

Effect of Sterically Protective Groups on the Aromaticity of Fully Unsaturated Oligoquinanes

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Abstract

Oligoquinane derivatives have unique aromatic properties, which dictate the stability of the molecules and their potential applications in various devices. Due to the challenge in their synthesis, systematic studies of these molecules are still lacking. In this work, we perform density function theory and nucleus-independent chemical shift (NICS) calculations on 24 oligoquinane derivatives that are composed of two, four, five, and six five-membered rings. Pentaquinane without any protection groups was predicted to be aromatic and stable. It would be interesting to synthesize the molecule and carry out further electronic and optical measurements.

Among introducing various protection groups to the bare oligoquinanes, single bond protection was found to be the least effective in the change of aromaticity of oligoquinane. In the protection of benzene rings, aromaticity change depends on the configuration of the molecule formed. HOMO-LUMO energy gap and UV-Vis absorption also depends on the molecular shape. The results show the potential application of the oligoquinanes as they can be diversely tuned for specific applications, and therefore is worthy of future studies.

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1. Introduction

Fullerene derivatives, such as C₆₀,¹ have been widely used as electron acceptors in solar cells.²⁻
²³ As a receptor material, the energy of the empty orbitals is required to be lower than the donor materials. There are many organic small molecules (OSMs) as electron donor materials²⁴⁻⁶⁶ for solar cells as well as materials for sensors.⁶⁷⁻¹⁰⁴ Therefore, it is critical to develop derivatives of fullerenes so that the new electron acceptor materials have satisfactory energy levels and other desired properties to accept electrons and facilitate electron transfer. Synthesis and studies of acenes¹⁰⁵ and pentalene derivatives¹⁰⁶ are examples of such efforts.

One of the important properties of polyacene and oligoquinane derivatives is aromaticity, which dictate the stability of the molecule as well as its ability to transport electrons. As an important parameter, nucleus-independent chemical shift (NICS) has been widely used to measure the aromaticity of organic molecules.¹⁰⁶⁻¹⁴⁴ Okazawa et al used NICS values to characterize a series of stacked antiaromatic molecules and found the aromaticity of these materials.¹¹¹ In the study of helicenes, Huang, et al used NICS values as one of the reliable parameters to confirm the aromaticity of these molecules.¹¹² In the chemically stable yet redox-switchable porphyrinoids, the ring current effects on redox-switchable rings and the details were studied using NMR measurements and NICS calculations.¹³⁵

Compared to polyacenes, oligoquinanes are less stable and challenging to synthesis. For instance, pentalene¹⁴⁵ and tetraquinane¹⁰⁶ were only synthesized when they are sterically protected. Hence, systematic computational investigations and predictions of oligoquinanes are critically important for potential synthesis and device studies. The objectives of the current work are three-folds. The first is to understand the change of aromaticity of oligoquinanes with the number of five-membered rings. Towards this, we select linear oligoquinanes **1**, **2**, **4**, and **6**, shown in Figure

1 in this work. The second is to investigate the effect of nonlinearity on the aromaticity. The molecules **3**, **5**, and **7-9** in Figure 1 were chosen to meet this goal. The third goal of the work is to understand how sterically protected groups can change the aromaticity as well as the electronic and optical properties of the oligoquinanes. To achieve this, we selected 18 molecules shown in Figures 2-4 to perform density functional theory (DFT) and NICS calculations to study their aromaticity and electro-optical properties in this work.

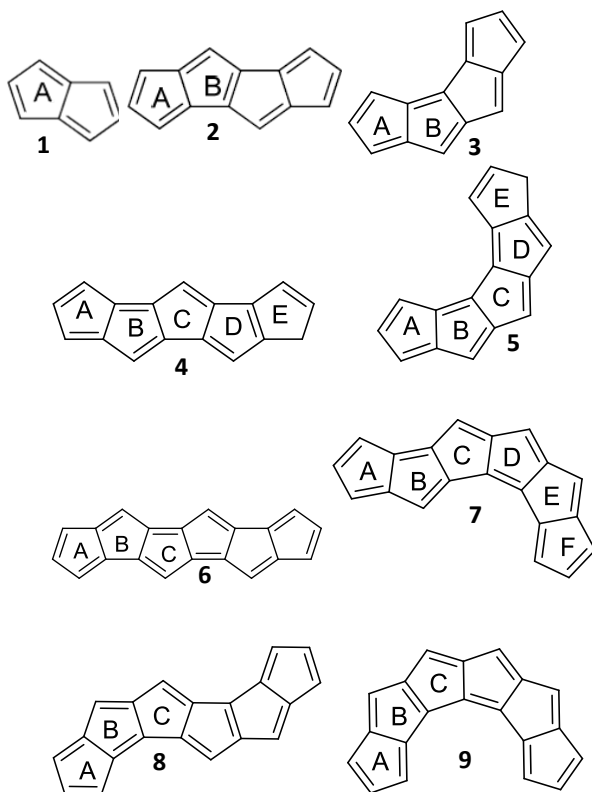


Figure 1. Structures of nine oligoquinanes. The letters denote the ring positions in the given molecule.

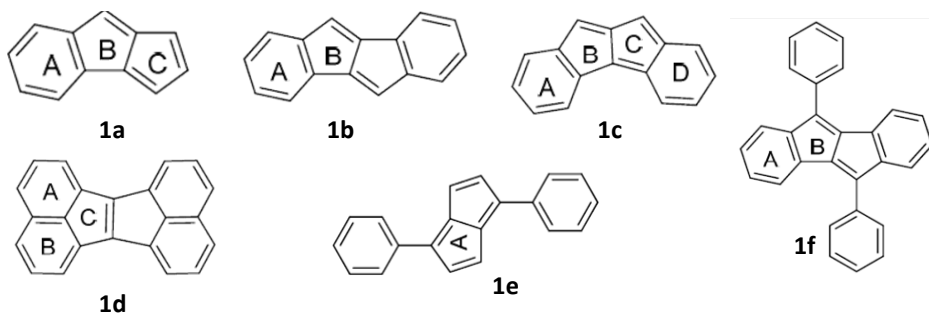


Figure 2. Structures of protected pentalenes. The letters denote the ring positions in the given molecule.

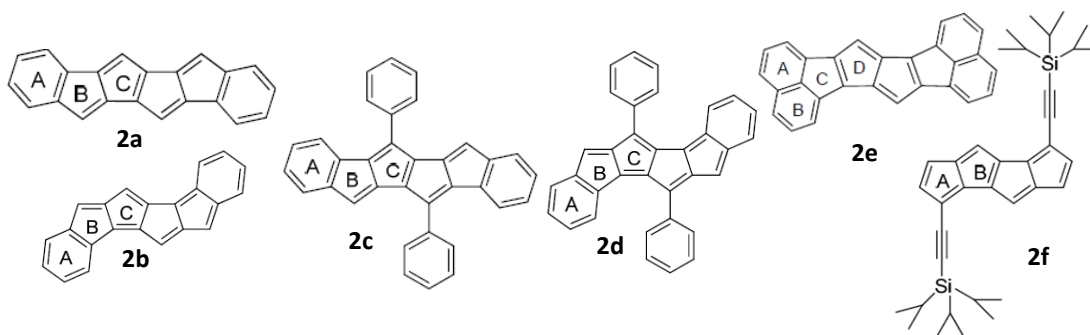


Figure 3. Structures of protected tetraquinanes. The letters denote the ring positions in the given molecule.

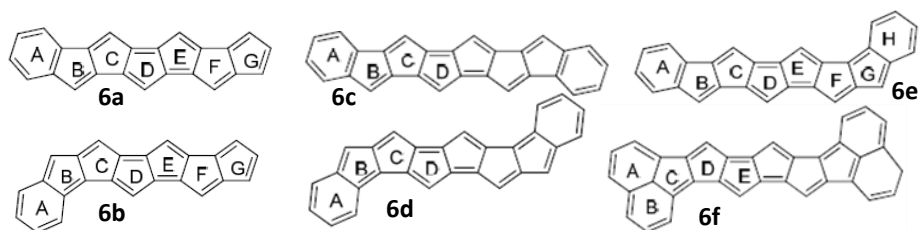


Figure 4. Structures of protected hexaquinanes. The letters denote the ring positions in the given molecule.

The DFT and NICS calculations were performed to study 24 molecules shown in Figures 1-4 to obtain aromaticity, electronic, and optical properties of the molecules. The details of the computations are described in the next section. The results and discussion are presented in section 3. Finally, the conclusions are drawn in section 4.

2. Computational Details

All geometry optimizations of the 24 molecules, **2-9** in Figure 1, **1a-1e** in Figure 2, **2a-2e** in Figure 3, and **6a-6f** in Figure 4, were performed using B3LYP/6-31+G(d,p) in chloroform. . All geometry optimizations were obtained with the default self-consistent field, gradient, and energy convergence of 10^{-8} , 10^{-4} , and 10^{-5} a.u., respectively. The optimized structures were confirmed by frequency analysis with no imaginary frequencies. Chloroform solvent was described using the polarized continuum model (PCM). The UV-Vis spectra were obtained from TDDFT calculations using both B3LYP/6-31+G(d,p) and CAM-B3LYP/6-31+G(d,p) with the optimized structures by B3LYP/6-31+G(d,p) for molecules **6a-6f**. All the above mentioned DFT and TDDFT calculations were performed using the Gaussian03 or Gaussian 09 package.¹⁴⁶

Calculations of NICS were carried out using B3LYP/6-31+G(d,p) from the optimized structures using the AROMA 1.0 program package in the same way as we previously did for molecules **1**, **1f**, and **2f**.¹⁰⁶

3. Results

The results from DFT calculations as well as NICS calculations of 24 molecules are presented here. We first discuss the results of 8 bare oligoquinanes and make comparison of the NICS value of pentalene in 3.1.¹⁰⁶ we then discuss the effect of protected group on the aromaticity of the oligoquinanes in 3.2 followed by the discussion of the electronic and optical properties of the oligoquinanes in 3.3.

3.1 Aromaticity of Bare Oligoquinanes

The calculated NICS(1) values of 8 oligoquinanes are summarized in Table 1 together with that of pentalene. There are two observations. First, for linear oligoquinanes, the NICSs values

decreases, in general, with the increase of ring size from 2 to 6 (molecules **1**, **2**, **4**, **6**). Interestingly, pentaquinane was predicted to be aromatic and stable, though it has never been studied previously. With the development of synthesis method and studies of activating/coupling of C-H,¹⁴⁷⁻¹⁵⁵ C-C,^{148,156-161} C-O,¹⁶²⁻¹⁶⁶ O-O,¹⁶⁷ N-O,¹⁶⁸ and the catalysts,^{169,170} it would be interesting to synthesize and study pentaquinane.

The second observation is the drastic change in aromaticity when oligoquinanes are formed in bend configurations. For tetraquinanes, the NICS values of the bend structure (**3**) indicate that it is aromatic. In the case of pentaquinane, the bend structure (**5**) has decreased the NICS values of two most aromatic five-membered rings. For hexaquinanes, the most center rings are aromatic and the outmost rings of **7** and **9** are the most antoaramatic.

Table 1. NICS(1) values of the five-membered rings, **A-F**, of oligoquinanes.

Molecule	Number of Rings	A	B	C	D	E	F
1 *	2	19.4(2) ⁺					
2	4	15.7(2)	17.3(2)				
3	4	-12.6(2)	-7.9(2)				
4	5	-11.0	-10.0	-3.9	-5.7	-1.7	
5	5	-9.8	-4.9	-3.9	-5.7	-1.7	
6	6	1.3(2)	2.1(2)	-6.6(2)			
7	6	16.5	15.0	-3.9	-9.6	8.8	12.5
8	6	3.7(2)	3.3(3)	-4.6(2)			
9	6	15.6(2)	13.7(2)	-7.4(2)			

*data was taken from reference ...;

⁺ the number in prentices denote the number of rings of having the NICS(1) value.

3.2 Aromaticity of Protected Oligoquinanes

As being stated previously, oligoquinanes are mostly unstable.¹⁰⁶ They were mostly being studied using various protection groups. In this DFT studies, we studied five protected pentalenes, five protected tetraquinanes, and six hexaquinanes and the results are summarized in Tables 2-4,

respectively. In this section, we focus on the discussion of NICS values and the electronic and optical properties of these oligoquinanes will be discussed in 3.3.

Table 2. NICS(1), HOMO, LUMO, and HOMO-LUMO energy gap of protected pentalenes.

Molecule	NICS(1)	HOMO (eV)	LUMO (eV)	Gap (eV)
1*	A= 19.4	-5.51	-3.06	2.45
1a	A= -3.4 B= 10.7 C= 11.8	-5.62	-2.81	2.81
1b	A= -5.3 B= 6.6	-5.76	-2.66	3.10
1c	A= 7.4 B= 29.0 C= 34.7 D= 15.4	-5.03	-3.39	1.64
1d	A= -8.3 B= -8.3 C= 2.0	-5.54	-2.65	2.89
1e	A= 16.2	-5.37	-3.19	2.18
1f*	A= -5.6 B= 6.0	-5.71	-2.81	2.90

*data was taken from reference ...

As shown in Table 1, the antiaromaticity of the five-membered rings protected by one benzene ring (**1a**) is reduced with the five-member ring adjacent to benzene ring being reduced more. When two benzene rings protected at the both end of pentalene in a linear fashion, i.e. **1b**, the antiaromaticity is substantially reduced. However, when it is bend configuration (**1c**), the NICS values increase greatly and the molecule is highly unstable. When four benzene rings are introduced forming **1d**, the five-membered rings become nearly nonaromatic. In the case of **1e**, where single bond protection was formed, the aromaticity of the five-membered rings remains unchanged. The same trend holds for **1f** with respect to **1b**. These results indicate that single bond protection is less effective.

In the case of tetraquinane derivatives, the data in Table 3 shows some interesting trends. A slight change of configurations, see **2a**, and **2b**, aromaticity changes from aromatic to antiaromatic.

Similar to the case of pentalene, single bond protection does not change substantially the aromaticity of the five-membered rings (**2a** vs **2c**, **2b** vs **2d**, and **2** vs **2f**). Addition of four benzene rings with two at each end of tetraquinane (**2e**) makes the molecule aromatic.

Table 3. NICS(1), HOMO, LUMO, and HOMO-LUMO energy gap of protected tetraquinanes.

Molecule	NICS(1)	HOMO (eV)	LUMO (eV)	Gap (eV)
2	A= 15.7 B= 17.3	-4.76	-3.52	1.24
2a	A= -3.8 B= 8.9 C= 11.6	-4.93	-3.33	1.60
2b	A= -10.2 B= -10.1 C= -10.4	-4.91	-3.46	1.45
2c	A= -4.0 B= 8.4 C= 10.8	-4.95	-3.33	1.62
2d	A= -9.6 B= -8.3 C= -8.7	-4.81	-3.45	1.36
2e	A= -10.4 B= -10.1 C= -1.3 D= 11.8	-5.00	-3.07	1.93
2f*	A= 13.7 B= 18.2	-4.75	-3.73	1.02

*data was taken from reference ...

The aromaticity of hexaquinane protected by a benzene ring is sensitive to the configuration of the attachment, as the NICS values of **6a** and **6b** shown in Table 4. The similar conclusions can also be drawn for the protection of using two benzene rings with one at each end of hexaquinane (see **6c-6e**). When 4 benzene rings protection hexaquinane with two at each end (**6f**), the middle five-membered rings become aromatic and the end five-membered rings are nonaromatic. Finally, we note that the NICS values of all 27 oligoquinanes illustrate the complexity of the aromaticity of a molecule and offer the diverse opportunities to tune the properties as well.

Table 4. NICS(1), HOMO, LUMO, and HOMO-LUMO energy gap of protected hexaquinanes.

Molecule	NICS(1)	HOMO (eV)	LUMO (eV)	Gap (eV)
6	A= 1.3 B= 2.1 C= -6.6	-5.27	-3.09	2.18
6a	A= -7.2 B= 0.0 C= 0.6 D= -6.9 E= -5.3 F= -2.3 G= -2.6	-5.10	-3.12	1.98
6b	A= -2.8 B= 7.9 C= 9.0 D= -3.2 E= -3.7 F= 21.8 G= 21.7	-5.00	-3.44	1.56
6c	A= -8.0 B= -1.5 C= -2.3 D= -3.1	-5.06	-3.09	1.97
6d	A= -3.4 B= 8.5 C= 10.4 D= -1.7	-5.09	-3.29	1.80
6e	A= -2.3 B= 10.4 C= 15.1 D= -13.3 E= -8.2 F= -1.4 G= 0.2 H= -6.9	-4.91	-3.43	1.48
6f	A= -8.6 B= -8.1 C= 1.4 D= -8.6 E= -8.5	-4.86	-3.30	1.56

3.3 Electronic and Absorption Properties of Oligoquinanes

The oligoquinanes are considered potential candidates as electron acceptors for electronic device. The electronic and optical properties of the oligoquinanes are important. We summarized in Tables 2-4 the HOMO and LUMO energies of the oligoquinanes being studied here. The UV-

Vis absorption spectra of 7 hexaquinane derivatives are depicted in Figures 5-7. For pentalene derivatives **1a**, **1b**, and **1d-1f** the HOMO –LUMO energy gap fluctuate substantially (see Table 2). Similar fluctuations can also be observed for the tetraquinanes (Table 3) and hexaquinane derivatives (Table 4).

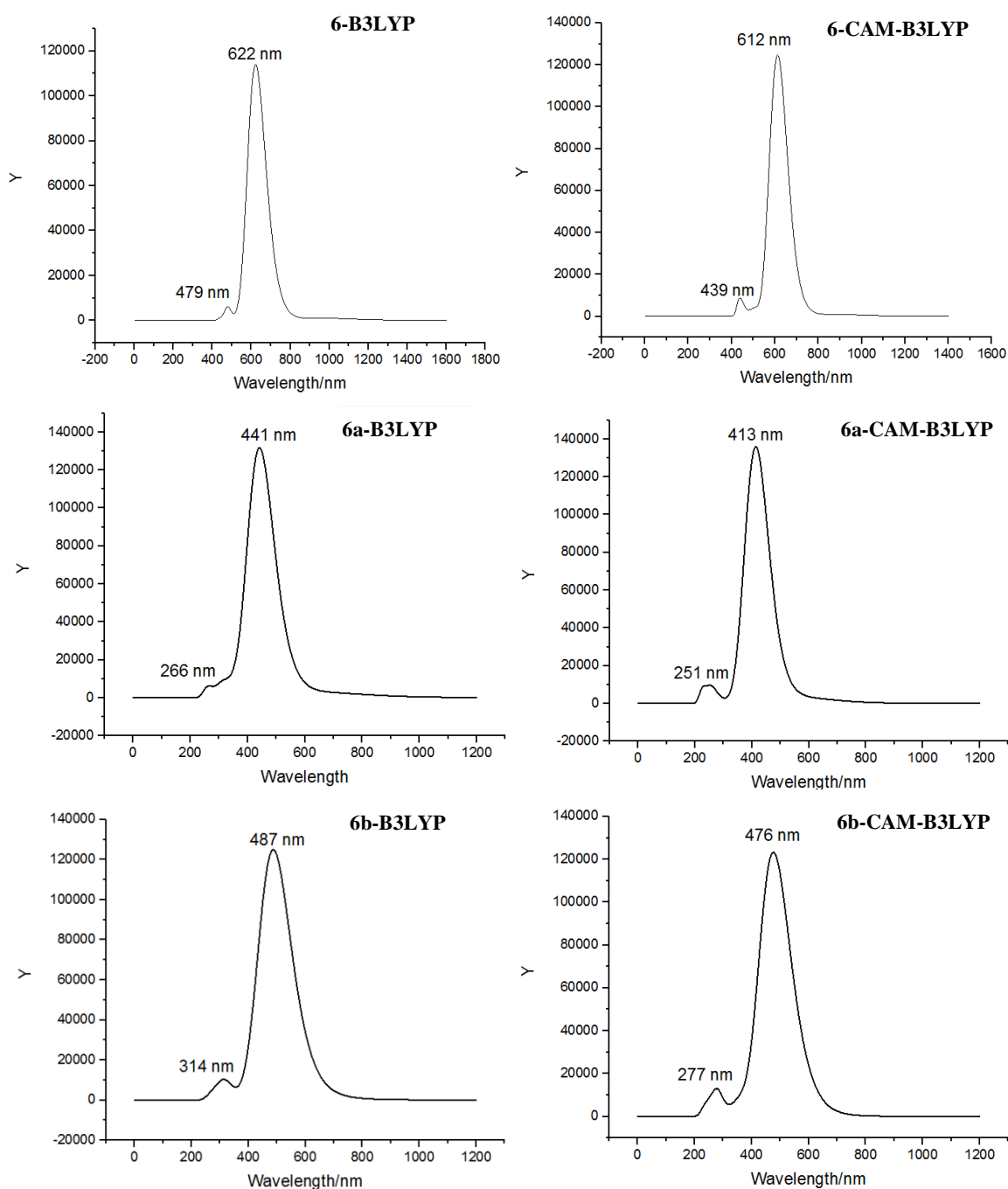


Figure 5. UV-Vis spectra of hexaquinane **6** and the hexaquinanes protected with one benzene ring (**6a** and **6b**) obtained from B3LYP and CAM-B3LYP calculations.

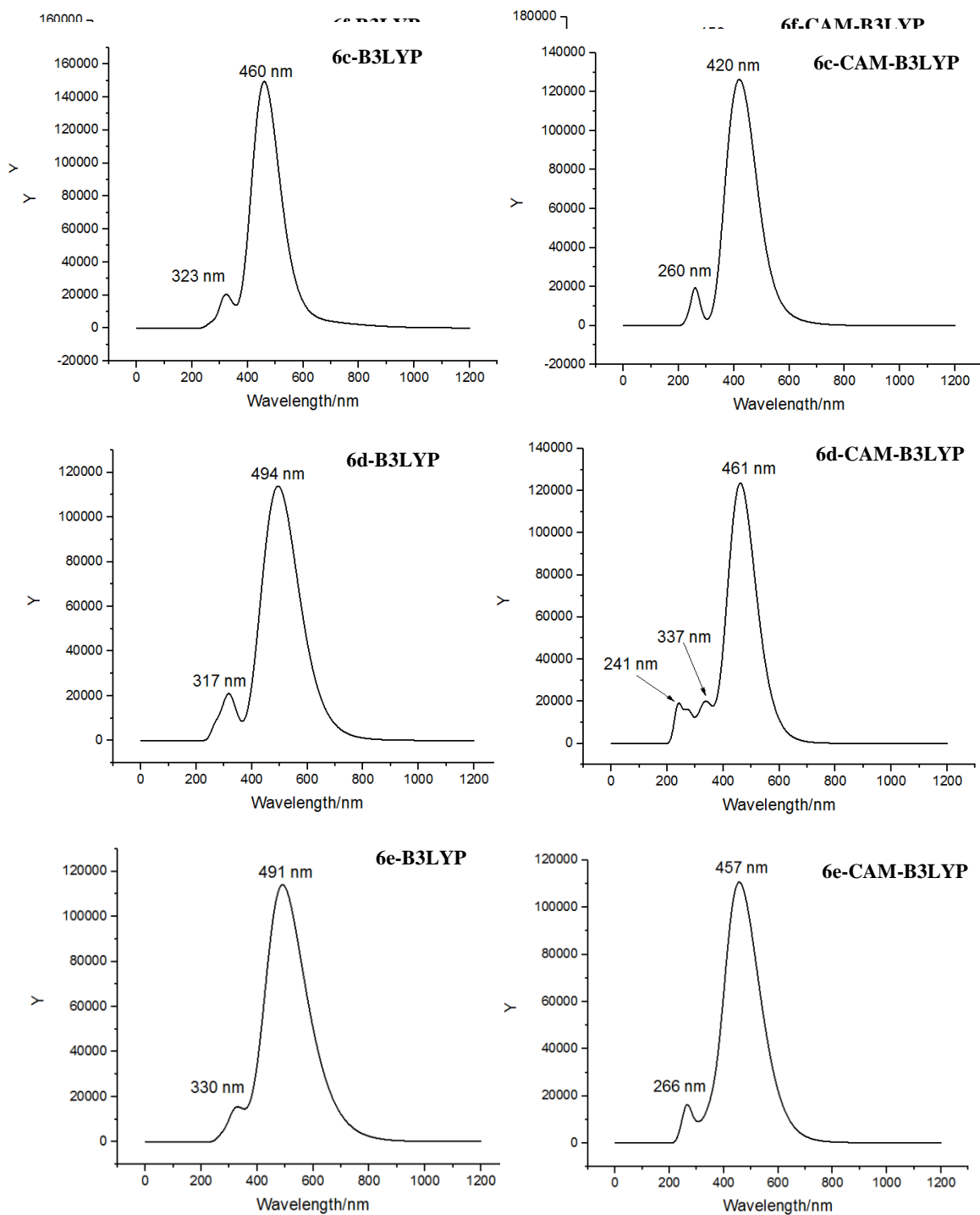


Figure 6. UV-Vis spectra of the hexaquinanes protected with two benzene rings (**6c**, **6d**, and **6e**) obtained from B3LYP and CAM-B3LYP calculations

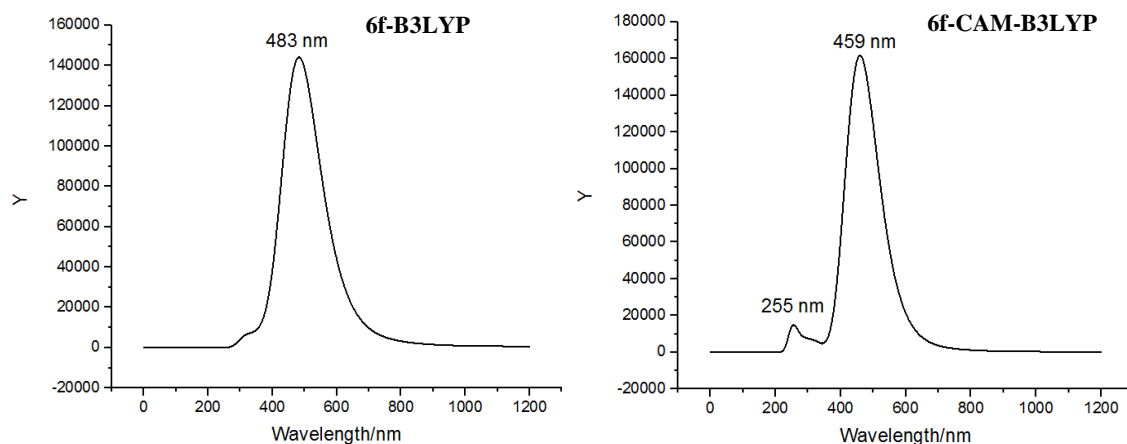


Figure 7. UV-Vis spectra of molecule **6f** obtained from B3LYP and CAM-B3LYP calculations.

While the HOMO-LUMO energy gaps fluctuate in the hexaquinanes derivatives, the UV-Vis absorption is all blue shifted when protection group is introduced, as the data shown in Figures 5-7. We note that B3LYP absorption wavelength is always longer than that of CAM-B3LYP results for all molecules studied here, although the exact difference in wavelength varies on individual molecules. As a general practice, spectra results from CAM-B3LYP calculations with B3LYP optimized structure are often used to compare with experimental measurements. Following this tradition, we will made comparisons of absorption spectra obtained from CAM-B3LYP calculations.

In the case of one benzene ring protection, a nonlinear configuration (**6b**) has a longer wavelength absorption than the linear configuration (**6a**). The same is true with the two benzene ring protected molecules (linear **6c** vs **6d** or **6e**). With four benzene rings protections (**6f**), the absorption length is not further blue shifted, rather it is similar to those of **6d** and **6e**. Finally, we note that the absorption wavelength does not correlate with the HOMO-LUMO energy gap as the excitation of these molecules does not correspond to the HIMO-LUMO transition, as we discussed previously.¹⁰⁶

4. Conclusions

DFT and NICS calculations were carried out to study 24 oligoquinane derivatives consisting of two, four, five, and six five-membered rings with various protection groups. Pentaquinane was predicted to be aromatic and stable. It would be interesting to synthesize the molecule and carry out further electronic and optical measurements.

Among the protection groups introduced to the oligoquinanes, single bond protection was found not to change the aromaticity of oligoquinane substantially. In the protection of benzene rings, aromaticity change depends on the configuration of the molecule formed. HOMO-LUMO energy gap and UV-Vis absorption also depends on the molecular shape. The results show the potential application of the oligoquinanes as they can be diversely tuned for specific applications, and therefore, this class of molecules is worthy of further studies.

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