Violently Twisted and Strained Organic Molecules: A Descriptor System for Simple Coronoid Aromatics with a Möbius Half-Twist and Semiempirical Calculations on the Möbius Analogs of Coronene

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A systematic descriptor system for simple coronoid molecules containing a Möbius half-twist is proposed. The system relies upon the fact that a Möbius band has only one continuous perimeter, with neither an interior nor an exterior surface. From this property of a Möbius band follows the method for the unambiguous designation of each of the Möbius analogs of simple coronoids. The method involves the labeling of the interior and exterior perimeter atoms of the non-Möbius parent molecule and then using the same labels to distinguish the analogous perimeter atoms of the Möbius analogs of the parent coronoid. The result is an unambiguous, unique designation for each of the Möbius analogs of the coronoid under consideration. The descriptor system also allows the comparison of potentially distinct analogs and provides a method for the elimination of duplicate Möbius analogs of coronoids. The application of the descriptor system to coronene itself results in two unique Möbius analogs. We have investigated each Möbius coronene analog using the semiempirical method MNDO (modified neglect of diatomic overlap). Both analogs, although much less thermodynamically stable than coronene, are stable minima on the MNDO potential energy surface.

INTRODUCTION

We have developed an interest in those planar, annular aromatic systems which are classed as coronoids. Coronoids are molecules composed of fused benzenoid hexagons which have a "hole in the middle". That is, coronoids are molecules which are missing at least two fused (or adjacent) hexagons in the interior of the molecule.[1] Two such molecules are [12]-kekulene (1) and [18]kekulene (2), depicted in Figure 1.[2] These molecules are large enough, at least theoretically, to be "cut" and then given a half-twist so as to form a Möbius band.

How many chemically-distinct Möbius analogs of 1 can potentially exist? When we first considered this problem, we (incorrectly) assumed that only one such analog was possible, since all Möbius bands are *topologically* equivalent. Believing that only one Möbius analog of 1 existed, we christened that molecule "Möbius-[12]kekulene". Upon more careful examination of the parent molecule, we realized that there were, in fact, *four* potentially chemically-distinct Möbius topomers (which are, in fact, constitutional isomers, each giving rise to two stereoisomers) of 1.[5] The existence of four Möbius analogs made our original simple descriptive nomenclature ambiguous. It became necessary to develop an *unambiguous* descriptor system for these interesting molecules. Herein we describe that system and, in addition, semiempirical calculations on the two Möbius analogs of coronene.

METHODS FOR "CUTTING" AND TWISTING CORONOIDS

The descriptor system to be described at present can only be applied to simple coronoids, molecules in which each benzenoid hexagon is fused to two and only two other hexagons at non-adjacent edges. Such coronoids have only two general classes of carbon atoms, either to be found on the external or on the internal perimeters of the molecule. Thus, the descriptor system will apply to molecules such as 3 and 4 (Figure 2), but 3a, 3b, 4a, and 4b cannot yet be included as proper simple coronoids for the following discussion.

In simple coronoids as described above, benzenoid hexagons can be described by the two hydrogen atoms attached to each hexagon: the hydrogen atoms are either para or ortho to each other (Figure 3). In each type of hexagon, two types of "cuts" (bond breakings) are possible: Cutting or breaking carbon–carbon bonds separated by only one edge of the hexagon, as shown in the pathways labeled a in Figure 3, and cutting carbon–carbon bonds separated by two hexagon edges, as in the pathways labeled b. We refer to the former as "meta" bond cuts and the latter as "para" bond cuts. (There are, of course, two ways to cut either ring when cutting meta bonds or para bonds; these may or may not be equivalent depending upon the symmetry of the coronoid under consideration.)

Only the types of bond breaking described in Figure 3 will produce Möbius analogs of simple coronoids. Cuts at carbon–carbon bonds "ortho" to each other result in no discernable change after twisting and re-forming the bonds. Cuts (other than the ortho cuts described above) which involve carbon–carbon bonds involved in ring fusion also do not produce Möbius analogs of simple coronoids. These latter cuts, after twisting, alter the number of carbon atoms in the ring being cut, and the molecules which result cannot be considered to be Möbius analogs of the coronoid.[7]

Finally, after breaking bonds as in Figure 3, the coronoid is given a half-twist at the position of the broken bonds and the bonds are re-formed. Depending upon the direction of the half-twist, the resulting Möbius analog will either be right- or left-handed, but these right- and left-handed analogs will be enantiomeric mirror images if formed from an identical cutting procedure.

APPLICATION OF THE DESCRIPTOR SYSTEM

The system for uniquely describing each possible Möbius analog of a simple coronoid is derivable from a fundamental topological property of any Möbius band: A Möbius band has only one perimeter, with neither an "outside" nor an "inside" surface. The proper labeling of that monocyclic perimeter results in an unambiguous description of the specific

1

2
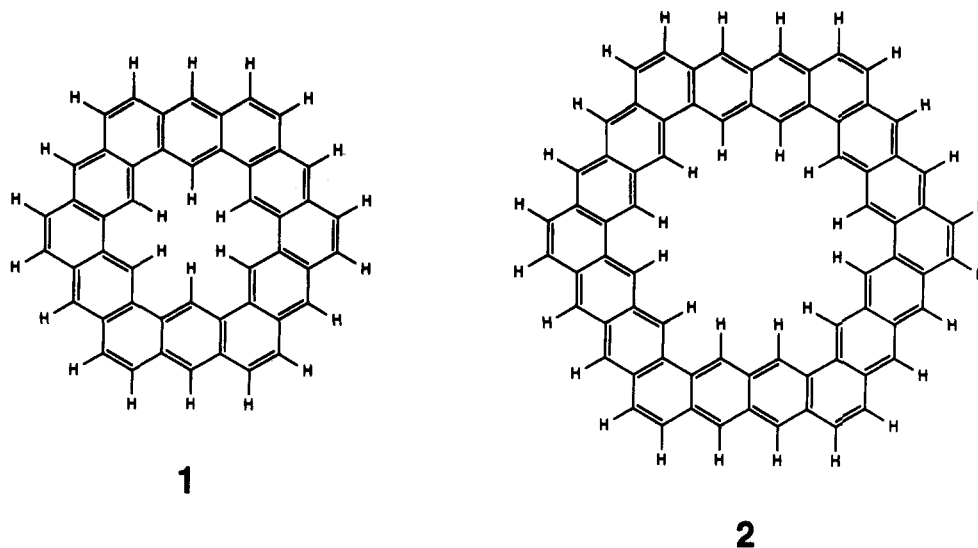
Figure 1. Two D_{6h}-symmetry simple coronoids: [12]kekulene (**1**) and [18]kekulene (**2**).

3   **4**

3a   **4a**

3b   **4b**
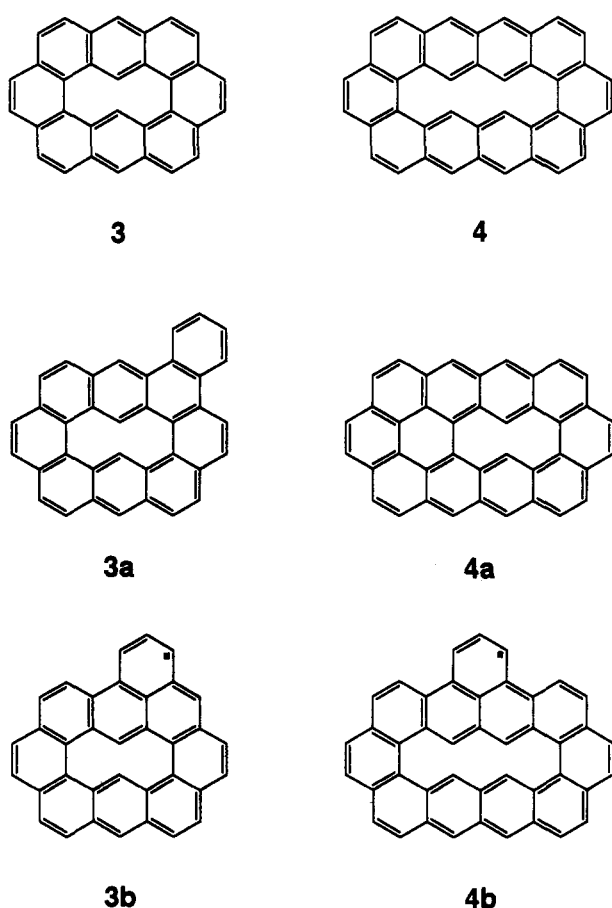
Figure 2. Two simple coronoids (**3** and **4**) and four coronoids (**3a**, **3b**, **4a**, and **4b**) which do not fit the definition of "simple".

Figure 3. Cutting and twisting simple coronoids.

Möbius analog under consideration. Further, this descriptor system allows any other potential Möbius analogs of a simple coronoid to be objectively tested for uniqueness and can be extended to include substituted as well as unsubstituted molecules.

To apply the descriptor system for Möbius analogs of molecules such as **1**, first consider the parent, planar, non-Möbius molecule. Classify each perimeter carbon atom[8] according to symmetry equivalent sets, just as is commonly done when classifying carbon atoms in a molecule prior to the interpretation of a ^{13}C-nuclear magnetic resonance spectrum.
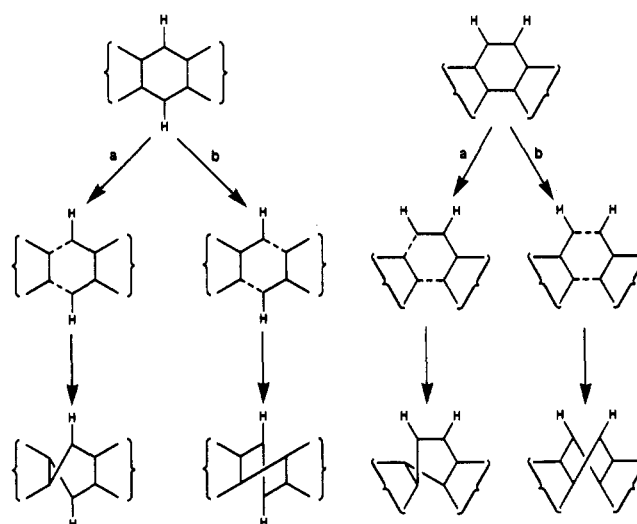
Assign upper-case letters to each class of carbon atoms (beginning with "A" and proceeding in alphabetical order).

Assign carbon atoms with attached hydrogen atoms priority over atoms without attached hydrogen atoms, and assign atoms in rings with ortho hydrogen atoms priority over rings with para hydrogen atoms. Use these assigned upper-case letters to label each perimeter carbon atom, consecutively, beginning with the external perimeter atoms, followed by the interior perimeter atoms. (This labeling is illustrated in the skeletal drawings of **1** and **1a–1d**, Figure 4).

Now perform the Möbius half-twist on the labeled molecule (without changing the labels on any of the perimeter atoms). Note that where there was once an inner perimeter and an outer perimeter, only one perimeter now exists in the Möbius molecule. (The total number of perimeter edges has not been altered. In **1**, there are 30 outer perimeter edges and 18 inner perimeter edges, while in **1a–1d**, there are 48 perimeter edges in each molecule.) Beginning with the atom on the "formerly external perimeter" nearest the position at which the half-twist was performed, list the labels for the atoms, in order, as a string of letters by following the edges along the perimeter. When a choice exists in the determination of the first letter of the string (as is the case for **1b**, "A" *versus* "B", and **1c** and **1d**, each with the choice of "B" *versus* "C", but is *not* the case with **1a**, where both twist atoms on the "formerly external
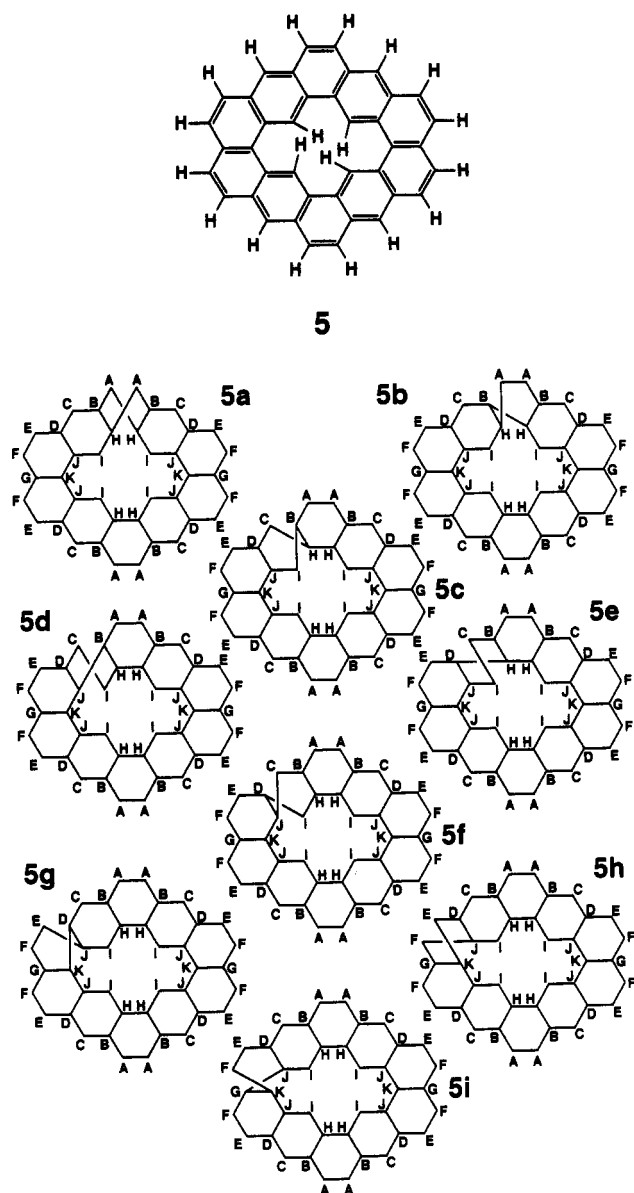
1a

(ABCBA)⁶(DED)⁶

1b

(AABCB)⁶(DED)⁶

1c

(BAABC)⁶(DDE)⁶

1d

(BAABC)⁶(EDD)⁶

Figure 4. Möbius analogs of [12]kekulene (1).

perimeter" are labeled "A"), begin with the perimeter atom whose label is the letter nearest the beginning of the alphabet. *This character string unambiguously and uniquely identifies the specific Möbius analog.* For the Möbius analogs of **1**, the strings are as follows:

1a: ABCBAABCBAABCBAABCBAABCBAABCB-
ADEDDEDDEDDEDDEDDED

1b: AABCBAABCBAABCBAABCBAABCBAABC-
BDEDDEDDEDDEDDEDDED

1c: BAABCBAABCBAABCBAABCBAABCBAAB-
CDDEDDEDDEDDEDDEDDE

1d: BAABCBAABCBAABCBAABCBAABCBAAB-
CEDDEDDEDDECDEDDEDD

Because the string for the perimeter of any Möbius analog is monocyclic and continuous, it is unimportant exactly where on the molecule the string of characters begins. However, beginning with one of the perimeter atoms which is on the "formerly external perimeter" nearest the twist and which is the letter nearest the beginning of the alphabet produces a string which is most obviously and easily abbreviated to a manageable length. (For molecules with moderately high symmetries, the strings always contain repeating units of labeled atoms. The strings for molecules of low symmetry, or substituted analogs of high symmetry parent molecules, will not be able to be abbreviated.) For the Möbius analogs of **1**, the abbreviated strings are as follows:

1a: (ABCBA)⁶(DED)⁶   **1b:** (AABCB)⁶(DED)⁶

1c: (BAABC)⁶(DDE)⁶   **1d:** (BAABC)⁶(EDD)⁶

Note that it is impossible to convert the string of **1a** into the string for **1b** (or **1c** or **1d**) without physically rearranging the labels on the atoms (which is the equivalent of breaking and re-forming bonds in the molecule). From these abbreviated strings, it becomes nearly trivial to distinguish between the originally apparently indistinguishable Möbius analogs of **1**.

Extrapolation of this systematic nomenclature to other molecules is straightforward. For example, [18]kekulene (**2**) has six unique Möbius analogs, **2a–2f**, as shown in Figure 5. The abbreviated strings for each of the Möbius analogs of **2**

2a

2b

2c

2d

2e

2f

Figure 5. Möbius analogs of [18]kekulene (2).

5

Figure 6. (a) D_{4h}-symmetry coronoid (**5**). (b) Nine Möbius analogs of **5**.

are easily determined to be as follows:

2a: $(ABCDCBA)^6(EFGFE)^6$

2b: $(AABCDCB)^6(EFGFE)^6$

2c: $(BAABCDC)^6(FEEFG)^6$

2d: $(BAABCDC)^6(EEFGF)^6$

2e: $(CBAABCD)^6(EEFGF)^6$

2f: $(CBAABCD)^6(FEEFG)^6$

Since both [12]kekulene and [18]kekulene are highly symmetric (formally D_{6h}) molecules, they might not be thought to be representative of other, less symmetrical arrangements of fused annular aromatic coronoid systems. However the systematic nomenclature described can be applied to molecules of lower symmetry in an identical manner to that employed for **1** and **2**. As an example, consider **5**, a D_{4h}-symmetry coronoid which has a total of nine Möbius analogs, **5a–5i**, as shown in Figure 6. The strings and their abbreviations for these nine Möbius molecules are immediately derivable from the structures and in abbreviated form are as follows:

5a: $(ABCDEFGFEDCBA)^2(HIJKJIH)^2$

5b: $(AABCDEFGFEDCB)^2(HIJKJIH)^2$

5c: $(BAABCDEFGFEDC)^2(HHIJKJI)^2$

5d: $(BAABCDEFGFEDC)^2(IHHIJKJ)^2$

5e: $(CBAABCDEFGFED)^2(HHIJKJI)^2$

5f: $(CBAABCDEFGFED)^2(IHHIJKJ)^2$

5g: $(DCBAABCDEFGFE)^2(JIHHIJK)^2$

5h: $(EDCBAABCDEFGF)^2(JIHHIJK)^2$

5i: $(FEDCBAABCDEFG)^2(JIHHIJK)^2$

An even less symmetrical coronoid is **6**, an isomer of **1** with one benzenoid hexagon rearranged so as to produce a C_{2v}-symmetry molecule. Coronoid **6** has 21 Möbius analogs! Again, each of these analogs is uniquely defined by the monocyclic perimeter of the Möbius band. Because of the lowered symmetry of **6**, the strings for these Möbius analogs cannot be abbreviated. The complete strings for the 21 Möbius analogs of **6** are listed below:

6a: ABCDEFGHIJKLMNOONMLKJIHGFEDCB-
APQRSTUVWXXWVUTSRQP

6b: AABCDEFGHIJKLMNOONMLKJIHGFEDC-
BPQRSTUVWXXWVUTSRQP

6c: BAABCDEFGHIJKLMNOONMLKJIHGFEDC-
PPQRSTUVWXXWVUTSRQ

6d: BAABCDEFGHIJKLMNOONMLKJIHGFEDC-
QPPQRSTUVWXXWVUTSR

6e: CBAABCDEFGHIJKLMNOONMLKJIHGFE-
DPPQRSTUVWXXWVUTSRQ

6f: CBAABCDEFGHIJKLMNOONMLKJIHGFED-
QPPQRSTUVWXXWVUTSR

6g: DCBAABCDEFGHIJKLMNOONMLKJIHGFE-
RQPPQRSTUVWXXWVUTS

6h: EDCBAABCDEFGHIJKLMNOONMLKJIHGF-
RQPPQRSTUVWXXWVUTS

6i: FEDCBAABCDEFGHIJKLMNOONMLKJIHG-
RQPPQRSTUVWXXWVUTS

6j: GFEDCBAABCDEFGHIJKLMNOONMLKJIH-
SRQPPQRSTUVWXXWVUT

6k: GFEDCBAABCDEFGHIJKLMNOONMLKJIH-
TSRQPPQRSTUVWXXWVU

6l: HGFEDCBAABCDEFGHIJKLMNOONMLKJI-
SRQPPQRSTUVWXXWVUT

6m: HGFEDCBAABCDEFGHIJKLMNOONMLKJ-
ITSRQPPQRSTUVWXXWVU

6n: IHGFEDCBAABCDEFGHIJKLMNOONMLKJ-
UTSRQPPQRSTUVWXXWV

6o: JIHGFEDCBAABCDEFGHIJKLMNOONMLK-
UTSRQPPQRSTUVWXXWV

6p: KJIHGFEDCBAABCDEFGHIJKLMNOONM-
LUTSRQPPQRSTUVWXXWV

6q: LKJIHGFEDCBAABCDEFGHIJKLMNOONM-
     VUTSRQPPQRSTUVWXXW

6r: MLKJIHGFEDCBAABCDEFGHIJKLMNOON-
     VUTSRQPPQRSTUVWXXW

6s: NMLKJIHGFEDCBAABCDEFGHIJKLMNOO-
     VUTSRQPPQRSTUVWXXW

6t: ONMLKJIHGFEDCBAABCDEFGHIJKLMNO-
     WVUTSRQPPQRSTUVWXX

6u: ONMLKJIHGFEDCBAABCDEFGHIJKLMNO-
     XWVUTSRQPPQRSTUVWX

THE PROBLEM OF ADJACENT TWISTS

Careful examination of **1b** and **1c** in Figure 4 appears to indicate that forcibly untwisting the half-twist in **1b** will result in the twist moving to the para-hydrogen ring adjacent to the originally-twisted ortho-hydrogen ring. The result of such an untwisting will apparently be the conversion of **1b** into **1c**. In drawings on paper such an operation appears to be straightforward and indicates that **1b** and **1c** are not truly isomers.

When models of either **1b** or **1c** are constructed, however, such an operation as described above becomes akin to the conversion of *cis*-2-butene into *trans*-2-butene: The conversion can be made to occur, but the energy barrier to conversion is large enough that the isomers do not readily interconvert. Although no double bond breaking or re-formation is necessary to convert **1b** into **1c** (or *vice versa*) models make such a conversion also appear to be a high-energy process.

Models, however, are not conclusive in a conversion such as this **1b** to **1c** concurrent untwisting and twisting. Another important factor to consider is atom connectivity. In **1b**, at the twist, an "A" carbon is attached to an "E" carbon and a "B" carbon is attached to a "D" carbon (regardless of the direction of the half-twist), while in **1c**, at the twist, a "B" carbon is attached to an "E" carbon, and a "C" carbon is attached to a "D" carbon (again, regardless of the direction of the twist). These connectivities also suggest that **1b** and **1c** are unique isomers.

Finally, although our data are not yet complete and conclusive (for example, the calculations of vibrational frequencies are not yet finished for all molecules), semiempirical studies of **1** indicate that indeed four distinct analogs of **1** are to be found on the relevant MNDO potential energy surfaces.

APPLICATION OF THE DESCRIPTOR SYSTEM TO CORONENE

The simplest seemingly coronoid-type molecule, coronene (**7**), is not actually a coronoid, as **7** has no "hole in the center" (is not missing two or more fused benzenoid hexagons in the interior of the molecule). Coronene, although the molecule from which the coronoids take their name, is a *pseudo*-coronoid.[1] Even so, **7** has two Möbius analogs, and these analogs may be designated using the nomenclature described above. The abbreviated strings for coronene follows naturally from the application of the descriptor system and are as follows:
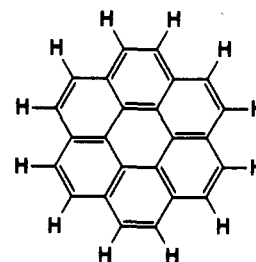
7a: (ABA)⁶C⁶   **7b**: (AAB)⁶C⁶

SEMIEMPIRICAL CALCULATIONS ON THE MÖBIUS ANALOGS OF CORONENE

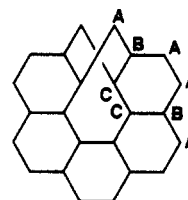**Methods.** Semiempirical calculations using the MNDO[10] (modified neglect of diatomic overlap) method were carried
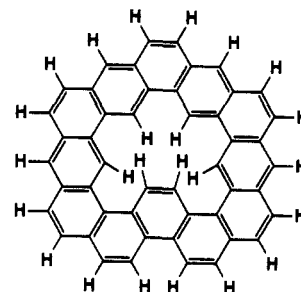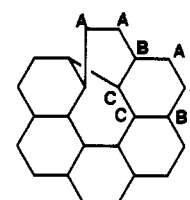

Figure 7. C_{2v}-symmetry coronoid (**6**) with 21 Möbius analogs.

7

7a   **7b**

(ABA)⁶C⁶   **(AAB)⁶C⁶**

Figure 8. Coronene (**7**) and its Möbius analogs.

Table 1. MNDO-Calculated Properties of the Two Möbius-Analogs of Coronene

property	[(AAB)⁶C⁶] "ortho" (7b)	[(ABA)⁶C⁶] "para" (7a)
heat of formation (kcal/mol)	252.8	301.7
HOMO energy (eV)	−7.289	−7.306
LUMO energy (eV)	−1.781	−1.943
dipole moment (D)	5.111	5.111
zero point vibrational energy (kcal/mol)	185.0	184.3
at 298 K and 1 atm		
translational enthalpy (kcal/mol)	0.889	0.889
rotational enthalpy (kcal/mol)	0.889	0.889
vibrational enthalpy (kcal/mol)	191.0	191.3
translational entropy (cal/(K·mol))	42.99	42.99
rotational entropy (cal/(K·mol))	33.87	32.46
vibrational entropy (cal/(K·mol))	37.96	38.03

out using the SPARTAN[11] suite of programs running on a Silicon Graphics Iris Indigo workstation. Full geometry optimizations without the imposition of any symmetry constraints were carried out. The initial trial geometries (ITGs) were built using the "front-end" force-field minimization routine of the Spartan package, at the "expert" level, before submitting the molecule for optimization under the MNDO method.

Results and Discussion. Table 1 contains the MNDO-calculated ground-state properties for the two Möbius analogs of coronene. For comparison, the properties of the parent molecule, coronene, were also calculated using the MNDO

Table 2. MNDO-Calculated Vibrational Frequencies for the Two Möbius Analogs of Coronene

[(AAB)^{6}C^6]-Möbius-Coronene (7b)					
93.25	99.56	139.71	169.30	224.53	238.52
259.00	289.85	304.83	350.94	368.55	377.68
396.07	399.87	412.08	444.20	474.16	505.16
520.38	551.58	561.79	573.84	580.40	600.93
624.48	635.47	671.92	681.91	696.62	713.95
722.07	763.38	777.26	803.05	836.39	855.67
862.73	880.87	897.17	902.33	915.28	918.14
935.53	952.53	985.33	994.66	1016.16	1018.68
1026.59	1034.59	1044.41	1051.05	1098.30	1117.27
1151.91	1161.52	1188.31	1199.48	1211.59	1230.18
1241.32	1272.78	1285.94	1301.12	1308.90	1326.88
1331.06	1352.13	1369.87	1389.63	1421.64	1428.31
1443.48	1467.95	1481.50	1510.57	1545.77	1560.65
1573.56	1662.71	1683.97	1700.77	1724.87	1732.08
1744.04	1749.55	1757.81	1786.69	1813.55	1926.32
3390.95	3393.46	3399.13	3399.27	3403.26	3403.81
3411.66	3414.33	3418.34	3429.34	3449.92	3463.01
[(ABA)^{6}C^6]-Möbius-Coronene (7a)					
86.93	93.82	175.42	192.06	217.79	241.80
267.26	290.80	309.38	317.65	368.73	376.92
393.44	394.19	413.41	460.95	463.22	470.92
503.41	523.67	527.90	565.96	569.32	603.90
620.62	648.31	649.20	693.29	697.04	718.14
727.26	759.82	782.24	786.59	811.39	845.94
858.20	879.45	886.37	896.21	909.88	917.88
929.57	943.39	949.94	972.12	1008.63	1009.25
1025.54	1044.23	1049.71	1049.89	1078.96	1125.48
1148.33	1168.35	1191.51	1236.33	1242.34	1253.94
1266.60	1273.49	1279.70	1298.49	1303.60	1329.95
1341.09	1345.73	1353.86	1379.83	1399.58	1403.25
1437.09	1451.01	1465.50	1503.04	1514.07	1515.74
1652.33	1653.63	1706.41	1710.27	1724.83	1728.63
1750.56	1759.66	1768.12	1779.42	1779.54	1790.44
3390.91	3391.67	3392.23	3401.48	3410.49	3411.17
3416.44	3416.52	3418.94	3418.95	3425.46	3426.07

Figure 9. [(AAB)^{6}C^6]-Möbius-coronene (7b). Open circles represent carbon atoms; solid circles represent hydrogen atoms.

Figure 10. [(ABA)^{6}C^6-Möbius-coronene (7a). Open circles represent carbon atoms; solid circles represent hydrogen atoms.
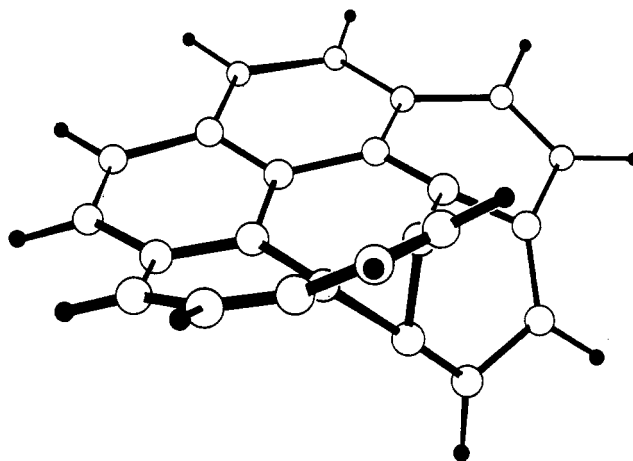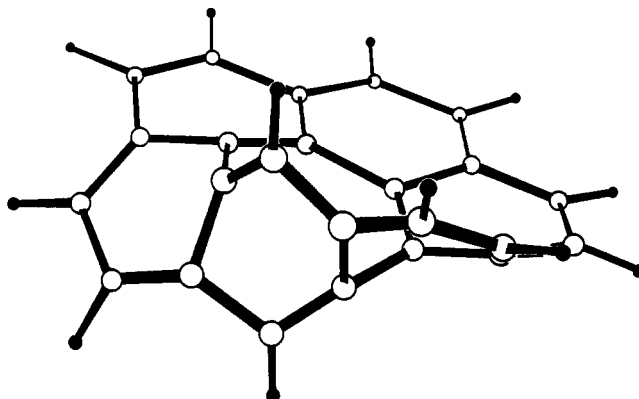
method. Under these computational conditions, with D_{6h} symmetry imposed, coronene was calculated to have a heat of formation of +83.063 kcal/mol. Thus, an intuitively expected, both Möbius analogs are significantly higher energy molecules than coronene, but the analog in which the hydrogen atoms remain *ortho* to each other after the half-twist is applied is more stable than the analog in which these hydrogens become *para* to each other after the half-twist has been applied (the difference between them is 48.9 kcal/mol).

The highest occupied molecular orbital (HOMO) for coronene was doubly degenerate at an energy of –8.077 eV, while the lowest unoccupied molecular orbital (LUMO) was also doubly degenerate at an energy of –1.013 eV. For the Möbius analogs of coronene, both the HOMO and LUMO are singly degenerate, as expected from the lack of imposed symmetry during the calculation (or, conversely, the imposition of C_1 symmetry).

The calculated vibrational frequencies for the two Möbius analogs of coronene are listed in Table 2; all vibrational frequencies are real, indicating that each of these molecules is a true minimum on the respective MNDO potential energy surface.

Figures 9 and 10 are pictorial representations of respectively [(AAB)^{6}C^6]-Möbius-coronene (7b, the "ortho" analog) and [(ABA)^{6}C^6]-Möbius-coronene (7a, the "para" analog). In each figure, the ring with the half-twist is in the foreground of the figure.

From Figures 9 and 10, some generalizations can be drawn. The ring with the half-twist in molecule 7b (Figure 9) is shaped much like a "chaise lounge" with a remarkably flat "seat". In 7a the twisted ring has a "twist-boat" conformation similar to the analogous cyclohexane conformer. Remarkably, in both

cases, the untwisted remainder of each molecule remains reasonably flat. Further, for rings which are distorted because of the half-twist in the shaded portion of the molecule, each distorted ring appears to favor preventing the distortion from spreading over the complete molecule. In other words, the distortions induced by the half-twist remain localized near the ring with the Möbius half-twist, and the remainder of the molecule attempts to maintain planarity.

POTENTIAL FLUXIONALITY OF MOBIUS CORONOIDS

Does the possibility of fluxionality exist for coronoids with a Möbius half-twist? If so, the chemical environment of the hydrogen atoms on the single perimeter of the molecule will change with time. Through studies of models and because of the computational results (*vide supra*), such fluxionality is probably impossible for the Möbius analogs of coronene or [12]kekulene.

Although no formal calculations have as yet been carried out for [18]kekulene or for higher kekulenes, depending upon the type of model used (and the flexibility of the model), the question remains open. By the time [24]kekulene or [30]-kekulene is reached, the molecules appear to become quite flexible, and some fluxionality appears to be possible.

The nature of fluxionality in Möbius analogs of large coronoids may actually involve the types of twisting earlier discussed with respect to potential conversions of one Möbius analog to another by forcibly untwisting and twisting an analog without bond breaking. The half-twist in these molecules may "move" around the molecule under appropriate circum-

stances such that the relative positions of the hydrogen atoms in the molecule become averaged on a certain time scale. This movement of the half-twist does not interconvert isomers but does in fact alter the chemical environment of inner and outer atoms in the molecule over time.

CONCLUSIONS

A descriptor system for the unambiguous designation of simple coronoid molecules with a Möbius half-twist has been described, and the system has been applied to a variety of such coronoids. The system allows Möbius analogs of coronoids to be evaluated for uniqueness, and also allows the number of Möbius analogs of a coronoid to be determined.

The two Möbius analogs of coronene, **7a** and **7b**, have been examined using the MNDO computational method. Both analogs are true, stable minima on the appropriate MNDO potential energy surface. The Möbius analog (**7b**) in which the hydrogen atoms attached to the ring with the half-twist remain *ortho* to each other is more stable than the analog (**7a**) in which these hydrogen atoms are twisted into a *para* configuration.

ACKNOWLEDGMENT

REFERENCES AND NOTES

(1) Cyvin, S. J.; Gutman, I. *Kekulé Structures in Benzenoid Hydrocarbons*; Lecture Notes in Chemistry 46; Springer-Verlag: Berlin, 1988; pp 9–10.

(2) The name of this molecule (**1**) "kekulene", was suggested by Professor Heinz Staab of the Max-Planck-Institute in Heidelberg.[3] Professor Staab also demonstrated the first unequivocal synthesis of kekulene, in 1978.[4] While we have no desire to usurp the privilege of experimental chemists to name their synthetic targets, we believe that the term kekulene may be applied to other members of a series of hexagonal symmetry molecules (benzene rings of benzene rings) which begins with Professor Staab's kekulene (as [12]kekulene, **1**), followed by [18]kekulene (**2**), then [24]-kekulene, [30]kekulene, etc. While there is no compelling reason to do so, with this system, benzene could be referred to as [1]kekulene and coronene as [6]kekulene.

(3) Nickon, A.; Silversmith, E. F.; *Organic Chemistry: The Name Game. Modern Coined Terms and Their Origins.* Pergamon: Oxford, U.K., 1987; pp 129–130.

(4) (a) Diederich, F.; Staab, H. A. *Angew. Chem., Int. Ed. Engl.* **1978**, *17*, 372. (b) Staab, H. A.; Diederich, F. *Chem. Ber.* **1983**, *116*, 3487.

(5) There are four Möbius analogs of **1** if stereochemistry is ignored. Each Möbius analog exhibits a "handedness" in the same way that a screw or helix exhibits handedness, and this right- or left-handedness may be described according to already existing rules for these types of chiral structures.[6] According to these rules, Möbius analogs which are "right-handed" enantiomers would be so designated with an upper-case Greek letter Δ, while the "left-handed" enantiomers would be designated with an upper-case Greek letter Λ.

(6) Purcell, K. F.; Kotz, J. C. *Inorganic Chemistry*; Saunders: Philadelphia, PA, 1977; pp 636–644 and especially Figure 11–5, p 639. In addition, see: *Nomenclature of Organic Chemistry*; Pergamon: Elmsford, NY, 1979.

(7) Specifically, a Möbius analog of a coronoid remains composed of six-membered benzenoid hexagons and is derived from the parent coronoid by the act of cutting and, after performing a half-twist, re-forming bonds as described in the text. If the carbon–carbon bonds involved in ring fusion are cut, the resulting molecule will not be composed solely of six-membered benzenoid hexagons.

(8) This method is applied here only to purely hydrocarbon molecules, but can easily be extended to include any type of perimeter atom by simply including *all* perimeter atoms in the initial classification of atoms. (When heteroatoms substitute for carbon atoms in the framework of the coronoid, the Cahn-Ingold-Prelog[9] system of priority for labelling atoms should be applied.) Since such hetero-substituted molecules will usually be less symmetric than the parent unsubstituted molecule, the strings for such molecules may not be able to be abbreviated.

(9) Cahn, R. S.; Ingold, C.; Prelog, V.; *Angew. Chem. Int. Ed. Engl.* **1966**, *5*, 385.

(10) Dewar, M. J. S.; Thiel, W.; *J. Am. Chem. Soc.* **1977**, *99*, 4899.

(11) Wavefunction, Inc., 18401 Von Karman, Irvine, CA 92715.