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Computational Studies of Cyclobutadiene and Benzocyclobutene Fused to *p*- and *o*-Quinone[†]

Michael L. McKee,*,[‡] Metin Balci,*,[⊥] Hamdullah Kilic,[§] and Ersin Yurtsever[||]

Department of Chemistry, Auburn University, Auburn, Alabama 36849, Department of Chemistry, Middle East Technical University, 06531 Ankara, Turkey, Department of Chemistry, Ataturk University, 25240 Erzurun, Turkey, and Department of Chemistry, Koç University, 80860 Istanbul, Turkey

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Cyclobutadiene and benzocyclobutenes fused to *o*- and *p*-quinone have been studied by computational methods. Geometries were optimized at the B3LYP/6-31G* level, and absolute NMR shielding values were calculated using the GIAO method with the HF/6-31G* basis set. NICS values of the compounds **8b,c** and **9b,c** indicate strong antiaromatic character for cyclobutadiene units. However, **8a** and **9a** show negative NICS values where the quinodal system reduces the antiaromaticity significantly by forcing these systems to possess a dimethylene-like structure. The calculated ^{13}C NMR chemical shifts of **6−9** and parent systems are in very good agreement with literature values.

Introduction

Aromaticity appears to be among the most controversial concepts in modern chemistry. The difficulty in determining the effects caused by aromaticity or antiaromaticity result from the inability to measure directly these effects by any physical or chemical experiment. Various criteria for aromaticity are known.[1−4] The most widely used quantitative measures of the degree of aromaticity are energetic, structural, and magnetic properties. Organic molecules that do not have permanent magnetic moments are weakly diamagnetic. This diamagnetism is caused by Larmor precession of the electrons, which produces small magnetic fields opposing the applied magnetic field.[5] Since the magnitudes of the diamagnetic susceptibility along the three axes in a molecule are not equal, most diamagnetic molecules are anisotropic. While the average magnetic susceptibility can be measured easily, the magnetic susceptibility tensor in a single crystal is dependent on the orientation of the three axes and is more difficult to measure. The magnetic susceptibility perpendicular to the plane of the ring is much greater than in the plane of the ring. Therefore, magnetic susceptibility anisotropy is another criterion for aromaticity.[6] However, χ_{anis} is only applicable to planar or nearly planar aromatic molecules and is useless for spherical systems. Another quantitative characteristic for aromaticity is magnetic susceptibility exaltation Λ (where χ_{m} is the experimentally determined molar susceptibility of the compound and $\chi_{\text{m}'}$ is the estimated molar susceptibility for the corresponding theoretical cyclic polyene).

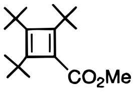
$$\Lambda = \chi_{\text{m}} - \chi_{\text{m}'}$$

A molecule is aromatic when $\Lambda < 0$ and antiaromatic when $\Lambda > 0$. Thus, benzene has $\Lambda = -13.4$ and naphthalene has $\Lambda = -28.2$.[3] In contrast, highly antiaromatic compounds such as cyclobutadiene and pentalene have positive magnetic susceptibility exaltation values ($\Lambda = 18.0$ and $\Lambda = 30.9$, respectively).[3] However, since the diamagnetic susceptibility exaltation (Λ) is highly dependent on the ring size, it requires suitable calibration.[7]

Schleyer et al.[8] has recently proposed the use of absolute magnetic shielding, computed at *ring centers* with available quantum mechanics programs as a new aromaticity/antiaromaticity criterion. NICS (nucleus-independent chemical shifts) values, which are the negative of the absolute magnetic shielding constants calculated at the ring or cage centers, have proven to be simple and efficient probes of aromaticity. Negative NICS values denote aromaticity (benzene, −11.5; naphthalene, −11.4; tropylium ion, −8.2) and positive NICS values denote antiaromaticity (cyclobutadiene, 28.8; heptalene, 21.7) while small NICS values (cyclohexane, −2.1; adamantane, −1.1) indicate nonaromaticity.[8] NICS values have the advantage that they are less dependent on ring size in contrast to the magnetic susceptibility exaltations.

Cyclobutadiene

Cyclobutadiene (**1**), the smallest annulene, has continued to attract the interest of both experimental and theoretical chemists.[9] According to theoretical and experimental evidence, cyclobutadiene (**1**) has a planar rectangular equilibrium structure with D_{2h} symmetry; the optimal square structure (D_{4h}) represents a transition state joining two equivalent minima on the potential energy surface.[1]



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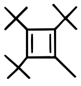

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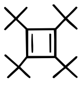

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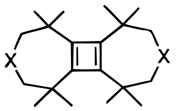

5a X = S
5b X = CH_2

Cyclobutadiene can be greatly stabilized by substituents. Some stable derivatives **2−5**[10] of cyclobutadiene have been synthesized and characterized. Several of these compounds have

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[†] Dedicated to Professor Waldemar Adam on the occasion of his 60th birthday.

[‡] Auburn University.

[⊥] Middle East Technical University.

[§] Ataturk University,

[||] Koç University.

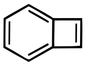
TABLE 1: Absolute Energies (hartrees), Zero-Point Energies (kcal/mol) and Relative Energies (kcal/mol) of *o*- and *p*-Quinone Fused with Cyclobutadienes (8a−c) and Benzocyclobutenes (9a−c)

compounds		HF/6-31G*//HF/6-31G*	ZPE[a]	B3LYP/6-31G*//B3LYP/6-31G*	HF/6-31G*	B3LYP/6-31G*	+ZPC[b]
cyclobutadiene	**1**	−153.641 17	41.68	−154.675 64			
benzene		−230.703 14	67.56	−232.248 65			
p-quinone		−379.235 57	58.00	−381.451 68	0.0	0.0	0.0
o-quinone		−379.221 35	57.97	−381.440 47	8.9	7.0	7.0
	6	−306.335 69	74.63	−308.360 33			
	7	−459.014 58	106.66	−462.032 00			
	8a	−454.897 09	65.39	−457.594 54	0.0	0.0	0.0
	8b	−454.842 31	64.65	−457.541 99	34.4	33.0	32.3
	8b′	−454.836 72	64.67	−457.541 95	37.9	33.0	32.3
	8c	−454.831 64	64.49	−457.535 73	41.1	36.9	36.0
	9a	−607.562 34	97.20	−611.252 28	0.0	0.0	0.0
	9b	−607.531 79	97.01	−611.221 47	19.2	19.3	19.1
	9b′	−607.461 55	96.30	−611.165 94	63.3	54.2	53.3
	9c	−607.521 27	96.95	−611.214 87	25.8	23.5	22.1

[a] Zero-point energy (kcal/mol) calculated at the HF/6-31G* level. [b] Relative energies at the B3LYP/6-31G* level with zero-point corrections at the HF/6-31G* level.

been subjected to X-ray analysis and do indeed show a clear alternation in bond lengths. The double bonds in the *tert*-alkyl cyclobutadienes (1.34 Å) are similar in length to that in ethene (1.33 Å), while the single bonds (1.60 Å), are markedly longer than that in ethane (1.54 Å). The chemical and physical properties of cyclobutadiene itself are also best explained as those of a rectangular singlet.[11]

1



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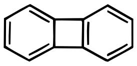
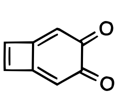
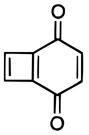


7

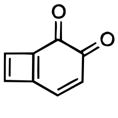
The cyclobutadiene unit **1** can be stabilized by incorporating one or both of the double bonds into a benzene ring. Benzocyclobutene (**6**)[12] and biphenylene (**7**)[13] are formally mono- and dibenzoderivatives of cyclobutadiene. Both **6** and **7** have overall 4n π-electrons and might therefore be expected to show antiaromatic behavior. This holds for benzocyclobutene, which can only be generated as a reactive intermediate,[14,15] but biphenylene is thermally stable and shows many of the properties associated with aromatic compounds. In this paper we discuss the NICS values of *p*- and *o*-quinone annulated cyclobutadiene and benzocyclobutene derivatives and the relationship between NICS values and antiaromaticity. We would like to determine the extent to which a quinone unit attached to cyclobutadiene and benzocyclobutene can stabilize the cyclobutadiene unit. To this effect, we have carried out calculations on **8** and **9**.



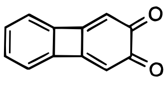
8a



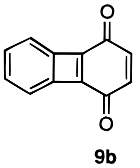
8b



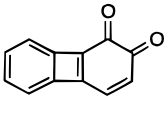
8c



9a



9b



9c

Computational Methods

Gaussian 94 was used throughout.[16] Geometries were first optimized at the HF/6-31G* level and frequencies calculated at that level. Using the HF/6-31G* geometries as starting guesses, structures were reoptimized at the B3LYP/6-31G* level. Total energies (hartrees) and relative energies (kcal/mol) are given in Table 1 while geometric parameters at the B3LYP/6-31G* level are given in Figure 1. Unless otherwise stated, relative energies given in the text will be at the B3LYP/6-31G*//B3LYP/6-31G*+ZPC/6-31G* level.

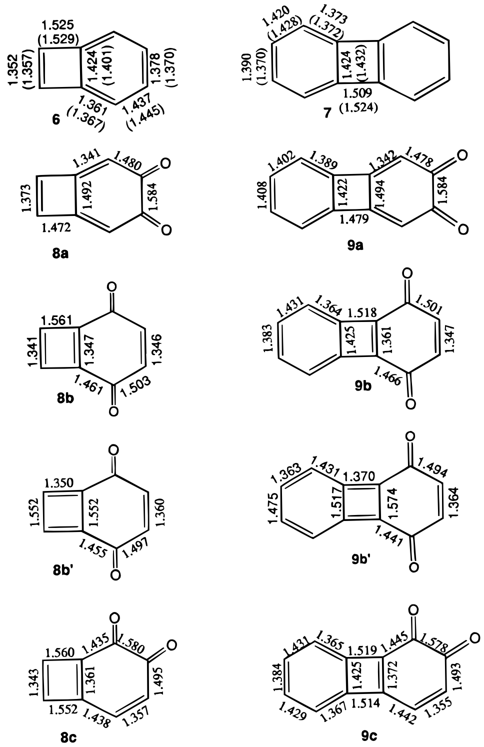


Figure 1. Geometric parameters for **6**, **7**, **8a-c**, and **9a-c** are given at the B3LYP/6-31G* level. Values in parentheses for **6**[20] and **7**[21] are experimental values.

Absolute NMR shielding values were calculated using the GIAO method[17] with the HF/6-31G* basis set at B3LYP/6-31G* optimized geometries. NICS values (Table 2) were obtained by calculating absolute NMR shielding at the ring centers (NICS(0)) and at 1 Å above the ring (NICS(1)). ^{13}C chemical shifts were obtained by relating the calculated absolute shielding to the experimental ^{13}C value of benzene (128.5 ppm).[18] Local shielding of nearby σ bonds complicate the analysis of the small-ring NICS values.[8] However, such local shielding is not a problem in larger, nonaromatic rings. The

TABLE 2: GIAO−SCF Calculated NICSs (ppm) for Cyclobutadiene and Benzocyclobutene Fused to *o*- and *p*-Benzoquinone (8a−c and 9a−c)[a]

	benzene ring		quinone ring		cyclobutadiene ring	
compounds	NICS(0)	NICS(1)	NICS(0)	NICS(1)	NICS(0)	NICS(1)
benzene	−11.5(−9.7)	−12.8				
p-quinone			7.4	0.1		
o-quinone			8.8	1.4		
cyclobutadiene (**1**)					25.8(27.6)	17.4
benzocyclobutene (**6**)	−4.2(−2.5)	−5.6			21.4(22.5)	12.1
8a			5.2	−0.8	3.3	−4.1
8b			5.8	−0.5	23.8	15.4
8b′			0.8	−3.7	25.1	16.7
8c			0.2	1.1	23.4	14.6
7	−6.5(−5.1)	−7.9			18.2(19.0)	8.5
9a	−10.6	−12.0	5.9	−0.2	4.5	−3.2
9b	−4.8	−6.1	6.0	−0.5	19.5	11.4
9c	−4.8	−6.2	7.1	0.4	19.5	11.0

[a] In parentheses are NICS at the HF/6-31+G* level at B3LYP/6-31G* optimized geometries from ref 8a.

maximum diatropic ring current effect for benzene is in the center of the ring, but is offset by the paratropic contributions of the CH and σ CC bonds. These paratropic effects fall off more rapidly than the diatropic effects away from the center, so that the maximum NICS value is about 0.8−1.0 Å above the ring.[19] Thus, the NICS(1) values minimize the paratropic effect and give a more reliable indication of aromaticity.

Results and Discussion

Since the geometries obtained at the HF/6-31G* level were similar to those obtained at B3LYP/6-31G*, we will discuss only B3LYP/6-31G* geometries below. The agreement between theory and experiment is good. For example, the B3LYP/6-31G* calculated distances deviate from experiment for **6** (X-ray of di-*tert*-butyltetramethyl derivative[20]) and **7** (gas-phase electron diffraction[21]) by usually only a few thousandths of an angstrom (Figure 1). Schulman and Disch[15] have recently studied **6** and a related valence isomer of **6**, the quinoid structure. They determined that the Hartree−Fock configuration was different for the two isomers and suggested that a barrier might exist between them. While **6** was favored over the quinoid structure by 47−52 kcal/mol (depending on level of theory), a synchronous transit based on MP2/3-21G geometries suggested that the quinoid structure should rearrange to **6** without barrier. However, Trahanovsky and Fischer[14] have measured the ^1H NMR chemical shifts of **6** and find them to be more consistent with the quinoid structure.

We have computed the fused-ring system between cyclobutadiene and quinone (**8a**−**c**) and between benzocyclobutene and quinone (**9a**−**c**). When *o*-quinone is fused at the 4,5 position to cyclobutadiene (to form **8a**) or to benzocyclobutene (to form **9a**), remarkably stable compounds result in which the antiaromaticity of the four-membered ring is dramatically reduced. While *o*-quinone is calculated to be 7.0 kcal/mol less stable than *p*-quinone, when cyclobutadiene is fused at the 4,5 position of *o*-quinone, the ortho isomer **8a** is 32.3 kcal/mol *more* stable than the para isomer **8b**. The total stability difference (39.3 kcal/mol), can be compared to the resonance destabilization energy in cyclobutadiene, estimated to be about 50 kcal/mol.[1] To a large extent the stability difference may be attributed to a reduction of antiaromatic destabilization.

When cyclobutadiene is fused to the 3,4 position of *o*-quinone, the resulting system (**8c**) does not enjoy enhanced stabilization. The ortho isomer **8c** is calculated to be 3.7 kcal/mol less stable than the para isomer **8b**, quite similar to the 7.0 kcal/mol energy difference between *o*- and *p*-quinone. In a similar fashion, the ortho isomer of fused benzocyclobutene−quinone (**9c**) is 3.0 kcal/mol less stable than the para isomer **9b**. Before exploring the enhanced stabilization of **8a** and **9a**, we turn to the question of resonance isomers.

As mentioned above, Schulman and Disch[15] were able to optimize a higher energy isomer of benzocyclobutene at lower levels of theory but concluded that the higher energy quinoid form would probably not exist at higher levels of theory. In the present study, all of the structures optimized with two exceptions (**8b′** and **9b′**) have a very short C═C bond opposite to the cyclobutadiene ring junction and are topologically related to the same isomer. Both exceptions (**8b′** and **9b′**) are confirmed to be minima at the HF/6-31G* levels. The structure **8b′** is calculated to have the same energy as its isomer **8b** (Table 2), which is in sharp contrast to the 50 kcal/mol separating the two isomers of **6**.[15]

The second isomer **9b′** is 43.2 kcal/mol higher in energy than **9b**. The long C−C bond in the four-membered ring of **8b′** opposite the ring junction (1.552 Å) does not present a favorable location for fusing a benzene ring to form **9b′**. Another way to view **9b′** is as the higher energy isomer of **6** fusing to *p*-quinone at the 2,3 position. In that case, the energy difference separating the two isomers of **6** (50 kcal/mol)[15] is reduced to 34.2 kcal/mol separating **9b** and **9b′**. It is possible that **9b′** will collapse without an activation barrier to **9b** at higher levels of theory. However, since the two isomers of **8b**/**8b′** have the same energy (Table 1), the existence of one form or two forms remains an open question.

Magnetic Properties

NICS(0) and NICS(1) values at the center of the benzene ring, quinone ring, and cyclobutadiene ring are given in Table 2. Negative values indicate aromaticity and positive values indicate antiaromaticity. The positive NICS(0) values for the quinone-ring are due to paratropic contributions of the CH and σ CC bonds, not antiaromaticity. The NICS(1) values are close to zero indicating little resonance stabilization. When cyclobutadiene is fused to benzene to form **6**, the NICS(1) value of the benzene ring becomes less negative (less aromatic: −12.8 → −5.6 ppm), while the NICS(1) value of the cyclobutadiene ring becomes less positive (less antiaromatic: 17.4 → 12.1 ppm). When cyclobutadiene is fused with two benzene rings to form biphenylene (**7**), the increase in the NICS(1) value of the benzene ring is less (−12.8 → −7.9 ppm), but the decrease in the NICS(1) value of the cyclobutadiene ring is greater (17.4

TABLE 3: Comparison of Calculated Bond Alternations in the Benzene and Cyclobutadiene Ring with Changes in NICS(0) and NICS(1) Values

	benzene ring			cyclobutadiene ring		
		ΔNICS (ppm)[b]			ΔNICS (ppm)[b]	
compound	bond alternation[a]	NICS(0)	NICS(1)	bond alternation[c]	NICS(0)	NICS(1)
cyclobutadiene (**1**)				0.245	0.0	0.0
benzene	0.0	0.0	0.0			
6	0.066(0.062)[d]	7.3	7.2	0.137(0.150)[d]	−4.4	−5.3
8a				0.040	−22.5	−21.5
8b				0.217	−2.0	−2.0
8b′				0.202	−0.7	−0.7
8c				0.202	−2.4	−2.8
7	0.042(0.058)[e]	5.0	4.9	0.085(0.092)[e]	−7.6	−8.9
9a	0.014	0.9	0.8	0.021	−21.3	−20.6
9b	0.059	6.7	6.7	0.125	−6.3	−6.0
9c	0.056	6.7	6.6	0.118	−6.3	−6.4

[a] Difference in angstroms between average of three long bonds and three short bonds in benzene ring. [b] Difference between NICS value in fused-ring system and NICS value in reference compound (either benzene or cyclobutadiene). [c] Difference in Å between average of two long bonds and two short bonds in cyclobutadiene ring. [d] Experimental value. Reference 20. [e] Experimental value. Reference 21.

TABLE 4: Calculated Reaction Energies (kcal/mol) for Fusing Cyclobutadiene or Benzocyclobutene to Benzene/Quinone

reaction		HF/6-31G*//HF/6-31G*	B3LYP/6-31G*//B3LYP/6-31G*	+ZPC[a]
1	**6** + *o*-quinone → benzene + **8a**	−27.1	−26.6	−26.3
2	**6** + *p*-quinone → benzene + **8b**	16.2	13.4	13.0
3	**6** + *o*-quinone → benzene + **8c**	14.0	10.3	9.8
4	**7** + **8a** → **6** + **9a**	8.6	8.7	8.5
5	**7** + **8b** → **6** + **9b**	−6.6	−4.9	−4.7
6	**7** + **8c** → **6** + **9c**	−6.7	−4.7	−4.3

[a] Relative energies at the B3LYP/6-31G* level with zero-point corrections at the HF/6-31G* level.

→ 8.5 ppm). Clearly, the reduction of antiaromaticity of the four-membered ring comes at the expense of loss of aromaticity in the six-membered ring.

The cause of the significant stabilization of **8a** (and **9a**) is revealed in the NICS values. The NICS(1) value of the cyclobutadiene-ring in **8a** has changed from 17.4 ppm (in **1**) to −4.1 ppm (in **8a**). The ring has become slightly aromatic! In **9a**, the NICS(1) of the cyclobutadiene ring changes from 17.4 ppm (in **1**) to −3.2 ppm. In contrast, the reduction of antiaromaticity in **8b**,**c** and **9b**,**c** is not nearly as large (Table 2).

Fusing a benzene ring to **8a** produces **9a**, where the aromaticity of the benzene ring remains virtually unchanged (NICS(1): −12.9 → −12.0 ppm). In **9b** and **9c**, the aromaticity of the benzene ring is reduced almost as much as found in benzocyclobutene (**6**). Presumably, the ring currents of the benzene rings in **9b** and **9c** are substantially disrupted in the presence of the fused four-membered ring.

Changes in NICS values as well as bond alternation between the long and short bonds of the benzene and cyclobutadiene rings are given in Table 3. Since all the bonds are equal in benzene, the bond alternation is zero. In cyclobutadiene, the short C=C bond (1.334 Å) and long C−C (1.579 Å) gives maximum bond alternation. Bond alternation increases in the six-membered ring and decreases in the four-membered ring when one or two benzene rings are fused to cyclobutadiene to form **6** and **7**, respectively. In addition, the computed bond alternations for **6** and **7** are in good agreement with experiment (Table 3). The computed bond alternation of the four-membered ring is drastically reduced in **8a** (0.245 → 0.040 Å) and in **9a** (0.245 → 0.021 Å), another indication of reduced antiaromaticity. In the benzene ring of **9a**, where aromaticity remains virtually unchanged, bond alternation is very small (0.014 Å), while it is much larger for the benzene rings of **9b** (0.059 Å) and **9c** (0.056 Å).

General

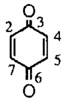
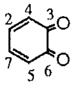
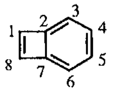
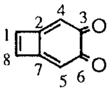
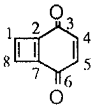
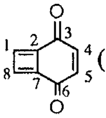
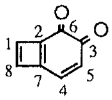
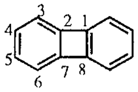
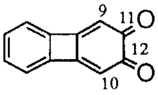
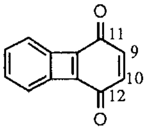
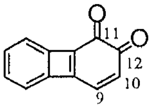
Herr[22] noted that formation of **8a** should be much easier than **8b** from the corresponding dihydroquinones due to the extra resonance stabilization in **8a**. While the isomer **8a** is unknown, the synthesis of isomer **8b**, 32.3 kcal/mol higher in energy, has been attempted.[23] We are currently attempting the synthesis of **8a**.

Of the three isomeric structures for biphenylenequinones containing one intact benzene ring, only isomer **9a**, containing a dimethylenecyclobutene group, has been synthesized and characterized so far.[24] The chemical reactivity of **9a** is completely in agreement with a decreased antiaromatic character of the cyclobutadiene ring. However, isomers **9b** and **9c** have cyclobutadiene units and are expected to be less stable than **9a**. Recent synthesis and trapping of **9b**[25] supports this finding. Attempts to observe **9b** even at lower temperatures (−70 °C) were unsuccessful. **9b** easily undergoes dimerization and Diels−Alder reactions with various dienophiles.

Six isodesmic reactions involving **8a**−**c** and **9a**−**c** are presented in Table 4. The first three reactions (1−3) show the preference of cyclobutadiene to fuse to benzene (to form **6**) or to fuse to quinone (to form **8a-c**). Reaction 1 to form **8a** is quite exothermic (−26.3 kcal/mol), which indicates that *o*-quinone stabilizes cyclobutadiene much better than benzene when fusion occurs at the 4,5 position. The second set of three reactions (4−6) shows the preference of benzocyclobutene to fuse to benzene (to form **7**) or to quinone (to form **9a**−**c**). The endothermicity of reaction 4 (8.5 kcal/mol) shows that **8a** is not significantly stabilized by fusing to a benzene ring.

The GIAO−SCF ^{13}C NMR absolute shieldings (ppm) have been converted to chemical shifts relative to the benzene which is given a chemical shift of 128.5 ppm (Table 5). Comparison of these values with the known chemical shifts indicates that the agreement is excellent. As mentioned above, the measured ^{1}H NMR chemical shifts of **6** were interpreted as supporting a

TABLE 5. Calculated (GIAO SCF) and Measured (in Parentheses) ^{13}C Chemical Shifts (ppm) of 6−9 and Parent Compounds[a]

Compounds	^{13}C Chemical Shifts[b]					
	1/8	2/7	3/6	4/5	9/10	11/12
Benzene[c]	128.5(128.5)					
		136.8(136.4)	187.0(187.0)			
		137.6(139.7)	179.2(180.4)	131.1(130.8)		
Cyclobutadiene	140.2					
 (6)	147.7	152.6	111.6	125.8		
 (8a)	151.7	154.7	178.0	111.1		
 (8b)	146.8	162.6	179.4	134.5		
 (8b′)	150.9	143.9	177.7	145.8		
 (8c)	160.5 131.4	138.4 187.3	181.2 165.3	127.9 138.5		
 (7)	152.5(151.9)		118.6(118.0)	128.0(128.8)		
 (9a)	154.4(156.9)	148.0(148.2)	129.0(124.6)	133.7(135.7)	114.2(116.3)	178.5(180.0)
 (9b)	164.8	149.3	137.6	128.4	135.7	180.8
 (9c)	149.0 179.0	153.8 144.8	115.5 120.0	132.0 124.7	129.4 136.5	169.3 180.7

[a] For references to experimental chemical shifts, see: ref 18. For **7**, see: Günther, H.; Tungal, B. D.; Regitz, M.; Scherer, H.; Keller, T. *Angew. Chem., Int. Ed. Engl.* **1971**, *10*, 563 and Günther, H.; Jikeli, G.; Schmickler, H.; Prestin, J. *Angew. Chem., Int. Ed. Engl.* **1993**, *12*, 762. For **9a**, see: Balci, M. Unpublished results. [b] Carbon positions (non IUPAC numbering) are given on the figure to the left. [c] Calculated absolute shielding of ^{13}C in benzene is referenced to the experimental value of 128.5 ppm.

quinoid structure which contradicts previous theoretical calculations as well as the present ones. If the ^{13}C NMR chemical shifts of **6** can be measured, a comparison with the calculated values in Table 5 may resolve this discrepancy. The calculated ^{13}C chemical shifts for **8b** and **8b′** in Table 5 are sufficiently different that the preferred resonance structure could be determined by a comparison with experiment. To that end, we are renewing our efforts to synthesize **8b**.

Conclusions

The fused ring systems between cyclobutadiene and quinone (**8a**−**c**) and between benzocyclobutene and quinone (**9a**−**c**) have been studied by computational methods. Energetic, structural and magnetic properties have been computed and compared. When *o*-quinone is fused at the 4,5 position to cyclobutadiene (**8a**) or benzocyclobutene (**9a**), a very stable compound is formed in which the antiaromaticity of the four-membered ring is completely eliminated. A second resonance structure (**8b′**, **9b′**) is calculated for **8b** and **9b** which is characterized by a different pattern of single and double C−C bonds. While **9b′** is much higher in energy than **9b**, the **8b** and **8b′** pair is calculated to have the same energy. Computed ^{13}C NMR chemical shift are reported and found to be in excellent agreement with available experimental data.

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Supporting Information Available: Cartesian coordinates for relevant structures optimized at the B3LYP/6-31G* level (5 pages). Ordering information is given on any current masthead page.

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