900 0.12228800
6    -6.93149300 -1.82387600 0.09900700
6    -6.22891400 -3.03576200 0.24708800
6    -4.81638900 -2.97562000 0.43978600
6    -2.00780300 1.94357100 0.51017000
6    -2.67037200 3.19362000 0.32254400
6    -4.06887700 3.18368100 0.14592100
6    -4.79310500 1.92853700 0.14552600
6    -4.10194300 0.71272000 0.32172400
6    -2.68817500 0.76452500 0.50980300
6    0.16538300 5.65771200 0.44290400
6    -0.48930000 6.91082100 0.25033300
6    -1.89008800 6.91279300 0.10157500
6    -2.62455300 5.66399600 0.12414100
6    -1.94178200 4.44404400 0.30840300
6    -0.52535800 4.48516600 0.47359000
6    2.37230700 9.34133100 0.26085400
6    1.72655000 10.59607100 0.08331500
6    0.32390200 10.62220900 -0.01136300
6    -0.42195800 9.38348200 0.03386700
6    0.25210500 8.15385800 0.20534800
6    1.66979700 8.17571400 0.32587700
6    0.37234200 13.06431400 -0.18365000
6    -0.32752200 11.90127600 -0.14585800
6    6.06193100 15.48403400 -0.09820000
6    4.70994700 15.49431900 -0.14685200
6    11.05704800 11.83163800 0.15729300
6    10.37163900 12.99708200 0.10963700
6    0.32502200 -11.90158900 0.14398600
6    -0.37484200 -13.06462700 0.18177800
6    -6.06443100 -15.48434600 0.09632900
6    -4.71244600 -15.49463100 0.14498000
6    -11.05954800 -11.83195100 -0.15916500
6    -10.37413900 -12.99739500 -0.11150900
6    11.12328400 6.86004400 0.18833800
6    10.46642700 5.67221200 0.14929200
6    9.01264700 3.08008200 0.10002200
6    8.34581400 1.89180700 0.07221200
6    6.88272900 -0.68830300 0.04163400
6    6.20582100 -1.87146600 0.03211500
6    4.72483300 -4.43808300 0.03136700
6    4.03911700 -5.61617000 0.04027500
6    2.53730600 -8.17405200 0.06959600
6    1.84204100 -9.34594000 0.09667400
6    -10.46892800 -5.67252500 -0.15116700
6    -11.12578500 -6.86035700 -0.19021200
6    -8.34831400 -1.89212000 -0.07408800
6    -9.01514700 -3.08039400 -0.10189800
6    -6.20832200 1.87115400 -0.03399200
6    -6.88522900 0.68799000 -0.04351100
6    -4.04161700 5.61585700 -0.04215300
6    -4.72733200 4.43777000 -0.03324500
6    -1.84454000 9.34562700 -0.09854900
6    -2.53980600 8.17373900 -0.07147300
1    2.01641500 15.21798200 -0.23885500
1    4.41361900 10.90394200 0.11416100
1    8.75153300 15.16736200 0.00648100
1    6.28117500 10.88575100 0.00326500
1    12.16543600 9.36104500 0.24669500
1    7.23098100 9.27852000 -0.10775000
1    -4.41611800 -10.90425500 -0.11603300
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1    -2.01891500 -15.21829500 0.23698300
1    -6.28367500 -10.88606300 -0.00514100
1    -8.75403200 -15.16767400 -0.00835200
1    -7.23348200 -9.27883100 0.10587400
1    -12.16793600 -9.36135800 -0.24856800
1    6.31508900 7.64196900 -0.35810900
1    5.16342100 5.55526100 -0.46840300
1    4.23966300 3.88980700 -0.57529200
1    3.06759300 1.81531600 -0.62866000
1    2.11963600 0.15209000 -0.66335700
1    0.92820100 -1.91273700 -0.66384200
1    -0.03732200 -3.56563600 -0.63110000
1    -1.24696600 -5.61861200 -0.57874100
1    -2.22632000 -7.25100500 -0.47302400
1    -3.45728700 -9.29243600 -0.36434400
1    -5.16592100 -5.55557300 0.46652400
1    -6.31758900 -7.64228100 0.35623100
1    -3.07009300 -1.81562900 0.62677800
1    -4.24216300 -3.89012000 0.57341000
1    -0.93070100 1.91242400 0.66196400
1    -2.12213600 -0.15240300 0.66147700
1    1.24446600 5.61829900 0.57686900
1    0.03482200 3.56532300 0.62922700
1    3.45478700 9.29212300 0.36247100
1    2.22382100 7.25069200 0.47115100
1    -0.15435700 14.01650300 -0.27537300
1    -1.41341200 11.94859600 -0.20878100
1    6.62137700 16.42191600 -0.11427000
1    4.16727200 16.44036900 -0.20419600
1    12.14766200 11.83512200 0.21519600
1    10.90375400 13.95071900 0.12706000
1    1.41091200 -11.94890900 0.20690800
1    0.15185700 -14.01681600 0.27350100
1    -6.62387700 -16.42222800 0.11240000
1    -4.16977200 -16.44068100 0.20232400
1    -12.15016200 -11.83543500 -0.21706800
1    -10.90625400 -13.95103100 -0.12893000
1    12.21125100 6.88029800 0.28008400
1    11.05089900 4.75577600 0.21116900
1    10.09249300 3.05883000 0.23615800
1    8.92483300 0.97691100 0.18509200
1    7.96144100 -0.71539900 0.18534500
1    6.77552600 -2.78896000 0.16811500
1    5.80427900 -4.47207000 0.16757500
1    4.60244500 -6.53650500 0.18382900
1    3.61913700 -8.21748300 0.18303200
1    2.40073400 -10.27024600 0.23282200
1    -11.05340000 -4.75608800 -0.21304400
1    -12.21375200 -6.88061100 -0.28195800
1    -8.92733400 -0.97722300 -0.18696800
1    -10.09499300 -3.05914200 -0.23803300
1    -6.77802600 2.78864800 -0.16999100
1    -7.96394100 0.71508600 -0.18722100
1    -4.60494400 6.53619200 -0.18570900
1    -5.80677800 4.47175700 -0.16945500
1    -2.40323300 10.26993300 -0.23469800
1    -3.62163600 8.21717100 -0.18491000
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25. [34]clarene <2,4,10,4,2,12>

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E(wB97XD/cc-pVDZ) = -5222.46372973
No imaginary frequency (B3LYP/6-31G*)

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6    1.25135800 15.03684800 0.00503700
6    0.49702800 13.85424100 0.00542800
6    1.16922400 12.60177800 0.00575000
6    2.57005300 12.60167300 0.00548800
6    7.62403500 13.76113900 0.00397400
6    6.90135900 14.96277800 0.00405000
6    5.50769400 14.98426600 0.00434200
6    4.79453600 13.74978300 0.00463700
6    5.52022800 12.56295900 0.00452000
6    6.92007100 12.52681900 0.00417200
6    11.95558800 6.35098400 0.00295800
6    11.25957900 7.56257800 0.00316800
6    9.83479100 7.54947900 0.00345100
6    9.18302800 6.31458600 0.00353700
6    9.86707900 5.09629000 0.00336400
6    11.29168400 5.12048000 0.00303300
6    1.20654500 -12.33267300 0.00039800
6    0.51617000 -11.08626300 0.00088400
6    -0.88096700 -11.10166300 0.00086000
6    -1.62549900 -12.28296100 0.00042500
6    -0.92543200 -13.52396700 -0.00000700
6    0.47184800 -13.52223400 -0.00002000
6    -7.39349700 -12.24236200 0.00031800
6    -8.12405100 -11.04770400 0.00072600
6    -9.51469900 -11.01184900 0.00068100
6    -10.22825000 -12.24601900 0.00014400
6    -9.51356900 -13.44267800 -0.00023500
6    -8.11159400 -13.46858700 -0.00014700
6    -9.63041100 -8.51138000 0.00182400
6    -10.32966600 -7.29756900 0.00218700
6    -11.75046200 -7.34035200 0.00180700
6    -12.39871600 -8.58432200 0.00118000
6    -11.69026200 -9.78422900 0.00085400
6    -10.26448500 -9.74897200 0.00113100
6    9.80484600 10.03923200 0.00353500
6    9.07600100 11.28463500 0.00370800
6    7.66564700 11.27415700 0.00399100
6    6.99929100 10.02313500 0.00406100
6    7.68947600 8.84546300 0.00388700
6    9.10652000 8.81521000 0.00363100
6    9.90247700 2.61069500 0.00307800
6    9.17294100 3.81297000 0.00347000
6    7.75339300 3.74433700 0.00398400
6    7.09250500 2.55261800 0.00404300
6    7.79153500 1.31381400 0.00354200
6    9.20367700 1.34426200 0.00304700
6    7.79634800 -1.16586100 0.00289200
6    7.08479100 0.05006500 0.00350200
6    5.65973000 -0.00220100 0.00405900
6    4.98685300 -1.18452900 0.00396400
6    5.67004600 -2.43632200 0.00328300
6    7.07991400 -2.42625900 0.00276100
6    5.64195400 -4.91535100 0.00238100
6    4.94641600 -3.68898100 0.00309200
6    3.52074000 -3.72226200 0.00358500
6    2.83249600 -4.89568400 0.00331500
6    3.49903800 -6.15633300 0.00254200
6    4.90790900 -6.16558900 0.00212400
6    3.43585800 -8.63830700 0.00152000
6    2.75710900 -7.39968000 0.00218000
6    1.33474800 -7.41237500 0.00243400
6    0.63212700 -8.57994800 0.00201400
6    1.28151400 -9.84414900 0.00135500
6    2.68751600 -9.87605900 0.00117500
6    -3.08577400 -12.28403400 0.00039400
6    -3.81942100 -11.07135300 0.00076600
6    -5.18441100 -11.06116100 0.00074100
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6    -5.93582300 -12.26302300 0.00034400
6    -5.24079000 -13.49032700 -0.00004900
6    -3.79778700 -13.50020900 -0.00002600
6    -7.58333800 -4.72808000 0.00416400
6    -8.29584700 -3.49632900 0.00432400
6    -9.70723300 -3.54035600 0.00372100
6    -10.39356700 -4.81457800 0.00309800
6    -9.65048000 -6.00936300 0.00291100
6    -8.23110500 -5.92607700 0.00345000
6    -5.51383200 -0.97487100 0.00642400
6    -6.20782500 0.27101300 0.00618900
6    -7.61757200 0.24959700 0.00541600
6    -8.32349300 -1.01702600 0.00488900
6    -7.60113100 -2.22660300 0.00501600
6    -6.17652900 -2.16251700 0.00583700
6    -3.38818800 2.74905700 0.00780600
6    -4.06342800 4.00550100 0.00724600
6    -5.47309600 4.00581200 0.00650400
6    -6.19860700 2.74983500 0.00622900
6    -5.49414300 1.52885100 0.00665600
6    -4.06839000 1.57160800 0.00751400
6    -1.20627900 6.43994100 0.00797400
6    -1.86222500 7.70619600 0.00724600
6    -3.27101200 7.72815800 0.00670500
6    -4.01588300 6.48402800 0.00674000
6    -3.33033100 5.25206500 0.00736400
6    -1.90437600 5.27279300 0.00804100
6    1.02864200 10.09884700 0.00694000
6    0.39208500 11.37023700 0.00626500
6    -1.01413900 11.41771200 0.00612900
6    -1.77552700 10.18690700 0.00639300
6    -1.10899300 8.94205400 0.00701800
6    0.31402300 8.93951700 0.00734500
6    -0.93824600 13.86380200 0.00548300
6    -1.65309000 12.70923500 0.00575100
6    4.76788600 16.22959000 0.00430300
6    3.41688000 16.24738600 0.00450300
6    11.93598200 8.83140700 0.00307300
6    11.24858900 10.00003600 0.00324500
6    3.34293500 -11.16125400 0.00066700
6    2.64342200 -12.32348900 0.00033000
6    -7.37083000 -14.69895400 -0.00053900
6    -6.01375300 -14.70849100 -0.00048600
6    -12.36658500 -11.06513500 0.00025700
6    -11.67661500 -12.22679800 -0.00004400
6    9.74571100 12.56249600 0.00356800
6    9.05994700 13.73360000 0.00367800
6    12.00108000 3.87088700 0.00274900
6    11.34327000 2.68453500 0.00273700
6    9.89108500 0.09022100 0.00248000
6    9.22410500 -1.09887000 0.00239100
6    7.75196500 -3.68667900 0.00207900
6    7.06954600 -4.86792100 0.00190000
6    5.56283200 -7.43609200 0.00142800
6    4.86559600 -8.60770700 0.00116600
6    -3.04284500 -14.73151500 -0.00044600
6    -1.68707500 -14.74347700 -0.00044100
6    -11.83161600 -4.90570100 0.00267400
6    -12.47518400 -6.10147500 0.00209100
6    -9.75039200 -1.09740300 0.00421300
6    -10.40630400 -2.29307300 0.00370300
6    -7.62564300 2.69140300 0.00547700
6    -8.29916800 1.50471600 0.00511700
6    -5.44367000 6.44752700 0.00609300
6    -6.13529500 5.27128400 0.00597900
6    -3.20524200 10.16989100 0.00595600
6    -3.91377900 9.00464400 0.00607300
1    0.72916200 15.99718000 0.00484700
1    3.08865000 11.64827700 0.00561500
1    7.44848900 15.90911800 0.00384500
1    4.97722500 11.62323000 0.00467400
1    13.04856400 6.36540600 0.00270000
1    8.09825300 6.29998500 0.00369200
1    -1.40977800 -10.15429900 0.00115300
1    1.00501800 -14.47644500 -0.00038800
1    -7.58194800 -10.10745300 0.00105400
1    -10.06016500 -14.38932600 -0.00063900
1    -8.54544700 -8.48506500 0.00208800
1    -13.49151100 -8.61121200 0.00093100
1    5.91201200 9.97952000 0.00422400
1    7.11980400 7.91833000 0.00393500
1    7.16117900 4.65730900 0.00438100
1    6.00498300 2.57111400 0.00446300
1    5.07753500 0.91662600 0.00458100
1    3.89957400 -1.15326900 0.00441400
1    2.95069900 -2.79585800 0.00418600
1    1.74569800 -4.85033500 0.00372600
1    0.77619500 -6.47901200 0.00293900
1    -0.45459500 -8.52281900 0.00222800
1    -3.30025200 -10.11503700 0.00106400
1    -5.68931300 -10.09721900 0.00101800
1    -6.49575100 -4.73475800 0.00455100
1    -7.62945500 -6.83277400 0.00331500
1    -4.42642300 -0.99725900 0.00704100
1    -5.58657500 -3.07629100 0.00604000
1    -2.30121900 2.71074700 0.00846300
1    -3.49212000 0.64916900 0.00796100
1    -0.11999500 6.38516500 0.00850100
1    -1.34238400 4.34154900 0.00860900
1    2.11466900 10.03055500 0.00721200
1    0.86246700 8.00028300 0.00788600
1    -1.45399900 14.82636300 0.00526500
1    -2.74001100 12.77281100 0.00575300
1    5.33315600 17.16406200 0.00406200
1    2.87633500 17.19637300 0.00441700
1    13.02798100 8.83905800 0.00284400
1    11.81232800 10.93124500 0.00314600
1    4.43051100 -11.21103800 0.00059300
1    3.17065200 -13.27978700 -0.00001500
1    -7.92390400 -15.64058300 -0.00089200
1    -5.50429100 -15.67045200 -0.00079900
1    -13.45871300 -11.07065900 0.00006700
1    -12.20409400 -13.18311900 -0.00047400
1    10.83360100 12.60093000 0.00334500
1    9.59974800 14.68290300 0.00353700
1    13.09289000 3.89152200 0.00252000
1    11.92959800 1.76722000 0.00250300
1    10.97947700 0.06648000 0.00205000
1    9.81123500 -2.01583400 0.00191300
1    8.84021300 -3.72277600 0.00165900
1    7.64462100 -5.79248400 0.00134800
1    6.65049700 -7.48682400 0.00108600
1    5.42956500 -9.53888300 0.00061700
1    -3.56781300 -15.68510500 -0.00079600
1    -1.14842400 -15.69341000 -0.00078100
1    -12.42934200 -3.99567000 0.00287100
1    -13.56668700 -6.13513000 0.00181600
1    -10.34601000 -0.18586300 0.00411200
1    -11.49494500 -2.27983400 0.00320500
1    -8.20777900 3.61158800 0.00516800
1    -9.38771400 1.53234000 0.00453300
1    -6.01153200 7.37660400 0.00563900
1    -7.22327000 5.31581700 0.00543700
1    -3.76021100 11.10653900 0.00543200
1    -5.00095700 9.06565500 0.00565200
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26. [36]clarene <2,2,14,2,2,14>

E(wB97XD/cc-pVDZ) = -5529.67607227
No imaginary frequency (B3LYP/6-31G*)

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6 3.63389900 16.13133900 -0.14957600
6 2.89736700 14.93817500 -0.09953900
6 3.58556300 13.69963300 0.02361000
6 4.98298400 13.72081900 0.05227600
6 10.01479900 14.89837600 0.03687700
6 9.29456900 16.09805600 0.00201800
6 7.89552000 16.12200400 -0.03315400
6 7.18561400 14.89128000 -0.01477100
6 7.91222800 13.70392200 0.00138900
6 9.30380900 13.66831300 0.01792700
6 12.15339000 11.21226100 0.15193600
6 11.46262200 12.42349400 0.10800100
6 10.04041000 12.40302300 0.02473000
6 9.39132600 11.17554100 -0.04959400
6 10.07154800 9.95465200 -0.02141200
6 11.48825100 9.97788100 0.10153400
6 -2.89736800 -14.93817600 0.10397700
6 -3.58556400 -13.69963300 -0.01916400
6 -4.98298400 -13.72081800 -0.04782400
6 -5.72155800 -14.89662200 0.02627700
6 -5.02823800 -16.13859500 0.10956300
6 -3.63390000 -16.13133900 0.15401100
6 -7.18561500 -14.89127900 0.01921100
6 -7.91222900 -13.70392200 0.00304500
6 -9.30381000 -13.66831300 -0.01348900
6 -10.01480000 -14.89837500 -0.03243400
6 -9.29457000 -16.09805500 0.00242700
6 -7.89552100 -16.12200300 0.03759800
6 -9.39132600 -11.17554100 0.05403500
6 -10.07154800 -9.95465200 0.02585000
6 -11.48825100 -9.97788100 -0.09710000
6 -12.15339000 -11.21226000 -0.14750300
6 -11.46262300 -12.42349300 -0.10356500
6 -10.04041100 -12.40302300 -0.02029200
6 10.08899400 7.47425900 0.00104900
6 9.37273300 8.67947500 -0.10105900
6 7.96390800 8.61925200 -0.28764300
6 7.29840000 7.43187400 -0.35109600
6 7.97956900 6.18965200 -0.21830700
6 9.38101800 6.21348900 -0.03965900
6 7.96108400 3.71564500 -0.09490500
6 7.26620500 4.92980800 -0.25806600
6 5.85443900 4.87454200 -0.45984200
6 5.17901600 3.69244500 -0.48751800
6 5.84464300 2.44329200 -0.30837500
6 7.24113200 2.45885500 -0.11175000
6 5.81043000 -0.02702100 -0.12981800
6 5.12296000 1.18820600 -0.32237800
6 3.71129600 1.13440700 -0.52814100
6 3.03113900 -0.04568300 -0.53513700
6 3.69124200 -1.29537400 -0.33472000
6 5.08658600 -1.28155500 -0.13337600
6 3.65293700 -3.76463200 -0.13298100
6 2.96724500 -2.54941200 -0.33454700
6 1.55492200 -2.60262100 -0.53479800
6 0.87293700 -3.78165100 -0.52735500
6 1.53219300 -5.03106300 -0.32141200
6 2.92843100 -5.01878400 -0.12906200
6 1.49086900 -7.50069600 -0.11019400
6 0.80612600 -6.28360800 -0.30705800
6 -0.60848400 -6.33174300 -0.48607900
6 -1.29457200 -7.50766700 -0.45800200
6 -0.63655300 -8.75790600 -0.25601900
6 0.76245200 -8.75258900 -0.09298000
6 -0.69085500 -11.23115200 -0.03712900
6 -1.37089800 -10.00560000 -0.21599200
6 -2.78725500 -10.03672600 -0.34875500
6 -3.48288800 -11.20669300 -0.28524000
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6 -7.96390800 -8.61925200 0.29208800
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6 -5.84464300 -2.44329200 0.31282200
6 -7.24113200 -2.45885500 0.11619000
6 -7.96108300 -3.71564500 0.09934300
6 -7.26620500 -4.92980900 0.26251100
6 -5.85444000 -4.87454200 0.46429400
6 -3.03114000 0.04568300 0.53959000
6 -3.69124100 1.29537400 0.33917000
6 -5.08658400 1.28155400 0.13782100
6 -5.81042900 0.02702100 0.13426100
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6 -3.71129600 -1.13440700 0.53259300
6 -0.87293600 3.78165000 0.53180800
6 -1.53219200 5.03106300 0.32586600
6 -2.92842900 5.01878400 0.13351600
6 -3.65293600 3.76463100 0.13743100
6 -2.96724400 2.54941100 0.33899800
6 -1.55492100 2.60262000 0.53925100
6 1.29457300 7.50766700 0.46245400
6 0.63655300 8.75790600 0.26047200
6 -0.76245100 8.75258900 0.09743400
6 -1.49086900 7.50069600 0.11465000
6 -0.80612500 6.28360700 0.31151200
6 0.60848600 6.33174300 0.49053100
6 3.48288700 11.20669400 0.28969200
6 2.83063900 12.45689700 0.10309000
6 1.42873900 12.47463200 0.00073900
6 0.69085500 11.23115200 0.04157900
6 1.37089800 10.00560000 0.22044400
6 2.78725500 10.03672700 0.35320800
6 1.46358700 14.91755200 -0.17251300
6 0.77062000 13.75016400 -0.13697700
6 7.14689800 17.36003200 -0.09337700
6 5.79435700 17.36715900 -0.13854700
6 12.14364900 13.70120300 0.14193600
6 11.46125700 14.86900200 0.09718100
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6 -7.14689900 -17.36003200 0.09782000
6 -5.79435700 -17.36715900 0.14298300
6 -12.14365000 -13.70120300 -0.13749900
6 -11.46125800 -14.86900100 -0.09273900
6 12.18726900 8.72583100 0.17405700
6 11.52271100 7.54204000 0.13845000
6 10.05167100 4.96006500 0.10606500
6 9.37735100 3.77620800 0.08550900
6 7.90351600 1.20805800 0.07222100
6 7.22344800 0.02743700 0.06595100
6 5.74638400 -2.53136300 0.06545200
6 5.06521200 -3.71110000 0.06567300
6 3.58778900 -6.26970700 0.06687400

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6    2.90529000 -7.44892400 0.07358800
6    1.41812200 -10.00938600 0.08766700
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6    -11.52271000 -7.54204000 -0.13401800
6    -12.18726900 -8.72583100 -0.16962600
6    -9.37735000 -3.77620900 -0.08107700
6    -10.05167000 -4.96006600 -0.10163500
6    -7.22344700 -0.02743700 -0.06151300
6    -7.90351400 -1.20805800 -0.06778500
6    -5.06521000 3.71110000 -0.06122800
6    -5.74638200 2.53136300 -0.06100900
6    -2.90529000 7.44892400 -0.06912900
6    -3.58778900 6.26970600 -0.06241500
6    -0.72995100 11.18524500 -0.10411400
6    -1.41812200 10.00938500 -0.08321400
1    3.09785800 17.08079200 -0.22791300
1    5.51320000 12.77769700 0.13116100
1    9.84121600 17.04478500 0.00220500
1    7.36979600 12.76440900 0.00099500
1    13.24367100 11.22263700 0.23021200
1    8.30945800 11.16333800 -0.12820600
1    -5.51320000 -12.77769500 -0.12669500
1    -3.09785900 -17.08079200 0.23234400
1    -7.36979800 -12.76440800 0.00342700
1    -9.84121700 -17.04478400 0.00224000
1    -8.30945900 -11.16333900 0.13265300
1    -13.24367100 -11.22263600 -0.22578200
1    7.38666500 9.53515300 -0.39923500
1    6.22147300 7.45500000 -0.50455100
1    5.28568700 5.79085800 -0.60491400
1    4.10348600 3.72064000 -0.65182700
1    3.14707800 2.05084400 -0.69071600
1    1.95602100 -0.01615100 -0.70248500
1    0.99161800 -1.68646800 -0.70244000
1    -0.20288300 -3.75143200 -0.68962100
1    -1.17080800 -5.41454000 -0.65065400
1    -2.37253900 -7.47335800 -0.60280800
1    -3.34572000 -9.11561600 -0.50221200
1    -4.56472000 -11.16462900 -0.39666800
1    -6.22147500 -7.45500100 0.50900200
1    -7.38666600 -9.53515400 0.40368300
1    -4.10348800 -3.72064000 0.65628600
1    -5.28568900 -5.79085700 0.60937200
1    -1.95602200 0.01615100 0.70694200
1    -3.14708000 -2.05084400 0.69517000
1    0.20288400 3.75143100 0.69407500
1    -0.99161800 1.68646700 0.70689300
1    2.37254000 7.47335900 0.60725800
1    1.17081000 5.41454000 0.65510300
1    4.56472000 11.16463000 0.40112000
1    3.34572000 9.11561800 0.50666700
1    0.93118300 15.86640400 -0.26591900
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1    7.70347800 18.29961500 -0.11087000
1    5.25001200 18.31235100 -0.19460800
1    13.23438000 13.70230000 0.19811300
1    11.99674300 15.82076100 0.11510100
1    0.31534600 -13.79121600 0.20764800
1    -0.93118300 -15.86640500 0.27034700
1    -7.70347900 -18.29961400 0.11531400
1    -5.25001300 -18.31235100 0.19904100
1    -13.23438000 -13.70229900 -0.19367800
1    -11.99674400 -15.82076100 -0.11065600
1    13.27523600 8.73912400 0.26714600
1    12.10148100 6.62225400 0.20425700
1    11.13058700 4.93337000 0.24836500
1    9.95008600 2.85891200 0.20941600
1    8.98041300 1.17900600 0.22767600
1    7.78936400 -0.89006000 0.21552800
1    6.82261300 -2.56109000 0.22439500
1    5.62923000 -4.62812200 0.22489200
1    4.66538200 -6.30084000 0.21616300
1    3.46903100 -8.36688500 0.22926200
1    2.49895000 -10.04650300 0.21141900
1    1.29261300 -12.10615900 0.25106100
1    -12.10147900 -6.62225300 -0.19982700
1    -13.27523500 -8.73912400 -0.26271800
1    -9.95008300 -2.85891300 -0.20499100
1    -11.13058400 -4.93337100 -0.24394100
1    -7.78936200 0.89005900 -0.21109400
1    -8.98041100 -1.17900700 -0.22324500
1    -5.62922700 4.62812200 -0.22045000
1    -6.82261100 2.56109000 -0.21995700
1    -3.46903200 8.36688500 -0.22479800
1    -4.66538200 6.30084000 -0.21170000
1    -1.29261400 12.10615800 -0.24661100
1    -2.49895000 10.04650200 -0.20696500
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27. [38]clarene <2,4,12,4,2,14>

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E(wB97XD/cc-pVDZ) = -5836.87344197
No imaginary frequency (B3LYP/6-31G*)

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6    1.53994900 15.73593400 -0.00046400
6    2.20931000 14.48186400 0.00036900
6    3.61035700 14.47885400 0.00032000
6    8.66695300 15.63464000 -0.00131100
6    7.94476300 16.83628900 -0.00169000
6    6.55131800 16.85818300 -0.00144200
6    5.83745500 15.62396600 -0.00071300
6    6.56289300 14.43671400 -0.00032300
6    7.96294900 14.40025800 -0.00062900
6    13.00835200 8.23283000 -0.00092900
6    12.30912000 9.44229500 -0.00078900
6    10.88429000 9.42566800 -0.00033100
6    10.23570500 8.18884300 -0.00009100
6    10.92327700 6.97226700 -0.00031300
6    12.34788800 7.00074100 -0.00070800
6    0.11120800 -14.19518000 -0.00309600
6    -0.57634100 -12.94711100 -0.00260500
6    -1.97372500 -12.95960500 -0.00254300
6    -2.72067700 -14.13963300 -0.00301600
6    -2.02279600 -15.38195300 -0.00356300
6    -0.62574500 -15.38307500 -0.00355600
6    -8.48961600 -14.09580800 -0.00387100
6    -9.22136100 -12.90161600 -0.00337900
6    -10.61226900 -12.86715200 -0.00392800
6    -11.32439400 -14.10229100 -0.00505000
6    -10.60865800 -15.29806700 -0.00544700
6    -9.20690000 -15.32259300 -0.00488200
6    -10.73350100 -10.36602200 -0.00220100
6    -11.43619300 -9.15392900 -0.00199100
6    -12.85694700 -9.20094800 -0.00323600
6    -13.50178000 -10.44641700 -0.00438400
6    -12.79024000 -11.64424000 -0.00450400
6    -11.36443400 -11.60548700 -0.00350500
6    10.85013400 11.91537700 -0.00070800
6    10.11984000 13.15973400 -0.00081500
6    8.70944400 13.14793500 -0.00036300
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6	8.04477400	11.89593800	0.00029800
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6	10.96818700	4.48682800	-0.00039100
6	10.23380700	5.68622100	-0.00020100
6	8.81449400	5.61120700	0.00004200
6	8.15867700	4.41644300	0.00005200
6	8.86294800	3.18054800	-0.00014200
6	10.27493400	3.21756800	-0.00030800
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1    -3.46044000 -4.18517100 -1.00098000
1    -4.66296600 -6.23365000 -0.80283900
1    -1.28742600 -0.40571300 -1.14346500
1    -2.47149300 -2.47441100 -1.12828300
1    0.84602300 3.39069900 -0.86270000
1    -0.31218100 1.31427100 -1.03310500
1    2.91378900 7.18780700 -0.35236400
1    1.78534600 5.10314300 -0.61172900
1    4.93634600 10.95641500 0.22776400
1    3.81451200 8.87253700 -0.06188900
1    1.10473400 15.55291400 0.28144600
1    -0.05318200 13.44076200 0.06602800
1    7.84436200 18.14418000 0.77892600
1    5.39885400 18.12764100 0.66451800
1    13.36186500 13.42251000 0.59304500
1    12.20222700 15.57341500 0.73450100
1    -1.76573400 -17.13130000 -0.02106300
1    -2.79232700 -19.31807100 0.14434700
1    -9.40982400 -22.18775900 0.87316400
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1    -15.05459800 -17.60998600 0.87636800
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1    13.07872800 8.40587800 0.09269600
1    11.71259600 6.41222200 -0.05866600
1    10.49742500 4.90837600 -0.50844700
1    9.05537000 3.04023900 -0.88831000
1    7.83306400 1.63973100 -1.41318500
1    6.40473700 -0.23470500 -1.78995700
1    5.22405300 -1.67882600 -2.19622300
1    3.93249700 -3.67695800 -2.34362500
1    2.98748500 -5.31890000 -2.34516900
1    1.91838400 -7.44380400 -2.18795600
1    1.27091300 -9.19166400 -1.77790100
1    0.37915700 -11.37179300 -1.39229000
1    -0.20894300 -13.13354800 -0.86685500
1    -1.08704000 -15.32245900 -0.47689000
1    -13.77537700 -10.53653000 0.25735100
1    -15.00951500 -12.60310900 0.49107000
1    -11.52443300 -6.85042800 -0.12520100
1    -12.75946800 -8.87573900 0.12850200
1    -9.31644200 -3.18438600 -0.48054000
1    -10.53511800 -5.22115900 -0.26867500
1    -7.16199000 0.49896700 -0.68048700
1    -8.35615100 -1.55804000 -0.58269500
1    -5.05522800 4.21083900 -0.63740800
1    -6.22441900 2.13819900 -0.69921700
1    -2.99949700 7.94931300 -0.39177300
1    -4.13897600 5.86506400 -0.57248500
1    -0.97192700 11.72292000 -0.04484100
1    -2.09392700 9.63044200 -0.27488200
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29. [42]clarene <2,2,16,2,2,18>

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No imaginary frequency (B3LYP/6-31G*)

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6    4.47312600 14.45850000 2.65752400
6    3.64300000 13.61737600 1.89000400
6    4.21528600 12.48730300 1.24738400
6    5.55351100 12.19270100 1.48694200
6    10.17720900 11.47657400 3.52710700
6    9.77305100 12.77555300 3.87846000
6    8.50254600 13.27186500 3.54239800
6    7.64580200 12.45605900 2.76326300
6    8.03415500 11.15838600 2.46423200
6    9.25335200 10.63229200 2.85780100
6    11.23524300 7.47902200 2.40191500
6    10.90968000 8.78046900 2.79225800
6    9.58312300 9.24017100 2.57181700
6    8.62408600 8.35380100 2.09457600
6    8.92599500 7.04039700 1.73434500
6    10.27910700 6.61259300 1.84307600
6    -5.13850100 -19.77014400 1.55451900
6    -6.17150000 -18.79348900 1.48426600
6    -7.45707800 -19.17208200 1.87164400
6    -7.75457200 -20.44630800 2.34179400
6    -6.70401600 -21.38642700 2.52140200
6    -5.41860500 -21.03454600 2.10206500
6    -9.12317800 -20.83470900 2.66544400
6    -10.18475100 -20.01550200 2.31881600
6    -11.49769700 -20.30440300 2.66073600
6    -11.77264200 -21.45928400 3.43364300
6    -10.71465600 -22.33763600 3.72086500
6    -9.39445800 -22.05987900 3.32852000
6    -12.31747000 -18.32163800 1.44729600
6    -13.22577000 -17.28486600 1.26002300
6    -14.46765000 -17.33737500 1.94732700
6    -14.77897700 -18.48302500 2.70647700
6    -13.84827700 -19.51149900 2.89853100
6    -12.56407800 -19.37915600 2.30554600
6    8.27943300 4.87346400 0.72757400
6    7.90521300 6.12773200 1.23590100
6    6.52210600 6.46626600 1.26273800
6    5.56089900 5.59900000 0.82953200
6    5.90038600 4.33495200 0.26999100
6    7.27069400 3.99771100 0.17391500
6    5.26864600 2.22984200 -0.86314500
6    4.88558400 3.40520200 -0.18975100
6    3.49151200 3.61105600 0.05356300
6    2.55758600 2.66792700 -0.27190800
6    2.91485100 1.46299900 -0.95086000
6    4.26462600 1.29767500 -1.32538900
6    2.33428700 -0.67283400 -2.05503800
6    1.95455300 0.41501300 -1.24418000
6    0.64321900 0.39255600 -0.67544300
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6    0.16821100 -1.80149000 -1.64097900
6    1.40470000 -1.74759200 -2.31653400
6    -0.25834800 -4.04688200 -2.59544100
6    -0.65751700 -2.99175600 -1.74938600
6    -1.84377800 -3.17869700 -0.97417500
6    -2.53411200 -4.35771900 -0.98435300
6    -2.11282900 -5.47254000 -1.77357400
6    -0.99230800 -5.29247300 -2.61052300
6    -2.19600100 -7.86803900 -2.38950500
6    -2.74907200 -6.77584200 -1.68974800
6    -3.90322000 -7.02510000 -0.88426600
6    -4.42761100 -8.27972600 -0.74489500
6    -3.81253700 -9.42370200 -1.34186000
6    -2.68308300 -9.20830100 -2.15632300
6    -3.46355000 -11.86949500 -1.48276200
6    -4.25871900 -10.77860000 -1.07387500
6    -5.47652600 -11.06684200 -0.38511600
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6    -4.98992300 -13.46108000 -0.36265400
6    -3.78624200 -13.21034100 -1.04822500
6    -4.34572400 -15.84135400 -0.06085100
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6    -6.56328500 -15.13716200 0.64869900
6    -6.84688600 -16.40641700 1.06367900
6    -5.88001500 -17.45024400 1.00022400
6    -4.61203300 -17.15910900 0.47181600
6    -11.14121100 -14.94797200 -0.78054900
6    -11.79682700 -13.70389800 -0.56437100
6    -13.06720900 -13.70739400 0.05688800
6    -13.60680600 -14.94053300 0.59061000
6    -12.83884100 -16.10974700 0.50408900
6    -11.64286900 -16.10250100 -0.26620600
6    -9.20241800 -11.25703000 -1.74215800
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6    -11.18752900 -9.99643600 -1.10958100
6    -11.84526400 -11.24104000 -0.77031000
6    -11.16604400 -12.46088800 -0.94566000
6    -9.82855200 -12.42894200 -1.44518000
6    -7.19102600 -7.53866100 -2.58932800
6    -7.82283200 -6.27871100 -2.36442900
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6    -9.18313900 -8.75434000 -1.87874000
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6    -5.75669100 -4.97020800 -2.97143500
6    -5.69477800 -2.54238800 -2.73602600
6    -7.05643800 -2.55622400 -2.37079900
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6    -2.62162600 4.77245700 -1.73908000
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6    -0.35476400 8.32722800 -0.83973300
6    -1.11923300 7.14422600 -1.17540500
6    -0.46358300 5.97287400 -1.61118200
6    0.95757100 6.00073000 -1.73093100
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6    3.39556600 11.56705300 0.48357400
6    1.99918900 11.68030000 0.52197700
6    1.19440000 10.60264200 -0.01414200
6    1.82080800 9.47457300 -0.59292100
6    3.23311100 9.49363800 -0.76431300
6    2.22003200 13.79210800 1.76345000
6    1.44273600 12.85699200 1.14884100
6    7.98690200 14.55796400 3.97659800
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6    11.85062900 9.68747500 3.42363700
6    11.49751600 10.94212800 3.80119000
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6    -3.83996200 -19.41308400 1.05418800
6    -8.28071300 -22.96070800 3.55627400
6    -7.02362900 -22.65732400 3.14523300
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6    -13.13175300 -21.63310000 3.91432900
6    10.60917300 5.29809400 1.36634200
6    9.66835300 4.49044100 0.81001200
6    7.61433000 2.78289900 -0.49419800
6    6.66363800 1.96084900 -1.01791000
6    4.60691200 0.18840900 -2.15442000
6    3.67739300 -0.72861100 -2.53587700
6    1.72713800 -2.79474800 -3.22961000
6    0.92467600 -3.88142600 -3.37702700
6    -0.56177400 -6.38979900 -3.41557600
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6    -13.74056600 -12.45416900 0.18431100
6    -11.20518900 -7.56493400 -1.23220300
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6    -9.80540900 -5.02548600 -1.71182500
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6    -3.25397700 5.98328900 -1.32432600
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6    -4.78885800 3.51797800 -1.77266200
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1    5.97806900 11.30723000 1.02932200
1    10.46286500 13.41224100 4.43900500
1    7.34930100 10.52167600 1.91773700
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1    3.15088700 4.51730600 0.55269600
1    1.51410100 2.86285600 -0.02313900
1    0.30497400 1.22331000 -0.05737500
1    -1.16437300 -0.65128500 -0.34360900
1    -2.20674600 -2.37474200 -0.33557800
1    -3.41774500 -4.44250600 -0.35358800
1    -4.39604400 -6.20011900 -0.37125600
1    -5.31351900 -8.40141200 -0.12294700
1    -6.14987200 -10.25543500 -0.10790200
1    -6.79324200 -12.50133700 0.42734500
1    -7.33567400 -14.37568100 0.74879400
1    -7.83308400 -16.59768400 1.48392100
1    -10.22262900 -14.99426400 -1.36188600
1    -11.11111000 -17.03205600 -0.46224100
1    -8.17323900 -11.29957900 -2.09448400
1    -9.26769900 -13.35274000 -1.57332000
1    -6.16236500 -7.57866400 -2.94246400
1    -7.29188300 -9.64195900 -2.53627000
1    -4.03980500 -3.81705300 -3.38326400
1    -5.22395000 -5.88612100 -3.22155100
1    0.48122200 3.53654800 -2.50401100
1    -0.77287200 1.54608300 -2.90824800
1    2.75797200 7.06985500 -1.53070200
1    1.49986000 5.11273600 -2.05120200
1    5.06449200 10.47507300 -0.40645400
1    3.73363900 8.69867400 -1.31325400
1    1.75509400 14.66978400 2.21765300
1    0.36423800 13.01261800 1.13061300
1    8.63736800 15.20167800 4.57316400
1    6.34605400 15.90265600 4.09210100
1    12.86341800 9.32569400 3.61496800
1    12.22443300 11.58605000 4.30138900
1    -2.60145500 -17.97429100 0.14137100
1    -3.03844200 -20.15333500 1.10147200
1    -8.47775100 -23.91494000 4.05009200
1    -6.21161700 -23.37070100 3.30323300
1    -15.09403100 -20.84339500 4.11362500
1    -13.36181100 -22.52224300 4.50583600
1    11.64369500 4.95695400 1.44389300
1    9.97562100 3.50788900 0.45466300
1    8.66051800 2.50716300 -0.61653400
1    6.98932000 1.05315200 -1.52283900
1    5.62703300 0.07377100 -2.51659800
1    3.99611000 -1.54960400 -3.17480500
1    2.62807400 -2.73135500 -3.83674100
1    1.22359500 -4.64539200 -4.09092200
1    0.25107100 -6.26391900 -4.12705600
1    -0.74313200 -8.42526500 -3.92411100
1    -1.12021000 -10.20966100 -3.31372600
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1    -1.93465800 -14.13014700 -1.75990700
1    -2.38255300 -16.31665300 -0.89635400
1    -15.53680800 -14.15770700 1.28343500
1    -16.28358000 -16.19304100 2.36211600
1    -13.72817400 -10.36371000 -0.08520000
1    -14.73431200 -12.41516500 0.62902300
1    -11.75866300 -6.63877600 -1.09176200
1    -12.87257500 -8.69610900 -0.61379900
1    -9.68619100 -2.92584200 -1.68334900
1    -10.84629600 -4.98888100 -1.39739600
1    -7.53956300 0.77000900 -1.82987100
1    -8.74725300 -1.28408100 -1.81814400
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1    -4.33532100 6.02367100 -1.21081100
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1    -2.04915700 9.56912700 -0.22996200
1    -1.80270400 -0.08959300 -3.21323700
1    -3.03909200 -2.12817700 -3.37136600
1    -5.32903700 4.41546000 -1.47883100
1    -6.56736900 2.39593900 -1.74412800
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30. [42]clarene <2,12,2,12,2,12>

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No imaginary frequency (B3LYP/6-31G*)

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6    13.68927000 6.19698600 0.00017600
6    14.37660600 4.97562400 -0.00000700
6    15.79786300 5.00502300 -0.00001300
6    14.33265000 9.92616800 0.00082700
6    13.63622500 11.13245100 0.00103500
6    12.23473700 11.17935400 0.00085400
6    11.49821200 9.96348500 0.00038500
6    12.21179100 8.75722700 0.00022200
6    13.60174400 8.70120300 0.00046500
6    3.56429500 -16.18559400 -0.00582800
6    2.87924400 -14.93996100 -0.00523100
6    1.47782800 -14.95501200 -0.00522200
6    0.73468100 -16.13095000 -0.00576400
6    1.43038400 -17.37627200 -0.00634700
6    2.82322800 -17.37601000 -0.00636700
6    14.42171400 2.49220100 -0.00041300
6    13.68710100 3.69237900 -0.00019300
6    12.26705400 3.61744200 -0.00016100
6    11.61147000 2.42308000 -0.00031900
6    12.31585500 1.18642100 -0.00054700
6    13.72748100 1.22273800 -0.00061100
6    12.33280000 -1.29282000 -0.00106100
6    11.61498300 -0.08051000 -0.00072900
6    10.19001300 -0.14088900 -0.00056400
6    9.52358700 -1.32708000 -0.00074200
6    10.21363300 -2.57537300 -0.00114900
6    11.62342800 -2.55696600 -0.00132400
6    10.20202500 -5.05399800 -0.00188800
6    9.49807700 -3.83271400 -0.00140100
6    8.07216600 -3.87644600 -0.00117000
6    7.39212700 -5.05462900 -0.00142400
6    8.06756300 -6.31120200 -0.00196000
6    9.47724100 -6.30982800 -0.00220000
6    8.02604700 -8.78968200 -0.00289200
6    7.33684000 -7.55974800 -0.00228400
6    5.91079600 -7.58636900 -0.00200600
6    5.21683800 -8.75662900 -0.00239900
6    5.87724900 -10.02076300 -0.00310000
6    7.28613800 -10.03620800 -0.00329000
6    5.80495200 -12.50178500 -0.00421900
6    5.13056900 -11.26117800 -0.00360300
6    3.70738000 -11.26925100 -0.00352000
6    3.00075100 -12.43410800 -0.00403000
6    3.64593600 -13.70136400 -0.00466600
6    5.05266100 -13.73767400 -0.00474600
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6    -16.45845400 6.24193300 0.00021300
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6    -14.37660600 4.97562400 -0.00000600
6    -11.49821200 9.96348500 0.00038600
6    -12.23473700 11.17935400 0.00085500
6    -13.63622500 11.13245100 0.00103700
6    -14.33265000 9.92616700 0.00082900
6    -13.60174400 8.70120300 0.00046600
6    -12.21179100 8.75722700 0.00022300
6    -0.73468100 -16.13095000 -0.00576400
6    -1.47782800 -14.95501200 -0.00522200
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1    4.31619200 6.26853600 1.82207100
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1    15.64622400 16.63908600 0.49176600
1    14.59251800 18.80608700 0.92155800
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1    -2.63373600 -19.08876500 -0.20396400
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32. [46]clarene <2,2,18,2,2,20>

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33. [46]clarene <2,4,16,4,2,18>

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1    -13.90709300 -5.87415900 -0.10420400
1    -10.67682800 0.02628800 0.12410300
1    -11.83442300 -2.06294800 0.05369600
1    -8.53828400 3.80373900 0.17516800
1    -9.72004800 1.72705900 0.15028000
1    -6.35649200 7.55692100 0.14893800
1    -7.56272800 5.49424900 0.17324100
1    -4.13224700 11.28409700 0.04682600
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1    -5.36221200 9.23653200 0.11792400
1    -1.86730200 14.98476400 -0.11885500
1    -3.11954300 12.95259700 -0.00908000
1    0.43391200 18.65877000 -0.32820700
1    -0.83654500 16.64234500 -0.19200600
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37. [52]clarene <2,2,22,2,2,22>

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No imaginary frequency (B3LYP/6-31G*)

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6    7.68275700 22.77384600 0.81730000
6    7.16211800 21.47689800 0.65392200
6    8.05481000 20.38010400 0.49376300
6    9.41691300 20.65585900 0.38750400
6    14.16468400 22.48055500 0.47522400
6    13.31759200 23.55433000 0.80000000
6    11.91886600 23.43622800 0.73789900
6    11.36060000 22.19022300 0.35360200
6    12.20331500 21.18846600 -0.09600600
6    13.58523700 21.29742300 -0.04622500
6    16.42362900 18.86698400 0.08550000
6    15.75841500 20.09879200 0.08811300
6    14.40816300 20.13516200 -0.35072400
6    13.84640100 19.00571100 -0.92457700
6    14.47711900 17.76545400 -0.88745000
6    15.77480400 17.68232500 -0.31395500
6    -7.16212500 -21.47697900 -0.65288400
6    -8.05481500 -20.38015900 -0.49289300
6    -9.41693300 -20.65588800 -0.38672200
6    -9.92992600 -21.94383300 -0.47942200
6    -9.05662700 -23.02608600 -0.76859800
6    -7.68276700 -22.77393400 -0.81618300
6    -11.36065800 -22.19022300 -0.35295500
6    -12.20343500 -21.18842200 0.09644400
6    -13.58535400 -21.29735400 0.04642000
6    -14.16472900 -22.48052200 -0.47503100
6    -13.31759900 -23.55433300 -0.79957700
6    -11.91888400 -23.43624700 -0.73725600
6    -13.84664000 -19.00552500 0.92445000
6    -14.47734100 -17.76526600 0.88705300
6    -15.77493200 -17.68219700 0.31333700
6    -16.42370100 -18.86689800 -0.08607300
6    -15.75849600 -20.09871200 -0.08842400
6    -14.40831800 -20.13504600 0.35064900
6    14.20605100 15.31759800 -0.80176600
6    13.73592200 16.56541400 -1.23181600
6    12.48508300 16.64022900 -1.90552400
6    11.67002800 15.55409500 -2.01169800
6    12.02629200 14.30813300 -1.42260300
6    13.31529000 14.17884300 -0.85349600
6    11.43690000 12.01501300 -0.71375900
6    11.08416200 13.20987300 -1.36867000
6    9.77539800 13.30609400 -1.93422800
6    8.88801700 12.27265400 -1.87524100
6    9.20352300 11.05292200 -1.20640400
6    10.46836200 10.94752600 -0.58867000
6    8.58451300 8.81072800 -0.37503500
6    8.26897900 9.94590700 -1.14579700
6    7.03881700 9.93243700 -1.87437100
6    6.22144200 8.83846400 -1.88721100
6    6.51234500 7.67204000 -1.11711000
6    7.66570700 7.69897200 -0.30769600
6    5.94952100 5.42561900 -0.25142100
6    5.66303600 6.49521800 -1.12264300
6    4.53875900 6.35215300 -1.99161300
6    3.78360700 5.21273300 -2.01506200
6    4.05508000 4.10659500 -1.15405300
6    5.12944600 4.23961600 -0.25186300
6    3.55875000 1.86252800 -0.23764800
6    3.26758700 2.88530800 -1.16205600
6    2.18891800 2.65630300 -2.06921900
6    1.46532100 1.49537500 -2.05677300
6    1.74022600 0.43848800 -1.13658200
6    2.79561300 0.63977900 -0.22523100
6    1.31410000 -1.79346100 -0.15280000
6    0.98450000 -0.80359800 -1.10058300
6    -0.10166800 -1.08471700 -1.98347300
6    -0.80107400 -2.25934100 -1.92240300
6    -0.48161600 -3.28588300 -0.98272300
6    0.58824900 -3.03765800 -0.10020800
6    -0.77850700 -5.53477000 0.00784100
6    -1.19900600 -4.54877300 -0.90753800
6    -2.33702800 -4.85252900 -1.71468600
6    -3.00349800 -6.04314700 -1.60890500
6    -2.56046900 -7.08335500 -0.73673100
6    -1.41760400 -6.82655400 0.04600800
6    -2.59615600 -9.41565900 0.07930100
6    -3.21122100 -8.37937800 -0.65140100
6    -4.47313900 -8.66458500 -1.25897800
6    -5.06888900 -9.88969200 -1.14011300
6    -4.41422600 -10.98560500 -0.49745600
6    -3.14336300 -10.75057300 0.05923800
6    -4.17247700 -13.40436000 -0.03558700
6    -4.98092200 -12.31951700 -0.43572200
6    -6.34886900 -12.58770900 -0.74325200
6    -6.86449200 -13.85108000 -0.66834900
6    -6.04079400 -14.98339200 -0.37876100
6    -4.67841900 -14.75562400 -0.10935000
6    -5.66306700 -17.43802500 -0.29705100
6    -6.55185600 -16.34100400 -0.38483000
6    -7.94650400 -16.61281800 -0.46356700
6    -8.42150400 -17.89242800 -0.45844000
6    -7.54651400 -19.01631700 -0.44274400
6    -6.16163200 -18.79104400 -0.40221800
6    -11.67037900 -15.55377900 2.01138000
6    -12.02651500 -14.30791700 1.42199600
6    -13.31542000 -14.17869600 0.85266300
6    -14.20620800 -15.31743100 0.80101400
6    -13.73617600 -16.56518400 1.23135200
6    -12.48544700 -16.63991100 1.90527200
6    -8.88825700 -12.27244000 1.87473300
6    -9.20361400 -11.05283800 1.20558600
6    -10.46833900 -10.94753800 0.58760500
6    -11.43693000 -12.01496800 0.71275800
6    -11.08434200 -13.20969800 1.36798800
6    -9.77567800 -13.30584000 1.93378800
6    -6.22164100 -8.83829700 1.88654100
6    -6.51239000 -7.67200900 1.11617900
6    -7.66559200 -7.69907500 0.30654200
6    -8.58441200 -8.81081600 0.37389200
6    -8.26904000 -9.94585500 1.14492900
6    -7.03902000 -9.93226600 1.87373800
6    -3.78377100 -5.21262300 2.01421500
6    -4.05514200 -4.10656600 1.15307400
6    -5.12938600 -4.23967000 0.25075300
6    -5.94942800 -5.42569800 0.25028300
6    -5.66308100 -6.49519200 1.12168400
6    -4.53892600 -6.35203900 1.99079300
6    -1.46546400 -1.49532700 2.05590800
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6    -1.74030300 -0.43846700 1.13567000
6    -2.79565000 -0.63975600 0.22427300
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6    -3.26766300 -2.88527500 1.16109700
6    -2.18908700 -2.65623500 2.06835800
6    0.80104600 2.25927700 1.92156500
6    0.48163100 3.28583900 0.98189500
6    -0.58824300 3.03767200 0.09937100
6    -1.31413300 1.79349500 0.15193500
6    -0.98455900 0.80360500 1.09970000
6    0.10160300 1.08467700 1.98261000
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6    2.56061700 7.08323700 0.73604900
6    1.41775100 6.82650400 -0.04671000
6    0.77861200 5.53473800 -0.00860600
6    1.19907700 4.54869400 0.90673700
6    2.33712500 4.85236500 1.71387900
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6    4.41437600 10.98550400 0.49713900
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6    6.34900100 12.58760000 0.74314800
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6    7.54652800 19.01626300 0.44349100
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6    12.76218000 11.90058700 -0.18975200
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6    0.29069000 -5.23029200 0.89995500
6    -0.89068500 -7.87461800 0.85768300
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6    -2.39177100 -11.86002700 0.55086000
6    -2.86229700 -13.13259900 0.45798400
6    -3.81790400 -15.88605400 0.04637400
6    -4.27825300 -17.16083200 -0.08370500
6    -15.54979000 -15.25297900 0.27329200
6    -16.31133400 -16.36615500 0.08657900
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6    -13.65990000 -12.92280500 0.26714600
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6    -7.07213400 -5.53638000 -0.62298200
6    -7.90184600 -6.61091900 -0.58248500
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6    0.89085600 7.87462700 -0.85832100
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1    13.75632700 24.49163900 1.15274800
1    11.76300600 20.25900700 -0.43604900
1    17.44409400 18.80837100 0.47340700
1    12.83681700 19.06289500 -1.31669600
1    -10.10347600 -19.82778900 -0.24656000
1    -6.99108000 -23.60091600 -0.99760000
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1    -13.75628900 -24.49166500 -1.15232000
1    -12.83711500 -19.06265600 1.31672800
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1    12.16453200 17.57830100 -2.35706400
1    10.72243700 15.66654800 -2.53458900
1    9.45973600 14.22060100 -2.43263900
1    7.90572600 12.40823800 -2.32474100
1    6.74503300 10.80077400 -2.46204400
1    5.30639100 8.88392700 -2.47640800
1    4.26755300 7.16407600 -2.66516600
1    2.93995600 5.16757000 -2.70287300
1    1.91784600 3.42414700 -2.79264000
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1    -0.40267400 -0.34437800 -2.72357200
1    -1.62699400 -2.40391900 -2.61850400
1    -2.71818300 -4.10911900 -2.41387200
1    -3.88270100 -6.20218000 -2.23312200
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1    -6.05700200 -10.03094500 -1.57814300
1    -7.01858400 -11.76507300 -0.99496900
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1    -9.49991600 -18.03617500 -0.50214900
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1    -12.16499000 -17.57791400 2.35702400
1    -7.90604300 -12.40795800 2.32442300
1    -9.46012900 -14.22025100 2.43244800
1    -5.30672700 -8.88365200 2.47595800
1    -6.74536900 -10.80049400 2.46163800
1    -2.94020000 -5.16739500 2.70212200
1    -4.26779700 -7.16389700 2.66445600
1    -0.64815100 -1.39061000 2.76899600
1    -1.91810700 -3.42403900 2.79185600
1    1.62695700 2.40382500 2.61768500
1    0.40256700 0.34432200 2.72271200
1    3.88285000 6.20193200 2.23236600
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1    5.01301800 7.87356200 1.78017400
1    7.92594400 13.98451600 0.87310800
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1    7.01872900 11.76494300 0.99476100
1    9.49995000 18.03615500 0.50271300
1    8.66306000 15.79282100 0.49861600
1    5.05322000 22.02865000 0.76970000
1    4.20405900 19.77709500 0.50410000
1    11.40676500 25.48623200 1.32202300
1    8.98338100 25.15689900 1.26925700
1    17.39676900 21.34805000 0.83540400
1    16.06704600 23.38446400 1.08656800
1    -4.20405100 -19.77720300 -0.50312500
1    -5.05323100 -22.02877900 -0.76847900
1    -11.40673800 -25.48630500 -1.32114800
1    -8.98335400 -25.15700100 -1.26807800
1    -17.39674100 -21.34802300 -0.83586000
1    -16.06699500 -23.38447200 -1.08661200
1    17.32626000 16.27098200 0.30427600
1    15.98010500 14.28309300 -0.02626200
1    14.65107700 12.77696600 0.15908800
1    13.08170700 10.97361400 0.28291800
1    11.70828200 9.67255500 0.68177800
1    10.12217100 7.89817900 0.88368800
1    8.75003900 6.63294500 1.26236000
1    7.30290900 4.74115700 1.32633600
1    6.18273300 3.27047300 1.40209600
1    4.86261500 1.29814900 1.42593800
1    3.89452300 -0.25928000 1.43886900
1    2.66021500 -2.28260800 1.50111900
1    1.73327900 -3.86435200 1.57134700
1    0.60136000 -5.95102900 1.65251200
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1    -0.97569300 -9.89021500 1.46503300
1    -1.39335600 -11.70639600 0.95568400
1    -2.23155200 -13.94720800 0.80948600
1    -2.75415800 -15.73770300 0.22435100
1    -3.56751400 -17.98037800 0.01070800
1    -15.98012600 -14.28300700 0.02509000
1    -17.32627500 -16.27091900 -0.30533300
1    -13.08152900 -10.97373100 -0.28443000
1    -14.65099000 -12.77699200 -0.16044800
1    -10.12180600 -7.89850200 -0.88532400
1    -11.70798200 -9.67281500 -0.68336400
1    -7.30249200 -4.74150500 -1.32786900
1    -8.74959200 -6.63331800 -1.26392500
1    -4.86235000 -1.29831500 -1.42722300
1    -6.18246600 -3.27063700 -1.40340700
1    -2.66032200 2.28274000 -1.50189800
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1    -0.60126200 5.95110500 -1.65324700
1    -1.73324100 3.86446600 -1.57216000
1    0.97586700 9.89026600 -1.46551400
1    0.01135300 7.70530000 -1.47470100
1    2.23172900 13.94721800 -0.80958400
1    1.39357000 11.70641800 -0.95607500
1    3.56754600 17.98031900 -0.01004400
1    2.75423700 15.73765800 -0.22405000
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38. [54]clarene <2,2,22,2,2,24>

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No imaginary frequency (B3LYP/6-31G*)

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6    11.90314500 25.45097600 -2.55084600
6    11.07095300 24.56605700 -1.83712200
6    11.65803900 23.46845700 -1.15158800
6    13.02182600 23.23999300 -1.30910100
6    17.51526800 22.43888600 -3.60022800
6    17.16401600 23.77575300 -3.85321200
6    15.93702900 24.31096800 -3.42424800
6    15.09781100 23.50763200 -2.61356600
6    15.44485800 22.18412200 -2.38521400
6    16.58737100 21.61167000 -2.91685700
6    18.27897500 18.26379900 -2.98728800
6    18.06558600 19.63136300 -3.18011700
6    16.80680800 20.17500100 -2.80907600
6    15.78590000 19.32415500 -2.40270800
6    15.96606900 17.94882400 -2.26261600
6    17.26454600 17.41765100 -2.50306800
6    -4.48393800 -19.78915400 -2.30376700
6    -5.58642500 -18.91518900 -2.08784000
6    -6.87150600 -19.43322000 -2.24256600
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6    -4.71748800 -21.09273200 -2.77868200
6    -8.46557900 -21.25707400 -2.76506100
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6    -11.12899100 -22.01781900 -3.30840200
6    -10.05459500 -22.82975800 -3.71117600
6    -8.72135100 -22.47834500 -3.43991900
6    -11.65722100 -18.93077100 -1.23283500
6    -12.52602400 -17.85152000 -1.10115000
6    -13.75814300 -17.88285800 -1.80829400
6    -14.11084900 -19.04865500 -2.51656100
6    -13.20735700 -20.10584700 -2.67909100
6    -11.92146200 -19.98801900 -2.08798400
6    15.12882200 15.72017100 -1.59201200
6    14.87013200 17.06978000 -1.87824000
6    13.52634700 17.53722600 -1.80785100
6    12.49029900 16.70140800 -1.50453900
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