Supplementary Information - The Polarization of Polycyclic Aromatic Hydrocarbons Curved by Pentagon Incorporation: The Role of the Flexoelectric Dipole

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S1. Strained corannulene

Electronic structure calculations were performed on a set of corannulene structures with constrained and equilibrium geometry (which we have previously applied to studying the strained induced coalescence of fullerenes[1]). The constrained variable was the internal dihedral angle ϕ between the pentagonal and the hexagonal rings (as shown in Figure S1). All other coordinates were optimized for geometries of varying ϕ ranging from 180° to 140° in 2° increments. Three of the constrained and optimized structures are shown in Figure S1. The total pyramidalization angle, $\boldsymbol{\theta}_{\text{tot}} = \sum_{\text{C}_{\text{hub}}} \theta_{\text{p}} \mathbf{v}_{\pi}$, was then computed (compare to Eq. 3). The magnitude of the dipole moment μ was calculated at the B3LYP/cc-pVQZ level of theory using the Gaussian 09 software.[2] The dependence of μ on θ_{tot} is shown in Figure S1. The linear model Eq. 3 is shown for comparison, with slope $f_{\theta_{\text{p}}} = 2.24$ D/rad, as determined in Figure 5. As seen, the dependence of μ on θ_{tot} shows non-linearity even at rather small values of the angle and the success of Eq. 3 seems to be due to fortuitous cancelation of effects at larger pyramidalization.

The ELF of the flat ($\phi = 180°$) and the relaxed ($\phi = 152.9°$) corannulene structures are compared in Figure S2. This figure clearly shows the squeezing of electron density to the convex side of the molecule and the resulting greater localization there.

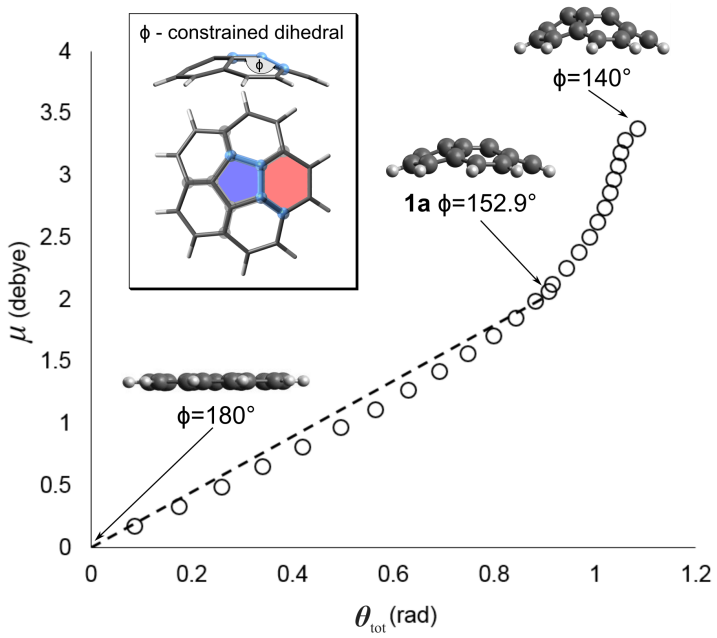

Figure S1: The magnitude of the dipole moment of the strained corannulene geometries are plotted versus the total pyramidalization angle $\boldsymbol{\theta}_{\text{tot}}$. The dihedral angle which is constrained in the geometry optimization is shown in the boxed inset. Three of the geometries with their corresponding dihedral angles are inset. The dashed line corresponds to Eq. 3.

S2. Distributed multipole expansion

The AIM analysis was performed on corannulene and dicircumcorannulene using the Multiwfn program[3] using a grid spacing of 0.06 Bohr. Figure S3 shows a xy cross section through the molecules. The blue lines show the interface of the two atomic volumes in cross section calculated using the AIM method.

As the flexoelectric dipole moment has been found in this study to be important, the atom-centered dipoles were compared between the GDMA(C_2H_2) method and the AIM method as the benchmark. For the molecule corannulene **1a**, the flexoelectric dipoles at the hub of the molecule were of similar magnitude (<10%) and direction for the different decompositions. Figure S4 shows a vector representation of the atom-centered dipole moments for dicircumcorannulene **1b** using two variants of GDMA, where the length is proportional to the magnitude of the moment. The GDMA(C_2H_2) method produces dipoles at the hub C atoms that are 40-50% larger than the AIM method, Figure S4a. In addition, it produces

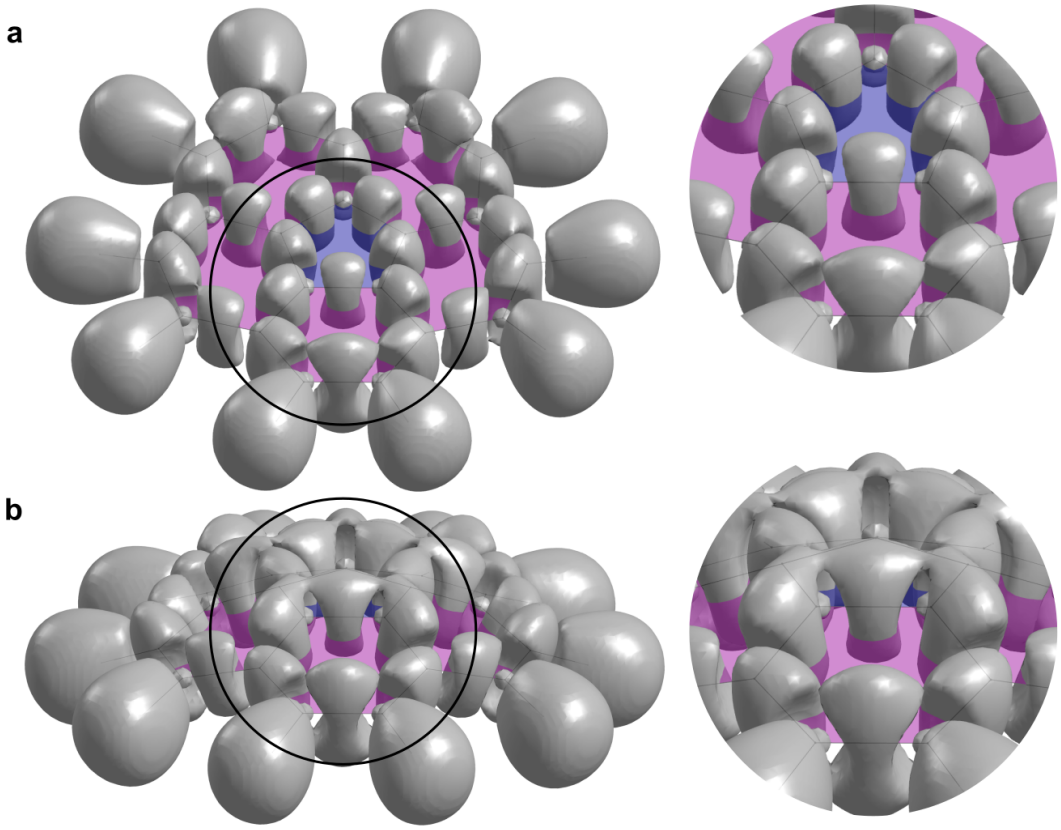

Figure S2: Plot of the iso-surfaces of the electron localization function for corannulene **1a** at iso=0.66 for a) flattened and b) relaxed corannulene. Insets on the right are expanded views near the π bonding region at the hub showing the asymmetry of the bond.

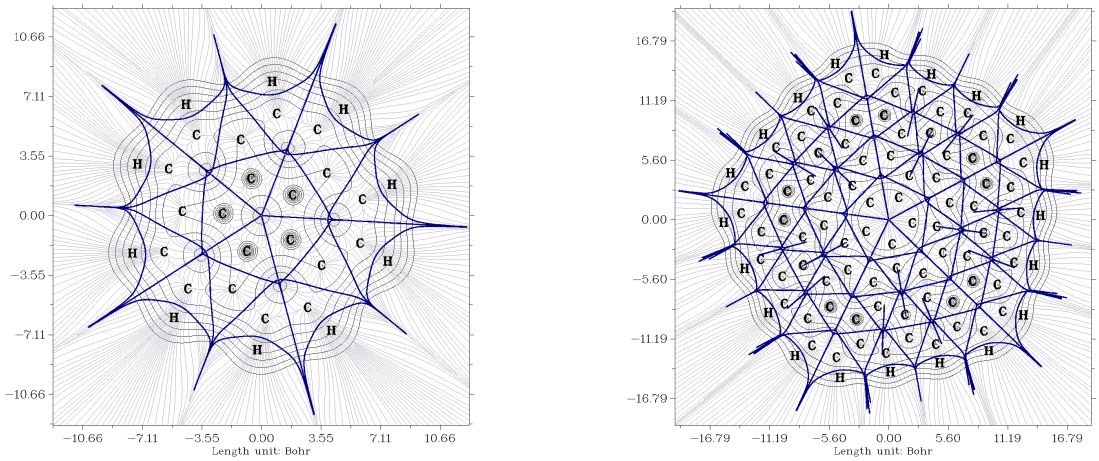

Figure S3: Cross section of the molecular volumes/basins calculated using the atoms in molecules approach for the molecules **1a** and **1b**.

a very high dipole moment at the hydrogen atoms (in addition to the positive point charge) that has no intuitive physical explanation. The second variant of the Gaussian distributed multipole decomposition, GDMA(C_2H_0), is with multipole rank at the H atoms set to 0 (point charges only). GDMA(C_2H_0) compares very well with the "benchmark" AIM multipoles, Figure S4b and produces intuitively reasonable values of the point charges and dipoles, as discussed in Section 4.

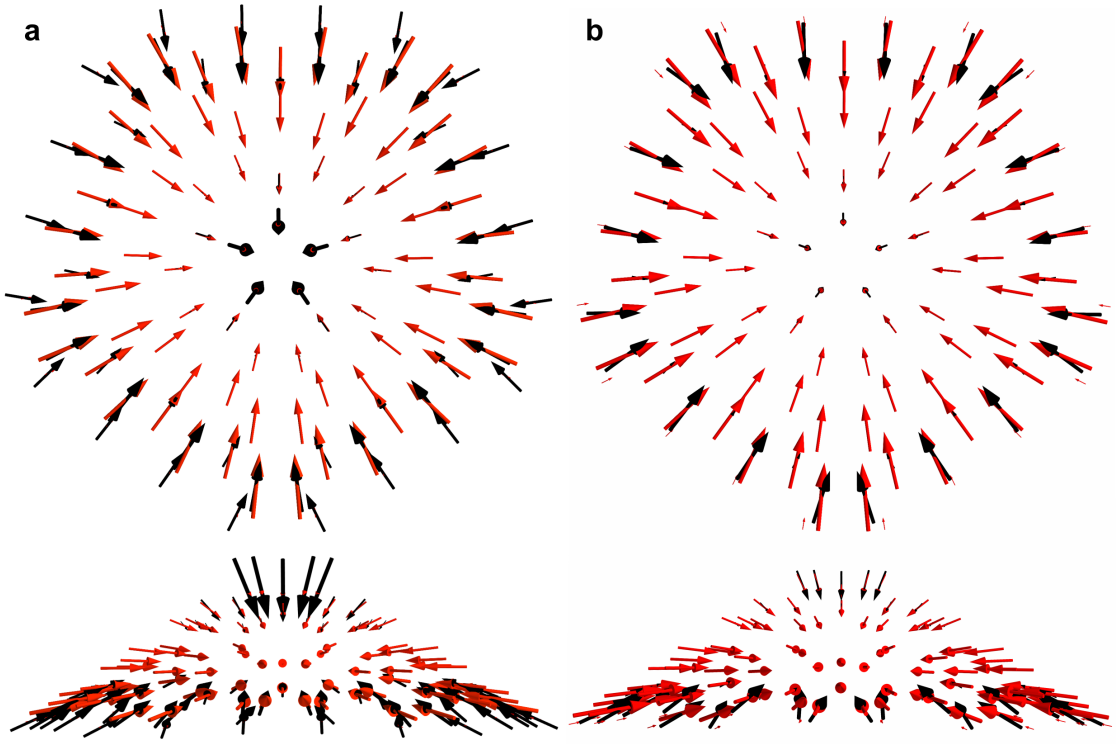

Figure S4: Atom-centered dipole moments plotted as vectors for circum-2-corannulene calculated using the AIM approach (red arrows) and the GDMA method (black arrows). In a, GDMA(C_2H_2) is shown with rank=2 multipoles on all atoms, hydrogens included. In b, the GDMA(C_2H_0) dipoles are given, where restricted expansion (rank=0) of the atomic multipoles on the hydrogen atoms is utilized.

S3. Geometries

Coordinates are in Å
Dipole moments (x, y and z components) are in debye

1a
30
0.0004 0.0012 -2.0616
C 1.01982 0.64144 0.62896
C 0.92512 -0.77156 0.62898
C -0.44785 -1.11828 0.62895
C -1.20187 0.08047 0.62912
C -0.29484 1.16799 0.62928
C 2.10034 1.32116 0.09730
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C 3.12803 -0.90428 -0.25919
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C 0.10664 -3.25438 -0.25952
C -0.92266 -2.30349 0.09781
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C -3.06214 -1.10706 -0.25898
C -2.32384 -2.28087 -0.25903
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H 0.38806 4.22195 -0.62457
H 2.63370 3.32275 -0.62478
H 4.13569 0.93517 -0.62442
H 3.97386 -1.47822 -0.62441
H 2.16722 -3.64330 -0.62658
H -0.17772 -4.23569 -0.62609
H -2.79584 -3.18735 -0.62472
H -4.08371 -1.14000 -0.62443
H -3.89564 1.67421 -0.62382

1b
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