Supporting Information

Understanding Molecular Switching Properties of Octaphyrins
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This PDF files includes:

I. Performance of several density functionals in geometry determination of neutral and diprotonated meso-octakis(pentafluorophenyl) [36]octaphyrins.
II. Dependence of the relative energies with the functional.
III. Conformational analysis of neutral unsubstituted [36]octaphyrin.
IV. Interconversion pathways of neutral unsubstituted [36]octaphyrin.
V. Substituent effect on the conformation of neutral [36]octaphyrins.
VI. Conformational changes upon protonation and redox reactions
VII. Conformational changes of meso-octakis(pentafluorophenyl) octaphyrins upon protonation and redox reactions.
VIII. Aromaticity.
IX. Cartesian coordinates of M06/6-31G(d,p) optimized geometries.
I. Performance of several density functionals in geometry determination of neutral and diprotonated \textit{meso-octakis(pentafluorophenyl)} [36]octaphyrins

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure_s1.png}
\caption{X-ray crystal structures of the \textit{meso-octakis(pentafluorophenyl)} [36]octaphyrin(1.1.1.1.1.1.1.1) in the neutral and diprotonated states.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure_s2.png}
\caption{Comparison of the B3LYP, M06, \(\omega\)B97XD optimized geometries of the figure-eight conformation and the Möbius, overlaid with the X-ray structure of the neutral and diprotonated \textit{meso-octakis(pentafluorophenyl)} [36]octaphyrin. The all-heavy atom RMS (in Å) are displayed.}
\end{figure}

\begin{table}[h]
\centering
\caption{Root-mean-square deviations (RMS in Å) and mean absolute errors (MUE) of the DFT optimized geometries relative to the X-ray structure of diprotonated \textit{meso-octakis(pentafluorophenyl)} [36]octaphyrin.}
\begin{tabular}{lcccc}
\hline
Functionals & 
\textit{T} & \textit{MUE} \text{bonds} & \text{MUE} \text{angles} & \text{MUE} \text{torsions} & \text{RMS} \text{heavy} \\
\hline
B3LYP & 0.033 & 1.259 & 3.453 & 0.272 & 0.620 \\
PBE & 0.036 & 1.290 & 3.419 & 0.256 & 0.523 \\
M06 & 0.034 & 1.279 & 3.542 & 0.243 & 0.606 \\
\(\omega\)B97XD & 0.036 & 1.322 & 3.766 & 0.332 & 0.887 \\
B3LYP-D & 0.033 & 1.322 & 3.488 & 0.270 & 0.583 \\
BP86 & 0.037 & 1.282 & 3.526 & 0.263 & 0.590 \\
\hline
\end{tabular}
\end{table}
Table S2. Torsional descriptors (Ψ_{MAX}, Ψ_{SMC} and Π) and bond-length alternation descriptors (Δr_{C,N}, Δr_{C,C} and HOMA) and the corresponding mean unsigned error relative to the X-ray structure of the Möbius [36]octaphyrin.[a]

<table>
<thead>
<tr>
<th>[36]T1</th>
<th>Ψ_{MAX}</th>
<th>Ψ_{SMC}</th>
<th>Π</th>
<th>Δr_{C,N}</th>
<th>Δr_{C,C}</th>
<th>HOMA</th>
<th>MUE Δr_{C,N}</th>
<th>MUE Δr_{C,C}</th>
<th>MUE HOMA</th>
</tr>
</thead>
<tbody>
<tr>
<td>RX</td>
<td>34.638</td>
<td>11.353</td>
<td>-0.286</td>
<td>0.058</td>
<td>0.099</td>
<td>0.720</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>B3LYP</td>
<td>32.145</td>
<td>9.773</td>
<td>-0.343</td>
<td>0.051</td>
<td>0.070</td>
<td>0.753</td>
<td>0.007</td>
<td>0.029</td>
<td>0.033</td>
</tr>
<tr>
<td>PBE</td>
<td>32.229</td>
<td>9.955</td>
<td>-0.340</td>
<td>0.063</td>
<td>0.081</td>
<td>0.661</td>
<td>0.005</td>
<td>0.018</td>
<td>0.059</td>
</tr>
<tr>
<td>M06</td>
<td>32.297</td>
<td>9.708</td>
<td>-0.338</td>
<td>0.060</td>
<td>0.113</td>
<td>0.698</td>
<td>0.002</td>
<td>0.015</td>
<td>0.022</td>
</tr>
<tr>
<td>ωB97XD</td>
<td>43.515</td>
<td>9.876</td>
<td>-0.260</td>
<td>0.092</td>
<td>0.115</td>
<td>0.576</td>
<td>0.034</td>
<td>0.016</td>
<td>0.144</td>
</tr>
<tr>
<td>B3LYP-D</td>
<td>30.701</td>
<td>9.559</td>
<td>-0.349</td>
<td>0.062</td>
<td>0.101</td>
<td>0.697</td>
<td>0.004</td>
<td>0.002</td>
<td>0.023</td>
</tr>
<tr>
<td>BP86</td>
<td>30.984</td>
<td>9.786</td>
<td>-0.356</td>
<td>0.062</td>
<td>0.08</td>
<td>0.645</td>
<td>0.004</td>
<td>0.019</td>
<td>0.075</td>
</tr>
</tbody>
</table>

[a] Ψ_{MAX} and Ψ_{SMC} are given in °; Δr_{C,N} and Δr_{C,C} in Å.

Table S3. Root-mean-square deviations (RMS in Å) and mean absolute errors (MUE) of the DFT optimized geometries relative to the X-ray structure of the neutral meso-octakis(pentafluorophenyl) [36]octaphyrin.

<table>
<thead>
<tr>
<th>[36]T2RX</th>
<th>MUE_{bonds}</th>
<th>MUE_{angles}</th>
<th>MUE_{torsions}</th>
<th>RMS_{Ag}</th>
<th>RMS_{heavy}</th>
</tr>
</thead>
<tbody>
<tr>
<td>B3LYP</td>
<td>0.037</td>
<td>0.951</td>
<td>2.926</td>
<td>0.206</td>
<td>0.724</td>
</tr>
<tr>
<td>PBE</td>
<td>0.041</td>
<td>1.313</td>
<td>3.110</td>
<td>0.174</td>
<td>0.665</td>
</tr>
<tr>
<td>M06</td>
<td>0.031</td>
<td>0.947</td>
<td>2.511</td>
<td>0.120</td>
<td>0.425</td>
</tr>
<tr>
<td>ωB97XD</td>
<td>0.035</td>
<td>0.956</td>
<td>2.406</td>
<td>0.192</td>
<td>0.438</td>
</tr>
<tr>
<td>B3LYP-D</td>
<td>0.034</td>
<td>1.008</td>
<td>2.679</td>
<td>0.196</td>
<td>0.542</td>
</tr>
<tr>
<td>BP86</td>
<td>0.045</td>
<td>1.030</td>
<td>2.817</td>
<td>0.133</td>
<td>0.665</td>
</tr>
</tbody>
</table>

Table S4. Torsional descriptors (Ψ_{MAX}, Ψ_{SMC} and Π) and bond-length alternation descriptors (Δr_{C,N}, Δr_{C,C} and HOMA) and the corresponding mean unsigned error relative to the X-ray structure of the twisted-Hückel conformations.

<table>
<thead>
<tr>
<th>[36]T2RX</th>
<th>Ψ_{MAX}</th>
<th>Ψ_{SMC}</th>
<th>Π</th>
<th>Δr_{C,N}</th>
<th>Δr_{C,C}</th>
<th>HOMA</th>
<th>MUE Δr_{C,N}</th>
<th>MUE Δr_{C,C}</th>
<th>MUE HOMA</th>
</tr>
</thead>
<tbody>
<tr>
<td>RX</td>
<td>20.244</td>
<td>7.888</td>
<td>0.618</td>
<td>0.084</td>
<td>0.119</td>
<td>0.684</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>B3LYP</td>
<td>19.177</td>
<td>6.114</td>
<td>0.699</td>
<td>0.059</td>
<td>0.095</td>
<td>0.697</td>
<td>0.025</td>
<td>0.024</td>
<td>0.014</td>
</tr>
<tr>
<td>PBE</td>
<td>16.439</td>
<td>6.636</td>
<td>0.680</td>
<td>0.041</td>
<td>0.078</td>
<td>0.690</td>
<td>0.043</td>
<td>0.041</td>
<td>0.006</td>
</tr>
<tr>
<td>M06</td>
<td>17.883</td>
<td>7.275</td>
<td>0.655</td>
<td>0.067</td>
<td>0.094</td>
<td>0.743</td>
<td>0.017</td>
<td>0.025</td>
<td>0.059</td>
</tr>
<tr>
<td>ωB97XD</td>
<td>16.375</td>
<td>7.625</td>
<td>0.631</td>
<td>0.088</td>
<td>0.115</td>
<td>0.596</td>
<td>0.004</td>
<td>0.005</td>
<td>0.068</td>
</tr>
<tr>
<td>B3LYP-D</td>
<td>15.700</td>
<td>7.432</td>
<td>0.630</td>
<td>0.065</td>
<td>0.092</td>
<td>0.727</td>
<td>0.019</td>
<td>0.027</td>
<td>0.043</td>
</tr>
<tr>
<td>BP86</td>
<td>16.627</td>
<td>6.427</td>
<td>0.691</td>
<td>0.042</td>
<td>0.079</td>
<td>0.667</td>
<td>0.042</td>
<td>0.040</td>
<td>0.017</td>
</tr>
</tbody>
</table>

Figure S3. (a) Root-mean-square deviations (RMS) and (b) mean unsigned errors (MUE) for the bond-length alternation parameters of the DFT optimized geometries relative to the X-ray structure of the diprotonated meso-octakis(pentafluorophenyl) [36]octaphyrin.
Table S5. $\pi-\pi$ stacking interactions distances of crystallographic and DFT-optimized neutral meso-octakis(pentafluorophenyl) [36]octaphyrin in the figure-eight conformation.

<table>
<thead>
<tr>
<th>[36]$T_{2nx}$</th>
<th>RX</th>
<th>M06</th>
<th>B3LYP</th>
<th>B3LYP-D</th>
<th>wB97XD</th>
<th>BP86</th>
<th>PBE</th>
</tr>
</thead>
<tbody>
<tr>
<td>phenyl-phenyl</td>
<td>3.13</td>
<td>3.13</td>
<td>3.22</td>
<td>3.06</td>
<td>3.20</td>
<td>3.27</td>
<td>3.59</td>
</tr>
<tr>
<td>pyrrol-pyrrol</td>
<td>3.41</td>
<td>3.33</td>
<td>3.71</td>
<td>3.06</td>
<td>3.52</td>
<td>3.61</td>
<td>3.23</td>
</tr>
<tr>
<td>pyrrol-phenyl</td>
<td>3.48</td>
<td>3.55</td>
<td>4.17</td>
<td>3.45</td>
<td>3.58</td>
<td>3.61</td>
<td>3.52</td>
</tr>
<tr>
<td>MUE</td>
<td>-</td>
<td>0.05</td>
<td>0.36</td>
<td>0.15</td>
<td>0.09</td>
<td>0.16</td>
<td>0.23</td>
</tr>
</tbody>
</table>

II. Dependence of the relative energies with the functional

Figure S4. Correlation between the relative energies (in kcal mol$^{-1}$) and the extent of $II$ conjugation computed with B3LYP and M06 functionals for unsubstituted [36]octaphyrins.
### Table S6. Relative and Gibbs free energies (in kcal mol\(^{-1}\)) together with the \(\pi\)-conjugation index (\(II\)) of the different conformations of neutral unsubstituted [36]octaphyrin 1 computed with M06 and B3LYP functionals.

<table>
<thead>
<tr>
<th>conf</th>
<th>(Tn^X)</th>
<th>M06(^a)</th>
<th>B3LYP(^b)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(E_{rel})</td>
<td>(\Delta G_{298})</td>
<td>(\Delta G_{THF})</td>
</tr>
<tr>
<td>1a</td>
<td>23.3</td>
<td>20.0</td>
<td>13.2</td>
</tr>
<tr>
<td>1b</td>
<td>43.7</td>
<td>41.3</td>
<td>47.3</td>
</tr>
<tr>
<td>1c</td>
<td>26.8</td>
<td>25.5</td>
<td>22.4</td>
</tr>
<tr>
<td>1e</td>
<td>47.1</td>
<td>45.0</td>
<td>40.1</td>
</tr>
<tr>
<td>1f</td>
<td>26.6</td>
<td>25.4</td>
<td>17.9</td>
</tr>
<tr>
<td>1g</td>
<td>17.3</td>
<td>17.3</td>
<td>12.5</td>
</tr>
<tr>
<td>1h</td>
<td>16.3</td>
<td>15.5</td>
<td>11.3</td>
</tr>
<tr>
<td>1i</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

\[\text{MAD} = 6.3, 5.3, 5.6, 5.8\]

\(^a\) ZPE-corrected relative energies and Gibbs free energies at the M06/6-311+G(d,p)/M06/6-31G(d,p) level of theory.\(^b\) ZPE-corrected relative energies and Gibbs free energies at the B3LYP/6-311+G(d,p)/B3LYP/6-31G(d,p) level.\(^c\) MAD is the mean absolute difference of the energies computed with both functionals.

**Figure S5.** Correlation between the Gibbs free energy (in kcal mol\(^{-1}\)) computed with B3LYP and M06 in gas-phase and DMSO.

**Figure S6.** Correlation between the Gibbs free energy and the relative energy (in kcal mol\(^{-1}\)) computed with B3LYP and M06, respectively.
III. Conformational analysis of neutral unsubstituted [36]octaphyrin

Table S7. Relative energies ($E_{rel}$ in kcal mol$^{-1}$), relative Gibbs free energies ($\Delta G_{298}$ in kcal mol$^{-1}$), hydrogen bonding index ($N_H$), p-conjugation index ($\Pi$), ring strain ($\Phi_p$ and $\Psi_{SMC}$) and bond-length alternation ($\Delta r_{C-C}$ and $\Delta r_{C-N}$) of the conformers of the neutral unsubstituted [36]octaphyrin.

<table>
<thead>
<tr>
<th>conformers</th>
<th>$E_{rel}$[a]</th>
<th>$\Delta G_{298}$</th>
<th>$N_H$</th>
<th>$\Psi_{SMC}$</th>
<th>$\Phi_p$</th>
<th>$\Pi$</th>
<th>$\Delta r_{C-M}$</th>
<th>$\Delta r_{C-C}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a</td>
<td>23.3</td>
<td>20.0</td>
<td>3</td>
<td>3.54</td>
<td>13.0</td>
<td>0.83</td>
<td>0.055</td>
<td>0.094</td>
</tr>
<tr>
<td>1b</td>
<td>43.9</td>
<td>41.3</td>
<td>1</td>
<td>5.23</td>
<td>16.9</td>
<td>0.76</td>
<td>0.063</td>
<td>0.100</td>
</tr>
<tr>
<td>1c</td>
<td>26.8</td>
<td>25.5</td>
<td>3</td>
<td>7.57</td>
<td>23.6</td>
<td>0.58</td>
<td>0.061</td>
<td>0.096</td>
</tr>
<tr>
<td>1d</td>
<td>32.0</td>
<td>31.4</td>
<td>3</td>
<td>8.66</td>
<td>27.3</td>
<td>0.47</td>
<td>0.064</td>
<td>0.097</td>
</tr>
<tr>
<td>1e</td>
<td>54.6</td>
<td>45.5</td>
<td>0</td>
<td>9.56</td>
<td>30.3</td>
<td>-0.35</td>
<td>0.058</td>
<td>0.089</td>
</tr>
<tr>
<td>1f</td>
<td>26.6</td>
<td>25.4</td>
<td>2.5</td>
<td>7.58</td>
<td>31.5</td>
<td>-0.57</td>
<td>0.062</td>
<td>0.098</td>
</tr>
<tr>
<td>1g</td>
<td>17.3</td>
<td>17.3</td>
<td>3</td>
<td>4.70</td>
<td>18.4</td>
<td>0.76</td>
<td>0.064</td>
<td>0.090</td>
</tr>
<tr>
<td>1h</td>
<td>16.3</td>
<td>15.5</td>
<td>3</td>
<td>4.70</td>
<td>15.0</td>
<td>0.80</td>
<td>0.054</td>
<td>0.095</td>
</tr>
<tr>
<td>1i</td>
<td>0.0</td>
<td>0.0</td>
<td>4</td>
<td>4.28</td>
<td>15.1</td>
<td>0.78</td>
<td>0.052</td>
<td>0.090</td>
</tr>
<tr>
<td>1j</td>
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<td>26.5</td>
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<td>-0.35</td>
<td>0.051</td>
<td>0.084</td>
</tr>
<tr>
<td>1k</td>
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<td>0.59</td>
<td>0.065</td>
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<td>16.3</td>
<td>0.64</td>
<td>0.103</td>
<td>0.093</td>
</tr>
</tbody>
</table>

[a] ZPE-corrected relative energies and Gibbs free energies at the M06/6-311+G(d,p)//M06/6-31G(d,p) level of theory

Figure S7. Relationship between the relative energy and the Gibbs free energies of neutral [36]octaphyrin conformers (1a-m) and the hydrogen bonding index ($N_H$).
Figure S8. Relationship between the Gibbs free energies of neutral [36]octaphyrin conformers (1a-m) and the torsional ring strain (Φr).

Figure S9. Evolution of the Gibbs free energy with the solvent computed at M06/6-311+G(d,p) (left) and at B3LYP/6-311+G(d,p) (right) level of theory.
<table>
<thead>
<tr>
<th>conf</th>
<th>Tn²</th>
<th>Eₑₑ[a]</th>
<th>ΔG₂₀₈</th>
<th>Nᵣ</th>
<th>Ψₛ</th>
<th>ΔG₉₆F</th>
<th>ΔG₀DCM</th>
<th>ΔG₀MSO</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a</td>
<td>T₀</td>
<td>11.5</td>
<td>12.0</td>
<td>3</td>
<td>11.8</td>
<td>5.9</td>
<td>5.1</td>
<td>4.4</td>
</tr>
<tr>
<td>1b</td>
<td>T₁</td>
<td>49.0</td>
<td>51.7</td>
<td>0</td>
<td>23.1</td>
<td>38.4</td>
<td>37.2</td>
<td>35.6</td>
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<tr>
<td>1c</td>
<td>T₀</td>
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<td>19.2</td>
<td>3</td>
<td>33.1</td>
<td>16.8</td>
<td>16.4</td>
<td>16.9</td>
</tr>
<tr>
<td>1d</td>
<td>T₀</td>
<td>22.9</td>
<td>23.6</td>
<td>3</td>
<td>39.0</td>
<td>19.9</td>
<td>19.2</td>
<td>19.6</td>
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<tr>
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<td>T₁</td>
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<td>42.3</td>
<td>0</td>
<td>34.3</td>
<td>30.7</td>
<td>29.6</td>
<td>28.7</td>
</tr>
<tr>
<td>1f</td>
<td>T₁</td>
<td>17.1</td>
<td>18.3</td>
<td>2.5</td>
<td>31.1</td>
<td>11.6</td>
<td>11.0</td>
<td>10.4</td>
</tr>
<tr>
<td>1g</td>
<td>T₁</td>
<td>11.7</td>
<td>12.1</td>
<td>3</td>
<td>18.1</td>
<td>7.3</td>
<td>6.7</td>
<td>6.2</td>
</tr>
<tr>
<td>1h</td>
<td>T₁</td>
<td>12.1</td>
<td>13.0</td>
<td>3</td>
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</table>

[a] ZPE-corrected relative energies and Gibbs free energies at the B3LYP/6-311+G(d,p)/B3LYP/6-31G(d,p) level of theory.

<table>
<thead>
<tr>
<th>conformers</th>
<th>T₀</th>
<th>Eₑₑ[a]</th>
<th>Nᵣ</th>
<th>Ψₛ ∈ GₛₐC</th>
<th>Ψₛ</th>
<th>ΔG₂₀₈</th>
<th>ΔG₀DCM</th>
<th>ΔG₀MSO</th>
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<td>T₁</td>
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<td>19.8</td>
<td>0.66</td>
<td>0.099</td>
<td>0.093</td>
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</tbody>
</table>

[a] Eₑₑ corresponds to the sum of the electronic energy computed at the B3LYP/6-311+G(d,p) level of theory and the zero-point vibrational energy obtained at the B3LYP/6-31G(d,p) level.
IV. Interconversion pathways of neutral unsubstituted [36]octaphyrin

Figure S10. Activation energy barriers ($\Delta G^\ddagger$ in kcal mol$^{-1}$) for the interconversions between the most relevant conformations in 1 computed at the M06/6-311+G(d,p)/M06/6-31G(d,p) level of theory. The relative Gibbs free energies of the different conformations with respect the global minima ($T_2_{RX}$) are also shown.

Figure S11. M06/6-31G(d,p) relaxed potential energy surface for the figure-eight conformation 1m ($T_2^{\text{th}}$) obtained by rotating the dihedral angles $\phi_1$ and $\phi_2$ (in °). The fully optimized geometries for the different minima and the corresponding Gibbs free energies and activation barriers ($\Delta G^\ddagger$ in kcal mol$^{-1}$) with respect to 1m are also shown.
Figure S12. M06/6-31G(d,p) potential energy curve for the figure-eight/Möbius interconversion in 1 as a function of dihedral angle $\phi_1$. The fully optimized geometries for the different minima and the corresponding relative Gibbs free energy and the activation barrier ($\Delta G^\dagger$ in kcal mol$^{-1}$) with respect to 1g are also shown.

Figure S13. M06/6-31G(d,p) potential energy curve for the Hückel/Möbius interconversions in 1 as a function of dihedral angle $\phi_1$. The fully optimized geometries for the different minima and the corresponding relative Gibbs free energy and the activation barrier ($\Delta G^\dagger$ in kcal mol$^{-1}$) with respect to 1k are also shown.
V. Substituent effect on the conformation of neutral [36]octaphyrins

**Figure S14.** Dependence of the relative energy on the intramolecular hydrogen bonding index ($N_H$) for unsubstituted (top) and substituted [36]octaphyrins (bottom).

**Figure S15.** Dependence of the relative energy on the torsional ring strain (in degrees) for substituted [36]octaphyrins.
Table S10. Relative energies ($E_{\text{rel}}$), Gibbs free energies ($\Delta G_{298}$ in kcal mol$^{-1}$), hydrogen bonding index ($N_H$), ring strain ($\Phi_p$ and $\Psi$), $\pi$-conjugation index ($\Pi$) and bond-length alternation ($\Delta r_{C-C}$ and $\Delta r_{C-N}$) of the neutral meso-trifluoromethyl-substituted [36]octaphyrins (R = CF$_3$).

<table>
<thead>
<tr>
<th>Conformers</th>
<th>$E_{\text{rel}}$</th>
<th>$\Delta G_{298}$</th>
<th>$N_H$</th>
<th>$\Phi_p$</th>
<th>$\Psi$</th>
<th>$\Pi$</th>
<th>$\Delta r_{C-N}$</th>
<th>$\Delta r_{C-C}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_0^{5,10,25,30}$</td>
<td>8.8</td>
<td>6.7</td>
<td>3</td>
<td>28.7</td>
<td>8.3</td>
<td>0.48</td>
<td>0.069</td>
<td>0.102</td>
</tr>
<tr>
<td>$T_0^{B,C,E,F,H}$</td>
<td>49.9</td>
<td>41.2</td>
<td>0</td>
<td>32.9</td>
<td>8.8</td>
<td>0.35</td>
<td>0.068</td>
<td>0.109</td>
</tr>
<tr>
<td>$T_0^{5,20,25,B,F}$</td>
<td>10.0</td>
<td>5.2</td>
<td>3</td>
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<td>10.2</td>
<td>0.30</td>
<td>0.075</td>
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<td>$T_1^{B,C,E,H}$</td>
<td>20.0</td>
<td>30.1</td>
<td>2.5</td>
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<td>9.7</td>
<td>-0.39</td>
<td>0.064</td>
<td>0.101</td>
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<td>0.131</td>
<td>0.102</td>
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<td>$T_2^{B,F}$</td>
<td>13.2</td>
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<td>$T_2^{C,G}$</td>
<td>7.3</td>
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<td>21.3</td>
<td>6.5</td>
<td>0.53</td>
<td>0.061</td>
<td>0.104</td>
</tr>
<tr>
<td>$T_2^{RX}$</td>
<td>0.0</td>
<td>0.0</td>
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<td>29.3</td>
<td>9.8</td>
<td>0.46</td>
<td>0.073</td>
<td>0.110</td>
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</table>

Table S11. Relative energies ($E_{\text{rel}}$), Gibbs free energies ($\Delta G_{298}$ in kcal mol$^{-1}$), hydrogen bonding index ($N_H$), ring strain ($\Phi_p$) and $\pi$-conjugation index ($\Pi$) of the neutral meso-aryl-substituted [36]octaphyrins.

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<th>$-\text{C}<em>6\text{F}</em>{5}$</th>
<th>$-\text{C}<em>6\text{H}</em>{3}\text{Cl}_2$</th>
<th>$-\text{C}_6\text{F}_3\text{-}F$</th>
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</thead>
<tbody>
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<td>$E_{\text{rel}}$</td>
<td>$\Delta G_{298}$</td>
<td>$N_H$</td>
<td>$\Phi_p$</td>
</tr>
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<td>a</td>
<td>$T_0^{5,10,25,30}$</td>
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<td>16.8</td>
</tr>
<tr>
<td>b</td>
<td>$T_0^{B,C,E,F,H}$</td>
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<td>41.4</td>
</tr>
<tr>
<td>c</td>
<td>$T_0^{5,20,25,B,F}$</td>
<td>20.2</td>
<td>18.3</td>
</tr>
<tr>
<td>d</td>
<td>$T_1^{B,C,F}$</td>
<td>19.3</td>
<td>10.1</td>
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<td>40.6</td>
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<tr>
<td>i</td>
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<tr>
<td>h</td>
<td>$T_2^{C,G}$</td>
<td>9.9</td>
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Figure S16. Evolution of the Gibbs free energy with the substituents at meso and β-positions, computed at the M06/6-311+G(d,p) level of theory.

Figure S17. The most stable conformations for meso-octakis(methoxy) [36]octaphyrin in neutral state. Intramolecular hydrogen bonds together with the torsional descriptors and the Gibbs free energies at the M06/6-311+G(d,p)//M06/6-31G(d,p) level of theory are also shown.
VI. Conformational changes upon protonation and redox reactions

![Diagram of octaphyrin structures](image)

Figure S18. Oxidation states available for the regular [36]octaphyrin.

Table S12. Relative energies ($E_{rel}$), Gibbs free energies ($\Delta G_{298}$ in kcal mol$^{-1}$), hydrogen bonding index ($N_H$), ring strain ($\phi_p$ and $\psi$), $\pi$-conjugation index ($\Pi$) and bond-length alternation ($\Delta r_{C-C}$) of the neutral unsubstituted [34]octaphyrins 3.

<table>
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<th>Conformers</th>
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<th>$E_{rel}$</th>
<th>$\Delta G_{298}$</th>
<th>$N_H$</th>
<th>$\psi_{SMC}$</th>
<th>$\phi_p$</th>
<th>$\Pi$</th>
<th>$\Delta r_{C-N}$</th>
<th>$\Delta r_{C-C}$</th>
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</thead>
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<td>2a</td>
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<td>14.8</td>
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<td>4.43</td>
<td>14.72</td>
<td>0.79</td>
<td>0.05</td>
<td>0.060</td>
</tr>
<tr>
<td>2b</td>
<td>$T_0^{B,C,E,F,H}$</td>
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<td>22.5</td>
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<td>16.5</td>
<td>3</td>
<td>6.7</td>
<td>34.9</td>
<td>0.59</td>
<td>0.034</td>
<td>0.078</td>
</tr>
<tr>
<td>2d</td>
<td>$T_0^{20,25,30}$</td>
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<td>3</td>
<td>8.0</td>
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<td>0.51</td>
<td>-0.30</td>
<td>0.069</td>
</tr>
<tr>
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<td>10.6</td>
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Table S13. Relative energies ($E_{rel}$), Gibbs free energies ($\Delta G_{298}$ in kcal mol$^{-1}$), hydrogen bonding index ($N_H$), ring strain ($\phi_p$ and $\psi$), $\pi$-conjugation index ($\Pi$) and bond-length alternation ($\Delta r_{C-C}$) of the neutral unsubstituted [38]octaphyrin 3.

<table>
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<th>$N_H$</th>
<th>$\psi_{SMC}$</th>
<th>$\phi_p$</th>
<th>$\Pi$</th>
<th>$\Delta r_{C-N}$</th>
<th>$\Delta r_{C-C}$</th>
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<td>14.8</td>
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<td>14.72</td>
<td>0.79</td>
<td>0.05</td>
<td>0.060</td>
</tr>
<tr>
<td>3b</td>
<td>$T_0^{B,C,E,F,H}$</td>
<td>50.0</td>
<td>48.8</td>
<td>0</td>
<td>5.9</td>
<td>22.5</td>
<td>0.59</td>
<td>0.038</td>
<td>0.085</td>
</tr>
<tr>
<td>3c</td>
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<td>16.5</td>
<td>3</td>
<td>6.7</td>
<td>34.9</td>
<td>0.59</td>
<td>0.034</td>
<td>0.078</td>
</tr>
<tr>
<td>3d</td>
<td>$T_0^{20,25,30}$</td>
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<td>20.4</td>
<td>3</td>
<td>8.0</td>
<td>38.8</td>
<td>0.51</td>
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<td>0.069</td>
</tr>
<tr>
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<td>39.6</td>
<td>0</td>
<td>9.5</td>
<td>35.1</td>
<td>-0.30</td>
<td>0.069</td>
<td>0.094</td>
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<tr>
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<td>16.6</td>
<td>2.5</td>
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<td>-0.56</td>
<td>0.110</td>
<td>0.100</td>
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<tr>
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<td>3.0</td>
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<td>14.9</td>
<td>0.81</td>
<td>0.050</td>
<td>0.070</td>
</tr>
<tr>
<td>3i</td>
<td>$T_2^{RX}$</td>
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<td>0.0</td>
<td>3.0</td>
<td>4.6</td>
<td>16.0</td>
<td>0.81</td>
<td>0.009</td>
<td>0.058</td>
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</tbody>
</table>
Table S14. Relative energies ($E_{rel}$), Gibbs free energies ($\Delta G_{298}$ in kcal mol$^{-1}$), hydrogen bonding index ($N_H$), ring strain ($\Phi_p$ and $\Psi$), $\pi$-conjugation index ($\Pi$) and bond-length alternation ($\Delta r_{C-N}$ and $\Delta r_{C-C}$) of the diprotonated unsubstituted [36]octaphyrin 4.

<table>
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<th>$\Delta G_{298}$</th>
<th>$N_H$</th>
<th>$\Psi_{SMC}$</th>
<th>$\Phi_p$</th>
<th>$\Pi$</th>
<th>$\Delta r_{C-N}$</th>
<th>$\Delta r_{C-C}$</th>
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</thead>
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<td>4a</td>
<td>$T_0^{8,10,25,30}$</td>
<td>5.5</td>
<td>4.3</td>
<td>3</td>
<td>4.9</td>
<td>16.4</td>
<td>0.74</td>
<td>0.054</td>
<td>0.094</td>
</tr>
<tr>
<td>4b</td>
<td>$T_0^{B,C,E,F,H}$</td>
<td>36.8</td>
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<td>0</td>
<td>7.0</td>
<td>26.1</td>
<td>0.52</td>
<td>0.069</td>
<td>0.089</td>
</tr>
<tr>
<td>4c</td>
<td>$T_0^{5,20,25,8,F}$</td>
<td>11.1</td>
<td>9.7</td>
<td>3</td>
<td>6.8</td>
<td>28.1</td>
<td>0.6</td>
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<td>0.076</td>
</tr>
<tr>
<td>4d</td>
<td>$T_0^{20,25,8,F}$</td>
<td>15.3</td>
<td>14.8</td>
<td>3</td>
<td>9.2</td>
<td>29.5</td>
<td>0.43</td>
<td>0.030</td>
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</tr>
<tr>
<td>4e</td>
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<td>38.8</td>
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<td>0.100</td>
</tr>
<tr>
<td>4f</td>
<td>$T_1^{B,C,F}$</td>
<td>3.6</td>
<td>2.7</td>
<td>2.5</td>
<td>7.7</td>
<td>29.5</td>
<td>-0.58</td>
<td>0.040</td>
<td>0.080</td>
</tr>
<tr>
<td>4g</td>
<td>$T_2^{B,F}$</td>
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<td>0.3</td>
<td>3</td>
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<td>0.0</td>
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<td>17.1</td>
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<tr>
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<td>3</td>
<td>4.9</td>
<td>17.4</td>
<td>0.73</td>
<td>0.069</td>
<td>0.087</td>
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</table>

Table S15. Relative energies ($E_{rel}$), Gibbs free energies ($\Delta G_{298}$ in kcal mol$^{-1}$), hydrogen bonding index ($N_H$), ring strain ($\Phi_p$ and $\Psi$), $\pi$-conjugation index ($\Pi$) and bond-length alternation ($\Delta r_{C-N}$ and $\Delta r_{C-C}$) of the diprotonated unsubstituted [38]octaphyrin 5.

<table>
<thead>
<tr>
<th>conformers</th>
<th>$T_n^\chi$</th>
<th>$E_{rel}$</th>
<th>$\Delta G_{298}$</th>
<th>$N_H$</th>
<th>$\Psi_{SMC}$</th>
<th>$\Phi_p$</th>
<th>$\Pi$</th>
<th>$\Delta r_{C-N}$</th>
<th>$\Delta r_{C-C}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5a</td>
<td>$T_0^{5,10,25,30}$</td>
<td>10.9</td>
<td>10.2</td>
<td>-</td>
<td>4.5</td>
<td>16.4</td>
<td>0.76</td>
<td>0.002</td>
<td>0.054</td>
</tr>
<tr>
<td>5b</td>
<td>$T_0^{B,C,E,F,H}$</td>
<td>6.5</td>
<td>4.9</td>
<td>-</td>
<td>6.6</td>
<td>25.1</td>
<td>0.56</td>
<td>0.004</td>
<td>0.064</td>
</tr>
<tr>
<td>5c</td>
<td>$T_0^{5,20,25,8,F}$</td>
<td>10.7</td>
<td>10.5</td>
<td>-</td>
<td>7.2</td>
<td>28.6</td>
<td>0.51</td>
<td>0.018</td>
<td>0.075</td>
</tr>
<tr>
<td>5d</td>
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<td>13.7</td>
<td>-</td>
<td>7.5</td>
<td>35.7</td>
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</tr>
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<td>13.0</td>
<td>-</td>
<td>10.0</td>
<td>33.3</td>
<td>-0.29</td>
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<td>0.095</td>
</tr>
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<td>5f</td>
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<td>9.2</td>
<td>-</td>
<td>7.1</td>
<td>28.5</td>
<td>-0.48</td>
<td>0.035</td>
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</tr>
<tr>
<td>5g</td>
<td>$T_2^{B,F}$</td>
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<td>2.2</td>
<td>-</td>
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<td>17.5</td>
<td>0.64</td>
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</tr>
<tr>
<td>5h</td>
<td>$T_2^{C,G}$</td>
<td>5.1</td>
<td>4.6</td>
<td>-</td>
<td>6.1</td>
<td>20.2</td>
<td>0.66</td>
<td>0.007</td>
<td>0.054</td>
</tr>
<tr>
<td>5i</td>
<td>$T_2^{RX}$</td>
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<td>0.0</td>
<td>-</td>
<td>4.4</td>
<td>14.1</td>
<td>0.79</td>
<td>0.006</td>
<td>0.052</td>
</tr>
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</table>
**Figure S19.** Dependence of the relative energy on the intramolecular hydrogen bonds of neutral unsubstituted [34] (top) and [38] octaphyrins (bottom).

**Figure S20.** Dependence of the relative energy on the ring strain of neutral unsubstituted [34] (left) and [38]octaphyrins (right).

**Figure S21.** Structural features of the neutral unsubstituted [34], [36] and [38]octaphyrins in the figure-eight $T_{2\text{ax}}$ conformation.
Figure S22. NCI analysis of the neutral unsubstituted [34] and [38]octaphyrins with a twisted-Hückel topology. (a) Plot of the reduced density gradient $\nabla\rho$ and (b) gradient isosurface ($s = 0.5$). The surfaces are coloured according to $\text{sign}(\lambda_2)\rho$ over the range $-0.03$ to $0.03$ a.u.

Figure S23. Dependence of the relative energy on the ring strain of diprotonated unsubstituted [38]octaphyrin 5.
Figure S24. Structural features of neutral [36] and diprotonated [36] and [38]octaphyrins in the figure-eight conformation.

Figure S25. NCI analysis of the diprotonated unsubstituted [36] and [38]octaphyrins with a twisted-Hückel topology. (a) Plot of the reduced density gradient $s(\rho)$ and (b) gradient isosurface ($s = 0.5$). The surfaces are coloured according to $\text{sign}(\lambda_2)\rho$ over the range -0.03 to 0.03 a.u.
VII. Conformational changes of meso-octakis(pentafluorophenyl) octa­phyrins upon protonation and redox reactions

Table S16. Relative energies ($E_{rel}$) and Gibbs free energies ($\Delta G_{298}$ in kcal mol$^{-1}$) in gas-phase and DCM solvent, hydrogen bonding index ($N_h$), ring strain ($\Phi$), $\pi$-conjugation index ($\Pi$) and bond-length alternation ($\Delta r_{CC}$ and $\Delta r_{CN}$) of the neutral meso-octakis(pentafluorophenyl)-substituted [36]octa­phyrins 6.

<table>
<thead>
<tr>
<th>conformers</th>
<th>$E_{rel}$</th>
<th>$E_{rel}^{DCM}$</th>
<th>$\Delta G_{298}$</th>
<th>$\Delta G_{298}^{DCM}$</th>
<th>$N_h$</th>
<th>$\Phi$</th>
<th>$\Pi$</th>
<th>$\Delta r_{CN}$</th>
<th>$\Delta r_{CC}$</th>
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<tbody>
<tr>
<td>6a</td>
<td>16.6</td>
<td>14.2</td>
<td>16.8</td>
<td>14.4</td>
<td>3</td>
<td>30.6</td>
<td>0.38</td>
<td>0.062</td>
<td>0.113</td>
</tr>
<tr>
<td>6b</td>
<td>48.7</td>
<td>30.7</td>
<td>41.4</td>
<td>23.4</td>
<td>0</td>
<td>35.6</td>
<td>0.47</td>
<td>0.061</td>
<td>0.101</td>
</tr>
<tr>
<td>6c</td>
<td>20.2</td>
<td>18.0</td>
<td>18.3</td>
<td>16.2</td>
<td>3</td>
<td>27.1</td>
<td>0.45</td>
<td>0.062</td>
<td>0.100</td>
</tr>
<tr>
<td>6d</td>
<td>29.7</td>
<td>27.5</td>
<td>25.4</td>
<td>23.2</td>
<td>3</td>
<td>31.6</td>
<td>0.19</td>
<td>0.087</td>
<td>0.127</td>
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<td>40.6</td>
<td>24.1</td>
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<td>33.9</td>
<td>-0.04</td>
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<td>0.979</td>
</tr>
<tr>
<td>6f</td>
<td>19.3</td>
<td>11.0</td>
<td>10.1</td>
<td>1.8</td>
<td>2.5</td>
<td>27.1</td>
<td>-0.48</td>
<td>0.024</td>
<td>0.070</td>
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<td>6h</td>
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<td>6.23</td>
<td>5.4</td>
<td>1.2</td>
<td>3</td>
<td>22.0</td>
<td>0.65</td>
<td>0.067</td>
<td>0.094</td>
</tr>
<tr>
<td>6i</td>
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<td>0.0</td>
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<td>4</td>
<td>21.6</td>
<td>0.60</td>
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<td>0.094</td>
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</table>

Table S17. Relative energies ($E_{rel}$) and Gibbs free energies ($\Delta G_{298}$ in kcal mol$^{-1}$) in gas-phase and DCM solvent, hydrogen bonding index ($N_h$), ring strain ($\Phi$), $\pi$-conjugation index ($\Pi$) and bond-length alternation ($\Delta r_{CC}$ and $\Delta r_{CN}$) of the neutral meso-octakis(pentafluorophenyl)-substituted [36]octa­phyrins 7.

<table>
<thead>
<tr>
<th>conformers</th>
<th>$E_{rel}$</th>
<th>$\Delta G_{298}$</th>
<th>$N_h$</th>
<th>$\Phi$</th>
<th>$\Pi$</th>
<th>$\Delta r_{CN}$</th>
<th>$\Delta r_{CC}$</th>
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<tbody>
<tr>
<td>7a</td>
<td>13.1 (14.3)</td>
<td>16.7(17.9)</td>
<td>3</td>
<td>30.3</td>
<td>0.38</td>
<td>0.015</td>
<td>0.073</td>
</tr>
<tr>
<td>7b</td>
<td>43.1 (28.3)</td>
<td>39.4 (24.6)</td>
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<td>31.2</td>
<td>0.45</td>
<td>0.037</td>
<td>0.083</td>
</tr>
<tr>
<td>7c</td>
<td>7.0 (7.5)</td>
<td>7.3 (8.7)</td>
<td>3</td>
<td>37.6</td>
<td>0.45</td>
<td>0.039</td>
<td>0.079</td>
</tr>
<tr>
<td>7d</td>
<td>17.9 (19.7)</td>
<td>19.5 (21.4)</td>
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<td>0.118</td>
</tr>
<tr>
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<td>44.1 (31.2)</td>
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<td>48.1</td>
<td>-0.21</td>
<td>0.067</td>
<td>0.093</td>
</tr>
<tr>
<td>7f</td>
<td>17.4 (13.0)</td>
<td>12.3 (8.0)</td>
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<td>28.6</td>
<td>-0.39</td>
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<td>0.102</td>
</tr>
<tr>
<td>7h</td>
<td>0.0 (0.0)</td>
<td>0.0 (0.0)</td>
<td>3</td>
<td>24.1</td>
<td>0.55</td>
<td>0.006</td>
<td>0.052</td>
</tr>
<tr>
<td>7i</td>
<td>5.3 (6.4)</td>
<td>7.5 (8.6)</td>
<td>3</td>
<td>21.1</td>
<td>0.57</td>
<td>0.012</td>
<td>0.058</td>
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Table S18. Relative energies ($E_{rel}$) and Gibbs free energies ($\Delta G_{298}$ in kcal mol$^{-1}$) in gas-phase and TFA solvent, hydrogen bonding index ($N_h$), ring strain ($\Phi$), $\pi$-conjugation index ($\Pi$) and bond-length alternation ($\Delta r_{CC}$ and $\Delta r_{CN}$) of the diprotonated meso-octakis(pentafluorophenyl)-substituted [36]octa­phyrins 8.

<table>
<thead>
<tr>
<th>conformers</th>
<th>$E_{rel}$</th>
<th>$\Delta G_{298}$</th>
<th>$N_h$</th>
<th>$\Phi$</th>
<th>$\Pi$</th>
<th>$\Delta r_{CN}$</th>
<th>$\Delta r_{CC}$</th>
</tr>
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<tbody>
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<td>8a</td>
<td>2.0 (5.8)</td>
<td>4.9 (8.6)</td>
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<td>0.104</td>
<td>0.104</td>
</tr>
<tr>
<td>8b</td>
<td>34.9 (26.0)</td>
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<td>0</td>
<td>35.2</td>
<td>0.34</td>
<td>0.087</td>
<td>0.087</td>
</tr>
<tr>
<td>8c</td>
<td>5.1 (10.7)</td>
<td>8.1 (13.6)</td>
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<td>39.6</td>
<td>0.43</td>
<td>0.086</td>
<td>0.086</td>
</tr>
<tr>
<td>8d</td>
<td>22.4 (24.5)</td>
<td>24.5 (22.8)</td>
<td>3</td>
<td>38.6</td>
<td>0.31</td>
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<td>0.084</td>
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<tr>
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<td>32.7 (26.8)</td>
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<td>-0.31</td>
<td>0.113</td>
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</tr>
<tr>
<td>8f</td>
<td>8.1 (5.1)</td>
<td>3.9 (1.0)</td>
<td>2.5</td>
<td>31.2</td>
<td>-0.43</td>
<td>0.070</td>
<td>0.070</td>
</tr>
<tr>
<td>8h</td>
<td>0.0 (0.0)</td>
<td>0.0 (0.0)</td>
<td>3</td>
<td>24.1</td>
<td>0.53</td>
<td>0.093</td>
<td>0.093</td>
</tr>
<tr>
<td>8i</td>
<td>12.2 (7.4)</td>
<td>15.8 (11.1)</td>
<td>3</td>
<td>21.6</td>
<td>0.57</td>
<td>0.091</td>
<td>0.091</td>
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</table>
Table S19. Relative energies ($E_{rel}$) and Gibbs free energies ($\Delta G_{298}$ in kcal mol$^{-1}$) in gas-phase and TFA solvent, hydrogen bonding index ($N_H$), ring strain ($\Phi_P$), $\pi$-conjugation index ($I I$) and bond-length alternation ($\Delta r_{C-C}$ and $\Delta r_{C-N}$) of the diprotonated meso-octakis(pentafluorophenyl)-substituted [38]octaphyrins 9.

<table>
<thead>
<tr>
<th>conformers</th>
<th>$E_{rel}$</th>
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<th>$N_H$</th>
<th>$\Phi_P$</th>
<th>$II$</th>
<th>$\Delta r_{C-N}$</th>
<th>$\Delta r_{C-C}$</th>
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<td>9a</td>
<td>6.9 (10.0)</td>
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<td>31.7</td>
<td>0.38</td>
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<td>0.057</td>
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<tr>
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<td>0.40</td>
<td>0.011</td>
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<td>0.41</td>
<td>0.028</td>
<td>0.075</td>
</tr>
<tr>
<td>9d</td>
<td>17.0 (22.6)</td>
<td>15.6 (20.3)</td>
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<td>26.9</td>
<td>-0.22</td>
<td>0.028</td>
<td>0.091</td>
</tr>
<tr>
<td>9f</td>
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<td>3.5 (5.7)</td>
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<td>-0.33</td>
<td>0.038</td>
<td>0.086</td>
</tr>
<tr>
<td>9h</td>
<td>0.0 (1.0)</td>
<td>0.0 (0.0)</td>
<td>0</td>
<td>28.5</td>
<td>0.49</td>
<td>0.006</td>
<td>0.052</td>
</tr>
<tr>
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<td>1.9 (0.0)</td>
<td>5.9 (3.0)</td>
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<td>35.9</td>
<td>0.45</td>
<td>0.002</td>
<td>0.058</td>
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</tbody>
</table>

Figure S26. Dependence of the relative energy with $N_H$ for meso-octakis(pentafluorophenyl) [36] (top) and [38]octaphyrins (bottom).
Figure S27. Dependence of the relative energy with $N_H$ for diprotonated meso-octakis(pentafluorophenyl) [36]octaphyrin $8$.

\[ E_{\text{rel}} = -8.591 N_H + 33.473 \]
\[ R^2 = 0.730 \]

Figure S28. Plausible conformations for meso-octakis(pentafluorophenyl) [36]octaphyrin in neutral state.

Figure S29. Experimental and computed $^1$H NMR shifts of the NH protons and $\beta$-protons for the neutral meso-octakis(pentafluorophenyl) [36]octaphyrin $8$ in different conformations.
In contrast to unsubstituted [36]octaphyrins, the relative Gibbs free energies of the different conformations of meso-octakis(pentafluorophenyl) octaphyrins in neutral and diprotonated state are strongly dependent on the functional used to evaluate the electronic energies in solvent. Whereas M06 predicts the twisted-Hückel topologies (i and h) as the most stable ones for the neutral [36] and [38]octaphyrins, B3LYP predicts that the Möbius f and the nonsymmetric Hückel c for 6 and 7, respectively. However, a doubly-twisted topology 6i with all the pyrrolic nitrogens pointing inward was revealed by the X-ray crystallographic structure for the neutral [36]octaphyrin. In the case of neutral [38]octaphyrin, no crystallographic structure is available, but the $^1$H-NMR spectra of the three plausible conformations (7c, 7d and 7h) (Figure 6) indicate that the most plausible structure for the neutral meso-octakis(pentafluorophenyl) [38]octaphyrin is the figure-eight conformation 7h with two inverted pyrrole rings. Therefore, M06 provides relative energies in better agreement with the experimental data than B3LYP.
By contrast, in the diprotonated species, B3LYP provides relative energies in better agreement with the experimental observations than M06, although it describes the overall Hückel and Möbius structures worse. According to B3LYP, the Möbius 8f and the Hückel 9b are the global minima. The main difference between both functionals is related to the relative stability of the figure-eight conformations, which seems to be overstabilized by M06 in the diprotonated state, whereas B3LYP underestimates the stability of the figure-eight conformations in the neutral state. Since both M06 and B3LYP describe well the degree of π-electron delocalization in Hückel and Möbius octaphyrins, the discrepancies between the different methodologies mainly arise from an overestimation of the noncovalent interactions stabilizing the figure-eight topologies, such us the π-π staking interactions. Therefore, the selection of a functional for describing the thermochemistry of neutral and protonated meso-substituted octaphyrins is a complex task.
VIII. Aromaticity

Scheme S1. Example of the isomerization reaction used to evaluate the ISE and other aromaticity indices of [36]octaphyrin. Syn-anti correction for the ISE. ISE and Δη are given in kcal mol$^{-1}$ and Λ in ppm cgs.

Table S21. Energetic, reactivity, magnetic and structural indices of aromaticity of the different conformations of the neutral unsubstituted [36]octaphyrins computed at M06/6-311+G(d,p) level of theory.[14][a]

<table>
<thead>
<tr>
<th>conformers</th>
<th>ISE</th>
<th>ISE$_{corr}$</th>
<th>Δη</th>
<th>Λ</th>
<th>NICS(0)</th>
<th>NICS$_{zz}(1)$</th>
<th>HOMA</th>
</tr>
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<td>1a</td>
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<td>-1.6</td>
<td>238.4</td>
<td>8.6</td>
<td>31.5</td>
<td>0.75</td>
</tr>
<tr>
<td>1b</td>
<td>18.4</td>
<td>/</td>
<td>-6.1</td>
<td>458.8</td>
<td>8.4</td>
<td>26.9</td>
<td>0.73</td>
</tr>
<tr>
<td>1c</td>
<td>8.4</td>
<td>-2.8</td>
<td>-8.4</td>
<td>295.0</td>
<td>13.2</td>
<td>22.9</td>
<td>0.76</td>
</tr>
<tr>
<td>1d</td>
<td>18.4</td>
<td>1.0</td>
<td>-2.9</td>
<td>102.5</td>
<td>6.1</td>
<td>22.6</td>
<td>0.73</td>
</tr>
<tr>
<td>1e</td>
<td>20.1</td>
<td>20.1</td>
<td>-1.0</td>
<td>-325.1</td>
<td>-6.1</td>
<td>-13.3</td>
<td>0.71</td>
</tr>
<tr>
<td>1f</td>
<td>21.3</td>
<td>2.2</td>
<td>1.6</td>
<td>-299.0</td>
<td>-13.4</td>
<td>-24.6</td>
<td>0.82</td>
</tr>
<tr>
<td>1g</td>
<td>23.2</td>
<td>-1.0</td>
<td>-5.3</td>
<td>62.8</td>
<td>3.8</td>
<td>-22.5</td>
<td>0.76</td>
</tr>
<tr>
<td>1h</td>
<td>27.3</td>
<td>0.3</td>
<td>-3.5</td>
<td>92.1</td>
<td>4.0</td>
<td>-17.3</td>
<td>0.72</td>
</tr>
<tr>
<td>1i</td>
<td>20.3</td>
<td>-13.3</td>
<td>-3.5</td>
<td>79.1</td>
<td>0.8</td>
<td>-19.3</td>
<td>0.76</td>
</tr>
</tbody>
</table>

[a] ISE and ISE$_{corr}$ are given in kcal mol$^{-1}$, Λ in ppm cgs and NICS indices in ppm.

Table S22. Energetic, reactivity, magnetic and structural indices of aromaticity of the different conformations of the neutral unsubstituted [34]octaphyrins computed at B3LYP/6-311+G(d,p) level of theory.[15]

<table>
<thead>
<tr>
<th>conformers</th>
<th>ISE</th>
<th>ISE$_{corr}$</th>
<th>Δη</th>
<th>Λ</th>
<th>NICS(0)</th>
<th>NICS$_{zz}(1)$</th>
<th>HOMA</th>
</tr>
</thead>
<tbody>
<tr>
<td>2a</td>
<td>27.4</td>
<td>-2.8</td>
<td>4.1</td>
<td>-444.9</td>
<td>-15.2</td>
<td>-34.2</td>
<td>0.81</td>
</tr>
<tr>
<td>2b</td>
<td>20.8</td>
<td>1.0</td>
<td>-0.1</td>
<td>-513.7</td>
<td>-6.5</td>
<td>-15.5</td>
<td>0.73</td>
</tr>
<tr>
<td>2c</td>
<td>23.4</td>
<td>-2.0</td>
<td>0.0</td>
<td>272.5</td>
<td>-12.7</td>
<td>-19.9</td>
<td>0.82</td>
</tr>
<tr>
<td>2d</td>
<td>16.1</td>
<td>-1.3</td>
<td>0.5</td>
<td>-192.0</td>
<td>-21.6</td>
<td>-29.1</td>
<td>0.79</td>
</tr>
<tr>
<td>2e</td>
<td>17.4</td>
<td>-0.4</td>
<td>-5.1</td>
<td>348.6</td>
<td>5.4</td>
<td>19.6</td>
<td>0.71</td>
</tr>
<tr>
<td>2f</td>
<td>15.1</td>
<td>-4.7</td>
<td>-6.2</td>
<td>347.0</td>
<td>10.8</td>
<td>33.5</td>
<td>0.78</td>
</tr>
<tr>
<td>2g</td>
<td>26.1</td>
<td>-13.3</td>
<td>-1.1[b]</td>
<td>-127.8</td>
<td>-12.7</td>
<td>-20.9</td>
<td>0.86</td>
</tr>
<tr>
<td>2h</td>
<td>25.7</td>
<td>-12.6</td>
<td>3.6</td>
<td>-126.9</td>
<td>-12.7</td>
<td>-20.9</td>
<td>0.84</td>
</tr>
<tr>
<td>2i</td>
<td>23.8</td>
<td>11.7</td>
<td>-1.2[c]</td>
<td>-30.1</td>
<td>-3.2</td>
<td>-9.3</td>
<td>0.85</td>
</tr>
</tbody>
</table>

[a] ISE and ISE$_{corr}$ are given in kcal mol$^{-1}$, Λ in ppm cgs and NICS indices in ppm.

[b] The large flexibility induces topology changes in the dihydrogen derivative of the methylene adducts of these conformations during the optimization.
Figure S31. Correlation between the relative hardness ($\Delta \eta$) (top) and the diamagnetic susceptibility exaltation ($\Lambda$ in ppm cgs) (bottom) computed with B3LYP and M06.
Figure S32. Correlation between the NICS(0) and ISE computed with B3LYP and M06 functionals.

Table S23. Energetic, reactivity, magnetic and structural indices of aromaticity of the different conformation of the neutral unsubstituted [38]octaphyrins computed at the B3LYP/6-311+G(d,p) level of theory.

<table>
<thead>
<tr>
<th>conformers</th>
<th>ISE</th>
<th>ISE_corr</th>
<th>Δη</th>
<th>Λ</th>
<th>NICS(0)</th>
<th>NICSZZ (1)</th>
<th>HOMA</th>
</tr>
</thead>
<tbody>
<tr>
<td>3a</td>
<td>29.3</td>
<td>-13.5</td>
<td>1.1</td>
<td>-491.7</td>
<td>-18.2</td>
<td>-37.3</td>
<td>0.84</td>
</tr>
<tr>
<td>3b</td>
<td>24.2</td>
<td>-12.3</td>
<td>3.7</td>
<td>-791.2</td>
<td>-9.5</td>
<td>-24.4</td>
<td>0.70</td>
</tr>
<tr>
<td>3c</td>
<td>33.9</td>
<td>-9.8</td>
<td>9.1</td>
<td>-158.7</td>
<td>-8.6</td>
<td>-9.0</td>
<td>0.82</td>
</tr>
<tr>
<td>3d</td>
<td>26.6</td>
<td>-</td>
<td>5.0</td>
<td>-215.3</td>
<td>-18.2</td>
<td>-25.7</td>
<td>0.83</td>
</tr>
<tr>
<td>3e</td>
<td>28.5</td>
<td>-9.4</td>
<td>4.9</td>
<td>307.1</td>
<td>5.0</td>
<td>18.3</td>
<td>0.73</td>
</tr>
<tr>
<td>3f</td>
<td>20.8</td>
<td>-6.2</td>
<td>-3.4</td>
<td>325.4</td>
<td>10.4</td>
<td>34.5</td>
<td>0.83</td>
</tr>
<tr>
<td>3g</td>
<td>29.1</td>
<td>-10.3</td>
<td>7.3</td>
<td>-136.3</td>
<td>-14.1</td>
<td>-19.1</td>
<td>0.81</td>
</tr>
<tr>
<td>3h</td>
<td>31.9</td>
<td>-12.1</td>
<td>4.9</td>
<td>-158.2</td>
<td>-15.8</td>
<td>-41.2</td>
<td>0.87</td>
</tr>
<tr>
<td>3i</td>
<td>27.9</td>
<td>-9.0</td>
<td>7.9</td>
<td>-107.2</td>
<td>-14.5</td>
<td>-44.1</td>
<td>0.88</td>
</tr>
</tbody>
</table>

[a] ISE and ISE_corr are given in kcal mol⁻¹, Λ in ppm cgs and NICS indices in ppm.
[b] The large flexibility induces topology changes in the dihydrogen derivative of the methylene adducts of these conformations during the optimization.
Table S24. Energetic, reactivity, magnetic and structural indices of aromaticity of the different conformations of the diprotonated unsubstituted [36]octaphyrins computed at the B3LYP/6-311+G(d,p) level of theory.\textsuperscript{[a]}

<table>
<thead>
<tr>
<th>conformers</th>
<th>ISE</th>
<th>ISE\textsubscript{corr}</th>
<th>(\Delta \eta)</th>
<th>(\Lambda)</th>
<th>NICS(0)</th>
<th>NICS\textsubscript{zz}(1)</th>
<th>HOMA</th>
</tr>
</thead>
<tbody>
<tr>
<td>4a</td>
<td>22.1</td>
<td>-13.5</td>
<td>-7.3</td>
<td>880.7</td>
<td>28.4</td>
<td>81.7</td>
<td>0.69</td>
</tr>
<tr>
<td>4b</td>
<td>26.1</td>
<td>2.9\textsuperscript{[b]}</td>
<td>-3.0</td>
<td>1199.1</td>
<td>16.1</td>
<td>49.3</td>
<td>0.76</td>
</tr>
<tr>
<td>4c</td>
<td>16.1</td>
<td>-15.5</td>
<td>-9.2</td>
<td>478.5</td>
<td>5.1</td>
<td>37.1</td>
<td>0.80</td>
</tr>
<tr>
<td>4d</td>
<td>21.9</td>
<td>-16.1</td>
<td>-9.8</td>
<td>469.6</td>
<td>9.7</td>
<td>37.5</td>
<td>0.81</td>
</tr>
<tr>
<td>4e</td>
<td>26.2</td>
<td>0.95</td>
<td>10.8</td>
<td>-558.8</td>
<td>-10.4</td>
<td>-26.0</td>
<td>0.80</td>
</tr>
<tr>
<td>4f</td>
<td>20.7</td>
<td>3.2</td>
<td>5.1</td>
<td>-361.1</td>
<td>-15.3</td>
<td>-30.9</td>
<td>0.71</td>
</tr>
<tr>
<td>4g</td>
<td>19.7</td>
<td>-1.7</td>
<td>-8.5</td>
<td>365.8</td>
<td>12.5</td>
<td>-17.9</td>
<td>0.79</td>
</tr>
<tr>
<td>4h</td>
<td>20.9</td>
<td>-1.5</td>
<td>-8.0</td>
<td>378.6</td>
<td>18.6</td>
<td>-17.1</td>
<td>0.78</td>
</tr>
<tr>
<td>4i</td>
<td>25.1</td>
<td>0.3\textsuperscript{[b]}</td>
<td>-3.4</td>
<td>70.0</td>
<td>1.2</td>
<td>-25.6</td>
<td>0.77</td>
</tr>
</tbody>
</table>

\[a\] ISE and ISE\textsubscript{corr} are given in kcal mol\textsuperscript{-1}, \(\Lambda\) in ppm cgs and NICS indices in ppm.

\[b\] The large flexibility induces topology changes in the dihydrogen derivative of the methylene adducts of these conformations during the optimization.

Table S25. Energetic, reactivity, magnetic and structural indices of aromaticity of the different conformations of the diprotonated unsubstituted [38]octaphyrins computed at B3LYP/6-311+G(d,p) level of theory.\textsuperscript{[a]}

<table>
<thead>
<tr>
<th>conformers</th>
<th>ISE</th>
<th>ISE\textsubscript{corr}</th>
<th>(\Delta \eta)</th>
<th>(\Lambda)</th>
<th>NICS(0)</th>
<th>NICS\textsubscript{zz}(1)</th>
<th>HOMA</th>
</tr>
</thead>
<tbody>
<tr>
<td>5a</td>
<td>27.7</td>
<td>-13.0</td>
<td>7.7</td>
<td>-638</td>
<td>-17.8</td>
<td>-39.2</td>
<td>0.88</td>
</tr>
<tr>
<td>5b</td>
<td>25.5</td>
<td>-7.1</td>
<td>9.6</td>
<td>-1081</td>
<td>-12.1</td>
<td>-32.5</td>
<td>0.84</td>
</tr>
<tr>
<td>5c</td>
<td>22.1</td>
<td>-9.6</td>
<td>6.7</td>
<td>-277.8</td>
<td>-18.5</td>
<td>-28.0</td>
<td>0.86</td>
</tr>
<tr>
<td>5d</td>
<td>27.4</td>
<td>-8.9</td>
<td>10.1</td>
<td>[c]</td>
<td>-7.4</td>
<td>-15.7</td>
<td>0.83</td>
</tr>
<tr>
<td>5e</td>
<td>29.3</td>
<td>-14.2</td>
<td>-2.6</td>
<td>707.0</td>
<td>12.8</td>
<td>40.5</td>
<td>0.76</td>
</tr>
<tr>
<td>5f</td>
<td>15.3</td>
<td>-15.6</td>
<td>-2.7</td>
<td>462.1</td>
<td>20.8</td>
<td>59.2</td>
<td>0.76</td>
</tr>
<tr>
<td>5g</td>
<td>23.8</td>
<td>0.0</td>
<td>8.1</td>
<td>-217.6</td>
<td>-16.9</td>
<td>-21.7</td>
<td>0.88</td>
</tr>
<tr>
<td>5h</td>
<td>27.8</td>
<td>-2.4</td>
<td>8.3</td>
<td>-283.0</td>
<td>-18.0</td>
<td>-21.1</td>
<td>0.87</td>
</tr>
<tr>
<td>5i</td>
<td>27.6</td>
<td>-13.0</td>
<td>10.3</td>
<td>-183.2</td>
<td>-14.4</td>
<td>-33.5</td>
<td>0.88</td>
</tr>
</tbody>
</table>

\[a\] ISE and ISE\textsubscript{corr} are given in kcal mol\textsuperscript{-1}, \(\Lambda\) in ppm cgs and NICS indices in ppm.

\[b\] The large flexibility induces topology changes in the dihydrogen derivative of the methylene adducts of these conformations during the optimization.

\[c\] Due to computational issues, the magnetic susceptibility exaltation of \(T_{B,F,20}^{\text{[36]}}\) is not reported.

\[
\begin{align*}
\Lambda &= 347.0 \\
\Delta \eta &= -3.4
\end{align*}
\]

\[
\begin{align*}
\Lambda &= 344.4 \\
\Delta \eta &= 3.8
\end{align*}
\]

\[
\begin{align*}
\Lambda &= 325.4 \\
\Delta \eta &= -3.4
\end{align*}
\]

Figure S33. Evolution of magnetic and reactivity descriptors of the Möbius topology \(T_{1B,C,F}^{\text{[36]}}\) (f) with the number of \(\pi\)-electrons.
Table S26. Correlation between several descriptors of aromaticity for unsubstituted octaphyrins (n=25).\[a\]

<table>
<thead>
<tr>
<th></th>
<th>$\Delta \eta$</th>
<th>$\Lambda$</th>
<th>NICS(0)</th>
<th>NICS(1)</th>
<th>HOMA</th>
<th>NICS$_{zz}$(1)</th>
<th>ISE$_{corr}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta \eta$</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\Lambda$</td>
<td>0.75</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>NICS(0)</td>
<td>0.83</td>
<td>0.92</td>
<td>1</td>
<td></td>
<td></td>
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<td>HOMA</td>
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<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>NICS(1)$_{zz}$</td>
<td>0.89$^{[b]}$</td>
<td>0.94$^{[b]}$</td>
<td>0.96$^{[b]}$</td>
<td>1</td>
<td>0.49$^{[b]}$</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>ISE$_{corr}$</td>
<td>0.01</td>
<td>0.04</td>
<td>0.07</td>
<td>0.04</td>
<td>0.03</td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

[a] Conformations with highly distorted methylene and methyl isomers in the isomerization reaction were not taken into account in this statistical analysis.

[b] The figure-eight topologies were left out because their NICS$_{zz}$(1) are not associated with the macrocyclic ring current.

Figure S34. Correlation between several aromaticity descriptors computed for neutral and diprotonated octaphyrins (n = 25).

Table S27. Energetic, reactivity, magnetic and structural indices of aromaticity of the most stable conformation of meso-octakis(pentafluorophenyl) [36] and [38]octaphyrins upon protonation.

<table>
<thead>
<tr>
<th></th>
<th>$\Delta \eta$</th>
<th>$\Lambda$</th>
<th>NICS(0)</th>
<th>NICS(1)$_{zz}$</th>
<th>HOMA</th>
<th>G$_{T2}^{[A]}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>[36]</td>
<td>$T_2^{C,G}$</td>
<td>-1.2</td>
<td>-30</td>
<td>-3.2</td>
<td>-9.3</td>
<td>0.85</td>
</tr>
<tr>
<td>[38]</td>
<td>$T_2^{C,G}$</td>
<td>4.9</td>
<td>-158</td>
<td>-15.8</td>
<td>-41.2</td>
<td>0.87</td>
</tr>
<tr>
<td>[36]$^{[2]}$</td>
<td>$T_1^{B,C,E,F,H}$</td>
<td>-559.00</td>
<td>-10.40</td>
<td>-26.00</td>
<td>0.80</td>
<td>5100</td>
</tr>
<tr>
<td>[38]$^{[2]}$</td>
<td>$T_0^{B,C,E,F,H}$</td>
<td>9.60</td>
<td>-1081.00</td>
<td>-12.10</td>
<td>-32.10</td>
<td>0.84</td>
</tr>
</tbody>
</table>

[a] $\Delta \eta$ is given in kcal mol$^{-1}$, $\Lambda$ in ppm cgs and NICS indices in ppm. [b] Two-photon absorption cross-section in GM measured experimentally (J. Am. Chem. Soc. 2010, 132, 3105).
Figure S35. Correlation between the two-photon absorption cross-section values ($\sigma_{\text{TPA}}$ in GM) and relative hardness and exaltation for meso-octakis(pentafluorophenyl) [36] and [38]octaphyrins in neutral and diprotonated states.

Table S28. Correlation between several descriptors of aromaticity for neutral unsubstituted octaphyrins ($n = 14$).

<table>
<thead>
<tr>
<th>$\Delta \eta$</th>
<th>$\Lambda$</th>
<th>NICS(0)</th>
<th>HOMA</th>
<th>NICS$_{zz}$(1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta \eta$</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\Lambda$</td>
<td>0.77</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NICS(0)</td>
<td>0.90</td>
<td>0.77</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>HOMA</td>
<td>0.78</td>
<td>0.73</td>
<td>0.80</td>
<td>1</td>
</tr>
<tr>
<td>NICS$_{zz}$(1)</td>
<td>0.89$^[b]$</td>
<td>0.91$^[b]$</td>
<td>0.96$^[b]$</td>
<td>0.73$^[b]$</td>
</tr>
</tbody>
</table>

[a] Conformations with highly distorted methylene and methyl isomers in the isomerization reaction were not taken into account in this statistical analysis.

[b] The figure-eight topologies were left out because their NICS$_{zz}$(1) are not associated with the macrocyclic ring current.

Table S29. Correlation between several descriptors of aromaticity for diprotonated unsubstituted octaphyrins ($n = 11$)$^[i]$.

<table>
<thead>
<tr>
<th>$\Delta \eta$</th>
<th>$\Lambda$</th>
<th>NICS(0)</th>
<th>HOMA</th>
<th>NICS$_{zz}$(1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta \eta$</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\Lambda$</td>
<td>0.77</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NICS(0)</td>
<td>0.82</td>
<td>0.91</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>HOMA</td>
<td>0.37</td>
<td>0.42</td>
<td>0.48</td>
<td>1</td>
</tr>
<tr>
<td>NICS$_{zz}$(1)</td>
<td>0.80$^[b]$</td>
<td>0.96$^[b]$</td>
<td>0.98$^[b]$</td>
<td>0.38$^[b]$</td>
</tr>
</tbody>
</table>

[a] Conformations with highly distorted methylene and methyl isomers in the isomerization reaction were not taken into account in this statistical analysis.

[b] The figure-eight topologies were left out because their NICS$_{zz}$(1) are not associated with the macrocyclic ring current.

Table S30. Correlation between several descriptors of aromaticity for unsubstituted [4$n$ + 2] $\pi$-electrons octaphyrins ($n = 13$)$^[i]$.

<table>
<thead>
<tr>
<th>$\Delta \eta$</th>
<th>$\Lambda$</th>
<th>NICS(0)</th>
<th>HOMA</th>
<th>NICS$_{zz}$(1)</th>
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<tr>
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<tr>
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<tr>
<td>HOMA</td>
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<tr>
<td>NICS$_{zz}$(1)</td>
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<td>0.72$^[b]$</td>
<td>0.93$^[b]$</td>
<td>0.73$^[b]$</td>
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</tbody>
</table>

[a] Conformations with highly distorted methylene and methyl isomers in the isomerization reaction were not taken into account in this statistical analysis.

[b] The figure-eight topologies were left out because their NICS$_{zz}$(1) are not associated with the macrocyclic ring current.
Table S31. Correlation between several descriptors of aromaticity for unsubstituted [4n] π-electrons octaphyrins (n = 12).[a]

<table>
<thead>
<tr>
<th></th>
<th>Δη</th>
<th>Λ</th>
<th>NICS(0)</th>
<th>HOMA</th>
<th>NICS_{zz}(1)</th>
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<td>0.91[b]</td>
<td>0.87[b]</td>
<td>0.53[b]</td>
<td>1</td>
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</table>

[a] Conformations with highly distorted methylene and methyl isomers in the isomerization reaction were not taken into account in this statistical analysis.

[b] The figure-eight topologies were left out because their NICS_{zz}(1) are not associated with the macrocyclic ring current.
VII Cartesian coordinates of M06/6-31G(d,p) optimized geometries

1a (Hückel $\pi^5\sigma^{10}\delta^{25}\delta^{30}$)

<table>
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<th>Y (Å)</th>
<th>Z (Å)</th>
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\[ E(RM06) = -1977.64678429 \quad \text{A.U. after 14 cycles} \]

1b (Hückel T0\textsuperscript{B,C,E,F,H})

| C     | 0.14091 | -5.38931 | 3.56325 |
| C     | 0.2508  | -5.94639 | 4.89117 |
| C     | 0.3072  | -4.93332 | 5.78731 |
| C     | 0.22472 | -3.67658 | 5.07989 |
| C     | 0.19376 | -2.42845 | 5.63357 |
| C     | 0.14825 | -1.17956 | 4.94163 |
| N     | -0.12892| -0.04714 | 5.57391 |
| C     | -0.13703| 0.92897  | 4.59452 |
| C     | -0.39492| 2.24894  | 4.86019 |
| C     | -0.64369| 3.20324  | 3.83249 |
| C     | -1.21501| 2.99782  | 2.57018 |
| C     | -1.18488| 4.20101  | 1.87787 |
| C     | -0.59841| 5.16502  | 2.7077 |
| C     | -0.26212| 6.52142  | 2.42883 |
| C     | -0.08106| 6.99301  | 1.15257 |
| N     | -0.11995| 6.15779  | 0.05907 |
| C     | 0.1355  | 6.90879  | -0.99758 |
| C     | 0.25471 | 6.37078  | -2.32157 |
| C     | 0.32886 | 5.02751  | -2.5807 |
| C     | 0.40876 | 3.92513  | -1.64168 |
| C     | 0.468   | 2.76888  | -2.33286 |
| C     | 0.42647 | 3.05747  | -3.75171 |
| C     | 0.37202 | 2.19299  | -4.80582 |
| C     | 0.47549 | 0.76597  | -4.68237 |
| N     | -0.0747 | -0.05232 | -5.56359 |
| C     | 0.15358 | -1.32949 | -5.07593 |
| C     | -0.36864| -2.43437 | -5.69378 |
| C     | -0.43226| -3.7487  | -5.15739 |
| C     | -0.6559 | -4.96568 | -5.81206 |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| C | -0.6687 | -5.97322 | -4.85063 |
| C | -0.46958 | -5.38258 | -3.59502 |
| C | -0.46072 | -6.02237 | -2.3309 |
| C | -0.15703 | -5.51476 | -1.0931 |
| N | -0.30697 | -6.3108 | 0.02954 |
| C | 0.04238 | -5.55807 | 1.06073 |
| C | 0.03384 | -6.08106 | 2.3917 |
| N | 0.16897 | -4.00815 | 3.72896 |
| C | 0.40229 | -0.96004 | 3.51483 |
| C | 0.21409 | 0.35913 | 3.29916 |
| N | -0.34363 | 4.54548 | 3.91641 |
| C | 0.20309 | 8.35625 | 0.72908 |
| C | 0.31831 | 8.31176 | -0.62112 |
| N | 0.36163 | 4.44225 | -3.83623 |
| C | 1.18153 | 0.03513 | -3.62565 |
| C | 0.96968 | -1.27683 | -3.86997 |
| N | -0.30619 | -4.0343 | -3.81567 |
| C | 0.34661 | -4.20236 | -0.7146 |
| C | 0.47278 | -4.22493 | 0.63264 |
| H | 0.28783 | 9.21866 | 1.38085 |
| H | -1.5551 | 4.41162 | 0.8854 |
| H | -1.65982 | 2.06579 | 2.24762 |
| H | 0.37726 | 0.91505 | 2.38439 |
| H | 0.78114 | -1.68458 | 2.80321 |
| H | 0.41497 | -5.00364 | 6.86293 |
| H | 0.30546 | -7.01035 | 5.08742 |
| H | 0.89784 | -3.44845 | 1.2594 |
| H | 0.20421 | 4.95451 | 4.65954 |
| H | -0.24481 | -3.38833 | 3.04869 |
| H | 0.5377 | 9.12821 | -1.3007 |
| H | 0.40065 | 4.07608 | -0.57189 |
| H | 0.4878 | 1.77157 | -1.91666 |
| H | 1.82403 | 0.46665 | -2.86753 |
| H | 1.41857 | -2.12181 | -3.3592 |
| H | -0.76419 | -5.07567 | -6.88354 |
| H | -0.79548 | -7.03644 | -5.01178 |
| H | 0.63935 | -3.38916 | -1.37022 |
| H | 0.28997 | 4.95059 | -4.70369 |
| H | -0.37978 | -3.32952 | -3.09677 |
| H | -0.7466 | -7.07338 | -2.34018 |
| H | -0.08309 | -7.15995 | 2.46753 |
| H | 0.15776 | -2.37128 | 6.71918 |
| H | -0.42351 | 2.5573 | 5.90579 |
| H | -0.10588 | 7.20307 | 3.26559 |
| H | 0.28909 | 7.07224 | -3.15461 |
| H | -0.81404 | -2.28334 | -6.67589 |
| H | 0.16107 | 2.57546 | -5.80368 |

SCF Done:  \( E(RM06) = -1977.59152008 \)  A.U. after  7 cycles

**1c (Hückel \( T0^{5,20,25,B,\ell} \))**

|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| C | 6.07536 | 2.20847 | 0.07551 |
| C | 6.25664 | 3.56169 | 0.54861 |
| C | 5.03514 | 4.09412 | 0.78356 |
| C | 4.02542 | 3.09827 | 0.49497 |
| C | 2.67537 | 3.29546 | 0.57728 |
C  1.6373  2.33841  0.37365
N  0.36084  2.70782  0.31026
C -0.33636  1.52776  0.15426
C -1.68578  1.37769 -0.00152
C -2.72136  2.34237 -0.08578
C -2.79317  3.74683  0.00053
C -4.11573  4.11162 -0.2316
C -4.86487  2.93484 -0.45628
C -6.21621  2.72582 -0.83584
C -6.77577  1.47787 -1.03453
N -6.08898  0.32294 -0.73318
C -6.77766  -0.69455 -1.25643
C -6.26201  -2.0275  -1.21898
C -5.15869  -2.36261 -0.46798
C -4.28883  -3.51956 -0.52867
C -3.22914  -3.13136  0.29698
C -3.42915  -2.05554  0.98523
C -2.74078  -1.42674  1.98628
C -1.407  -1.65967  2.43546
N -0.46226  -2.29245  1.74825
C  0.7036  -2.04249  2.45285
C  1.96834  -2.17291  1.94865
C  2.3374  -2.64622  0.66127
C  1.6939  -3.49801 -0.2509
C  2.53728  -3.657 -1.34585
C  3.6773  -2.8656 -1.13104
C  4.81474  -2.65177 -1.9456
C  5.749  -1.66008 -1.77826
N  5.62499  -0.59057 -0.8997
C  6.76435  0.0982 -1.0275
C  7.02804  1.36215 -0.42579
N  4.72122  1.96039  0.11469
C  1.80333  0.88797  0.26859
C  0.55976  0.38158  0.14153
N -3.98478  1.89505 -0.33938
C -8.00275  1.13919 -1.72387
C -7.99112 -0.21279 -1.89081
N -4.60639 -1.54354  0.48654
C -0.89562 -1.03937  3.65401
C  0.42803  -1.30316  3.67457
N  3.53579  -2.28537  0.10089
C  7.02083  -1.60626 -2.46661
C  7.67829  -0.53369 -1.96493
H  4.20364 -1.5942  0.43499
H  4.35292  1.1245 -0.32861
H -4.29206  0.94407 -0.54587
H -4.99731 -0.6229  0.6616
H  7.3605  -2.32273 -3.2062
H  8.66326 -0.16225 -2.22454
H  2.36166  -4.25855 -2.22909
H  0.72096  -3.93765 -0.07811
H  7.22409  4.03514  0.6626
H  4.79934  5.09164  1.13437
H -1.94103  4.38251  0.20194
H -4.5216  5.11587 -0.24626
H -8.74466  1.84618 -2.07782
H -8.73172 -0.82779 -2.38928
| C  | -2.37596 | -3.95543 | 0.47448 |
| H  | -4.46221 | -4.37253 | -1.17372 |
| H  | 2.72693  | 0.32563  | 0.33955 |
| H  | 0.24469  | -0.65619 | 0.07422 |
| H  | 4.96444  | -3.35433 | -2.7642 |
| H  | 8.0457   | 1.74259  | -0.47863 |
| H  | 2.34596  | 4.30403  | 0.81844 |
| H  | 2.77606  | -1.76217 | 2.55697 |
| H  | 1.17215  | -0.99326 | 4.39962 |
| H  | -1.48617 | -0.46925 | 4.3624 |
| H  | -6.69596 | -2.78179 | -1.87004 |
| H  | -3.24592 | -0.58083 | 2.45698 |
| H  | -6.81226 | 3.60959  | -1.05592 |
| H  | -2.02293 | 0.34222  | -0.09852 |

SCF Done: $E_{(RM06)} = -1977.63975611$ A.U. after 7 cycles

1d (Hückel $T_0^{20,25,8,5}$)

| C  | 5.75709  | 1.86238  | -1.01897 |
| C  | 6.03336  | 3.20908  | -0.72798 |
| C  | 4.9008   | 3.75374  | -0.14944 |
| C  | 3.8973   | 2.76348  | -0.11742 |
| C  | 2.57676  | 3.01703  | 0.32199 |
| C  | 1.36328  | 2.37404  | 0.22806 |
| N  | 0.26313  | 3.09387  | 0.65935 |
| C  | -0.80569 | 2.39193  | 0.30472 |
| C  | -2.06738 | 3.0519   | 0.457 |
| C  | -3.32883 | 2.86956  | -0.04407 |
| C  | -4.28354 | 3.95674  | -0.09925 |
| C  | -5.34586 | 3.57469  | -0.84301 |
| C  | -5.16372 | 2.19575  | -1.21963 |
| C  | -6.03578 | 1.42987  | -1.95183 |
| C  | -5.94293 | 0.02016  | -2.10622 |
| N  | -5.12993 | -0.71587 | -1.3494 |
| C  | -5.3485  | -2.03161 | -1.71352 |
| C  | -4.78479 | -3.08839 | -1.03299 |
| C  | -4.02313 | -2.93651 | 0.15046 |
| C  | -3.14311 | -3.80793 | 0.81615 |
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| C  | -3.04154 | -1.783   | 1.80947 |
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The table above shows the Cartesian coordinates of atoms in the molecule.
SCF Done:  E(RM06) = -1977.65391418  A.U. after 19 cycles
1h (Hückel T2\textsuperscript{c-o})

C  -7.0665  -0.22027  -0.06575
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H -7.2391 3.8836 1.23591
H 0.03619 2.42494 -1.60149
H -0.03619 2.42492 1.60107
H 5.23535 -3.94573 1.42377
H 8.22824 1.48463 -0.49573
H 2.30422 3.63055 -1.52697
H -2.30419 3.63059 1.52691
H 1.96046 0.95174 1.54679
H -8.2282 1.48464 0.49562
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H -3.33277 -0.21196 1.42269
H -4.97215 -0.28002 -0.42711
H 3.33273 -0.21199 -1.42256
H 4.97223 -0.27989 0.4273

\[ \text{Hückel } T_{266} \]

\begin{align*}
\text{C} & : 4.82693 -2.28698 0.4187 \\
\text{C} & : 4.93641 -3.69104 0.46872 \\
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SCF Done: $E_{(RM06)} = -1977.68236697$  A.U. after 22 cycles
\[ Z_2 \text{ (Hückel [34])} \] 

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C & \quad 7.55698 & 1.11776 & -0.00852 \\
N & \quad 6.77214 & -0.00014 & -0.00019 \\
C & \quad 7.55689 & -1.1181 & 0.00813 \\
C & \quad 7.08556 & -2.4347 & 0.00889 \\
C & \quad 5.75518 & -2.82015 & -0.04616 \\
N & \quad 4.71999 & -1.94202 & -0.14193 \\
C & \quad 3.60758 & -2.69747 & -0.16145 \\
C & \quad 2.34715 & -2.0823 & -0.29078 \\
C & \quad 1.08628 & -2.63603 & -0.15093 \\
N & \quad -0.01012 & -1.85998 & -0.38137 \\
C & \quad -1.07162 & -2.63114 & -0.11742 \\
C & \quad -2.36246 & -2.07769 & -0.22074 \\
C & \quad -3.59687 & -2.68909 & -0.0798 \\
N & \quad -4.73445 & -1.93326 & -0.08717 \\
C & \quad -5.74814 & -2.80357 & 0.02571 \\
C & \quad -7.10035 & -2.42543 & 0.06372 \\
C & \quad -7.56047 & -1.12714 & 0.03268 \\
C & \quad -8.92702 & -0.68043 & 0.02408 \\
C & \quad -8.92693 & 0.68024 & -0.02433 \\
C & \quad -7.56032 & 1.12141 & -0.03287 \\
C & \quad -7.10022 & 2.42511 & -0.06395 \\
C & \quad -5.74807 & 2.80343 & -0.02587 \\
N & \quad -4.73424 & 1.93331 & 0.08737 \\
C & \quad -3.59671 & 2.68933 & 0.07989 \\
C & \quad -2.3623 & 2.07818 & 0.22112 \\
C & \quad -1.07151 & 2.63166 & 0.11784 \\
C & \quad -0.66057 & 3.96858 & -0.32063 \\
C & \quad 0.68855 & 3.9705 & -0.29756 \\
C & \quad 1.08642 & 2.63631 & 0.15124 \\
C & \quad 2.34725 & 2.08239 & 0.29077 \\
C & \quad 3.60773 & 2.69743 & 0.16146 \\
N & \quad 4.72006 & 1.94185 & 0.14171 \\
C & \quad 5.75532 & 2.81987 & 0.04601 \\
C & \quad 7.08569 & 2.43437 & -0.00917 \\
C & \quad 8.91209 & 0.68603 & -0.00949 \\
C & \quad 8.91204 & -0.68647 & 0.00906 \\
C & \quad 5.27965 & -4.19254 & -0.02221 \\
C & \quad 3.93076 & -4.11963 & -0.08759 \\
C & \quad -3.9226 & -4.10856 & 0.03784 \\
C & \quad 0.68831 & -3.97001 & 0.29831 \\
C & \quad -0.6608 & -3.96796 & 0.32148 \\
C & \quad -5.27031 & -4.17908 & 0.0946 \\
N & \quad -6.77737 & -0.00021 & -0.00009 \\
C & \quad -5.27046 & 4.17899 & -0.09514 \\
C & \quad -3.92274 & 4.10871 & -0.03827 \\
N & \quad -0.01002 & 1.86033 & 0.38149 \\
C & \quad 3.93106 & 4.11956 & 0.08788 \\
C & \quad 5.27995 & 4.19233 & 0.02237 \\
H & \quad -5.75184 & -0.00051 & 0. \\
H & \quad -7.8522 & -3.21018 & 0.11791 \\
H & \quad -7.85213 & 3.20978 & -0.11824 \\
H & \quad -2.38465 & 1.01018 & 0.43528 \\
H & \quad 2.3659 & 1.01748 & 0.52114 \\
H & \quad 7.84281 & 3.21556 & -0.05278 \\
H & \quad 7.84268 & -3.21588 & 0.05256 \\
H & \quad 2.36591 & -1.01746 & -0.52146 \\
H & \quad -2.38494 & -1.00967 & -0.43476 \\
H & \quad -5.8957 & 5.0621 & -0.16783
\end{align*}
H  -3.22339  4.93399 -0.02451
H  -1.30507  4.77026 -0.65725
H   1.34297  4.77252 -0.61327
H   3.23043  4.94251  0.13722
H   5.90513  5.0769 -0.0265
H   9.76591  1.3521 -0.01625
H   9.76582 -1.35259  0.01581
H   5.90473 -5.07716  0.0268
H   3.23003 -4.94251 -0.13673
H   1.3427 -4.77195  0.61429
H  -1.30539 -4.76938  0.65855
H  -3.2231 -4.9337  0.0237
H  -5.8954 -5.06232  0.16697
H  -9.77996 -1.34752  0.04576
H  -9.77977  1.34746 -0.04608
H   5.74625 -0.00014 -0.00017

SCF Done: E(RM06) = -1976.38849696  A.U. after  7 cycles

2b (Hückel [34] T\textsuperscript{B,C,E,F,H})

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SCF Done: $E(RM06) = -1976.34405050$  A.U. after 8 cycles

$2c$ (Hückel [34]$\theta^{20,25,8,6,4}$)

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46
SCF Done: E(RM06) = -1976.38427789  A.U. after 7 cycles

2d (Hückel [34]7020,25,8R)

C  5.22334  2.12126  -1.12127
H  -1.3644  0.43241 -0.51796
H  4.79712 -4.20496 -1.32025
H  6.8799  1.81794 -2.42957
H  2.21788  4.04939  1.09717
H  3.07082  0.13038  2.28809
H  1.35521  1.69689  3.63698
H  -1.35431  1.6972  3.63662
H  -4.79659 -4.20519 -1.31993
H  -3.07005  0.1308  2.28765
H  -6.88044  1.81733 -2.42942
H  -2.21861  4.04914  1.09737
H  4.55243 -0.52874 -0.52778
H  -4.55249 -0.52886 -0.52773

SCF Done: E(RM06) = -1976.37659028  A.U. after 8 cycles

2e (Möbius [34] $T^RGEH$)

C  -7.07529  0.13943  -0.23783
N  -6.08816 -0.70511  0.24927
C  -6.57565 -1.92365  0.1209
C  -5.77535 -3.11087  0.28532
C  -4.49558 -3.14902  0.75037
N  -3.6934  -4.27063  0.54288
C  -2.48542  3.89615  0.91669
C  -1.34974 -4.73415  0.64075
C  -0.05904  -4.13158  0.50518
N  -0.95259 -5.21003  0.16757
C  2.04185 -4.47363  0.03978
C  3.29328  5.07072 -0.32566
C  4.46806 -4.40904 -0.55342
N  4.62357 -3.03702 -0.47411
C  5.90845  -2.80655 -0.67749
C  6.50346  1.50647  -0.608
C  5.79266 -0.34055 -0.53474
C  4.37852 -0.10683 -0.74306
C  4.10375  1.18648 -0.46233
C  5.32864  1.83816 -0.04453
C  5.50884  3.06788  0.52331
C  4.44479  3.9661  0.8583
N  3.22312  3.91864  0.35161
C  2.47994  4.80629  1.10658
C  1.13889  5.01308  0.93966
C  0.36393  4.5287  -0.15365
C  0.74362  4.2334  -1.46979
C  -0.41648  4.01157 -2.20663
C  -1.50948  4.09725 -1.33581
C  -2.8709  3.79502 -1.60729
C  -3.77946  3.22259 -0.75779
N  -5.05928  2.92785 -1.20964
C  -5.551  2.09142 -0.31468
C  -6.8175  1.4427 -0.54726
C  -3.73511 -2.08464  1.39454
C  -8.25899 -0.62299 -0.61052
C  -7.94612 -1.92005 -0.39221
C  -2.47987 -2.55366  1.51769
C  5.74992  5.04449  -0.84698
C  0.47993 -2.95592  0.5855
C  6.65718 -4.04638  -0.90901
C  1.79125 -3.05229  0.30284
N  6.33198  0.89424  -0.20885
C  4.55792  4.95601  1.93205
C  3.31281  5.44879  2.11341
C  -3.53912  2.59743  0.53541
N  -1.00545  4.42029  -0.09713
C  -4.64264  1.86115  0.80089
H  -1.64172  -2.07183  2.0034
H  3.70543  -0.88382  -1.07735
H  7.72311  -4.11442  -1.09721
H  5.46151  5.18426  2.48671
H  -4.84064  1.20865  1.64121
H  -8.55299  -2.79992  -0.57474
H  5.90736  -6.11044  -0.96578
H  1.77047  4.22553  -1.80855
H  -4.14343  -1.12957  1.69223
H  2.54508  -2.27915  0.26737
H  2.975  6.18698  2.83216
H  3.15824  1.71086  -0.50757
H  -0.07602  -2.05028  0.78192
H  -2.61856  2.62911  1.10645
H  -0.49042  3.75723  -3.25654
H  -9.17521  -0.2066  -1.01275
H  -6.17838  -4.04387  -0.10781
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H  7.58982  -1.46072  -0.53212
H  6.50619  3.33297  0.87484
H  0.62368  5.61138  1.69275
H  -3.20609  3.94181  -2.63365
H  -7.552  2.00019  -1.12765
H  7.25958  1.00432  0.17234
H  -1.57475  4.63537  0.70867
SCF Done: $E(RM06) = -1976.33206100$ A.U. after 7 cycles

$2f(M"obius [34]T^1RC)$

C  7.40991  0.34271  -0.56963
N  6.0895  0.74463  -0.58878
C  6.06711  1.88468  -1.27093
C  4.89809  2.69276  -1.45559
C  3.68576  2.53547  -0.847
N  2.62595  3.38382  -1.16049
C  1.59927  2.91629  -0.47964
C  0.32304  3.57673  -0.47221
C  -0.86598  2.99222  -0.15366
N  -1.99802  3.75947  0.08386
C  -2.95296  2.88851  0.35817
C  -4.22572  3.37038  0.79311
C  -5.37983  2.67835  1.02435
N  -5.62112  1.33764  0.76737
C  -6.90527  1.16435  1.06306
C  -7.6558  -0.01265  0.79758
C  -7.21368  -1.11309  0.11544
C  -8.04859  -2.16136  -0.42899
C  -7.27263  -2.96256  -1.1921
C  -5.90713  -2.49298  -1.09907
C  -4.82553  -3.05676  -1.71677
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SCF Done: E(RM06) = -1976.37180804  A.U. after 7 cycles

2g (Twisted-Hückel [34] T20,p)

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\[ \text{SCF Done: E(RM06) = -1976.39833799 \ A.U. after 9 cycles} \]

\[ \text{2h (Twisted-Hückel \{34\}72^{CG})} \]

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\end{align*}
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SCF Done: E(RM06) = -1976.39833799 A.U. after 8 cycles

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SCF Done: E(RM06) = -1976.38919013  A.U. after 10 cycles

3a (Hückel [38])\textsuperscript{70,10,25,30}
SCF Done: E(RM06) = -1978.88937663  A.U. after 8 cycles

3b (Hückel [38] T0,R,E,F,H)

C  5.14502  3.93851 -0.11212
C  5.62977  5.24925 -0.27116
C  4.54694  6.10841 -0.36231
C  3.36775  5.34664 -0.2433
C  2.03961  5.82267 -0.2187
C  0.88698  5.0682  -0.21522
C  0.68298  3.66335 -0.41967
C  -0.64373  3.38512 -0.28453
C  -1.34579  4.60097  0.00671
C  -2.69729  4.79  0.20582
C  -3.55661  3.70287  0.50038
C  -3.24645  2.48342  1.12877
C  -4.37712  1.68514  1.11576
C  -5.41319  2.3974  0.48788
C  -6.72475  1.98149  0.16531
C  -7.08082  0.64962  0.05504
N  -6.16209 -0.35884  0.13894
C  -6.82834 -1.49545 -0.0511
C  -6.19578 -2.76789 -0.11758
C  -4.82849 -2.94132 -0.12546
C  -3.78642 -1.94665 -0.107
C  -2.58519 -2.57383 -0.13869
C  -2.79638 -3.99526 -0.18925
C  -1.85746 -4.99666 -0.21395
C  -0.47449 -4.74086 -0.42927
C  0.16161 -3.70592  1.12472
C  1.54001 -3.86647 -0.9903
C  1.77475 -5.01654 -0.22188
C  2.98767 -5.61174  0.21133
C  4.18251 -4.94488  0.32292
C  5.47594 -5.47766  0.6462
C  6.36774 -4.45117  0.69101
C  5.68002 -3.22087  0.41054
C  6.22366 -1.96207  0.41519
C  5.61021 -0.71061  0.14236
N  6.30187  0.42059  0.3128
C  5.4484  1.44121 -0.01192
C  5.8824  2.7564  0.0347
N  3.75998  4.03198 -0.12245
N  -0.38152  5.59664 -0.01525
N  -4.8985  3.65059  0.18907
C  -8.40616  0.10545 -0.19492
C  -8.254 -1.24296 -0.23991
N  -4.17333 -4.16338 -0.16057
SCF Done: E(RM06) = -1978.83305137  A.U. after 7 cycles

3c (Hückel [38])

C  6.21226  2.04882 -0.02097
C  6.328  3.38943  0.4736
C  5.07348  3.85707  0.73177
C  4.12238  2.83837  0.38625
C  2.74872  2.95737  0.41408
C  1.79067  2.03796 -0.05603
C  1.90154  0.8132 -0.74702
C  0.62592  0.30517 -0.93085
C -0.30058  1.20967 -0.38618
C -1.70098  1.07317 -0.39846
C -2.70566  2.01713 -0.32005
C -2.73556  3.45319 -0.30316
C -4.03564  3.85796 -0.45022
C -4.87008  2.69301 -0.55445
C -6.22053  2.56553 -0.86676
C -6.83168  1.30064 -1.0344
N -6.20301  0.17746 -0.65292
C -6.92536 -0.88901 -1.12042
C -6.45824 -2.18846 -0.96275
C -5.30716 -2.48422 -0.19136
C -4.38574 -3.55443 -0.2043
C  -3.31451  -3.21703  0.62149  
C  -3.59333  -1.95646  1.1983  
C  -2.95605  -1.08577  2.11466  
C  -1.63162  -0.92338  2.42578  
C  -1.1138  0.04355  3.35123  
C  0.24305  0.01981  3.28826  
C  0.63885  -0.96099  2.32095  
C  1.91683  -1.18473  1.88269  
C  2.33828  -2.08628  0.88144  
C  1.7342  -3.21728  0.28073  
C  2.62068  -3.72625  -0.65905  
C  3.76631  -2.90463  -0.66797  
C  4.93802  -2.95063  -1.44244  
C  5.91351  -1.96625  -1.43672  
N  5.76943  -0.75435  -0.80026  
C  6.94964  -0.11816  -0.94407  
C  7.19402  1.19173  -0.47519  
N  4.86536  1.75524  -0.02625  
N  0.43321  2.26433  0.11176  
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C  -8.06374  0.9627  -1.72572  
C  -8.10388  -0.39768  -1.80486  
N  -4.80701  -1.57468  0.70464  
N  -0.53252  -1.56836  1.87663  
N  3.56  -1.94317  0.29087  
C  7.2312  -2.07159  -2.01917  
C  7.8923  -0.93286  -1.68113  
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H  4.55839  0.85164  -0.3722  
H  -4.38661  0.68496  -0.57496  
H  -5.2251  -0.64736  0.76901  
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H  8.9091  -0.64791  -1.92747  
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SCF Done:  E(RM06) = -1978.88616480  A.U. after 7 cycles
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3e (Möbius [38] Tj R,E,H)

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N    -6.2082    0.4436  -0.3806
N     -3.9765    4.009  -0.5193
N     0.7075   5.2334   0.1455
C     5.6624   5.2226   0.5079
C     6.6154   4.2655   0.4269
N     6.2904  -0.6212  -0.2288
N     3.3927  -3.9026  -0.4978
N    -0.7633  -4.4291   0.2079
C    -3.3512  -2.6873  -0.3986
C    -4.5127  -2.0524  -0.6901
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H      0.625   6.2338   0.0563
H      4.0148   0.8326   1.6018
H      7.6914   4.3859   0.3629
H      5.683   -5.2425  -2.4495
H    -4.7694  -1.5108  -1.5949
H    -8.9385   2.2666  -0.0585
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H     2.0646  -4.2916   1.8367
H    -4.1776   1.1388  -2.059
H     2.3618   2.3996   0.2839
H     3.2908  -6.4365  -2.6094
H     3.5778  -1.7898   1.1711
H    -0.2809   2.1108  -0.157
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H    -6.7199   3.7915  -0.5632
H    -1.9032   5.7442  -0.2499
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H      6.5611  -3.0074  -1.3163
H      0.828   -5.8682  -1.5268
H    -2.8618  -3.8592   2.8139
H    -7.4449  -2.3033   1.1829
H      7.0591  -0.6246  -0.883
H    -1.3694  -4.6747  -0.5614
H    -4.3107   4.7338   0.0985
H      2.9392  -3.0908  -0.1012

SCF Done: E(RM06) = -1978.82570394   A.U. after 6 cycles

3f (Möbius [38] T^{B,C})

C     7.4926   0.06196  -0.36018
C     8.37423   0.81902  -1.15329
C     7.64004   1.83957  -1.74351
C     6.29898   1.71727  -1.31775
C     5.20034   2.57377  -1.60917
C     3.88979   2.33952  -1.28645
C     3.2583   1.15891  -0.74412
C     1.94036   1.40324  -0.56365
C     1.65447   2.75646  -0.97583
C     0.4798   3.43983  -0.87762
C    -0.75384   2.81721  -0.48975
SCF Done: E(RM06) = -1978.87103986  A.U. after 7 cycles

3g (Twisted-Hückel [38] T20.7)

C  -6.0908  2.14861  0.51474
C  -6.02851  3.54697  0.77235
C  -4.72216  3.87394  1.03691
C  -3.93926  2.68213  0.98694
C  -2.57927  2.56065  1.26103
C  -1.83669  1.38848  1.42465
C  -2.20985  0.02044  1.55517
C  -1.07023  -0.73342  1.71031
C  0.0564  0.12874  1.65673
C  1.43173  -0.09026  1.64089
C  2.0957  -1.30343  1.47566
C  1.65044  -2.6572  1.38353
C  2.74729  -3.45725  1.16242
C  3.89572  -2.62414  1.06876
C  5.22146  -2.93423  0.7695
C  6.19403  -1.97031  0.48571
N  5.89813  -0.6536  0.29641
C  7.08439  -0.02466  0.08967
C  7.18068  1.34007  -0.21249
C  6.09083  2.14861  -0.51487
C  6.02854  3.54698  -0.77244
C  4.72218  3.87398  -1.03691
C  3.93926  2.68219  -0.98689
C  2.57925  2.56073  -1.26088
C  1.83667  1.38855  -1.42442
C  2.20985  0.02051  -1.55484
C  1.07022  -0.73336  -1.71002
C  -0.05642  0.1288  -1.65564
C  -1.43175  -0.09021  -1.64078
C  -2.0957  -1.30338  -1.47559
C  -1.65042  -2.65714  -1.38344
C  -2.74727  -3.45721  -1.16239
C  -3.89572  -2.62413  -1.06879
C  -5.22147  -2.93423  -0.79691
C  -6.19404  -1.97031  -0.48587
N  -5.89812  -0.65361  -0.29657
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C  -7.18065  1.34009  0.21227
N  -4.80311  1.67249  0.64892
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N  3.45477  -1.3444  1.29308
C  7.6185  -2.18778  0.38148
C  8.17861  -0.96549  0.16775
N  4.80313  1.67251  -0.64899
N  0.46124  1.40721  -1.54606
N  -3.45478  -1.34437  -1.29307
C  -7.61853  -2.18775  -0.38173
C  -8.17862  -0.96544  -0.16803
H  0.62448 -2.98719  1.47731  
H  2.75933 -4.53393  1.04358  
H  8.11762 -3.14445  0.48913  
H  9.22766 -0.72177  0.04113  
H  6.88356  4.21133 -0.74865  
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H -6.88351  4.21133  0.74852  
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H  4.10335 -0.56392  1.21199  
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H -2.04742  0.80035 -1.62997  
H  2.04854  3.50362 -1.3966  
H -3.22628 -0.35622  1.58153  
H -1.03674 -1.80451  1.85593  
H  0.11262  2.22109  1.38185  
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SCF Done: E(RM06) = -1978.90164996 A.U. after 17 cycles

3h (Twisted-Hückel [38]T2C,C)

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C  -6.28886 -1.92261 -0.72268  
C  -5.33994 -2.83314 -1.19807  
C  -4.01899 -2.50196 -1.4841  
C  -2.91742 -3.32569 -1.84435  
C  -1.80515 -2.5276 -1.97013  
C  -2.19279 -1.17706 -1.71752  
C  -1.48186  0.02213 -1.71333  
C  -0.09829  0.17296 -1.67678  
C  0.97137 -0.75485 -1.5612  
C  2.15302 -0.05835 -1.46687  
C  1.86593  1.3358 -1.53538  
C  2.6707  2.47624 -1.53093  
C  4.04237  2.57304 -1.31379  
N  4.89022  1.58252 -0.88976  
C  6.19291  2.03634 -0.84386  
C  7.27139  1.24567 -0.47008  
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SCF Done: E(RM06) = -1978.90146269  A.U. after 16 cycles

3i (Twisted-Hückel [38] \( T_{2_{20}} \))

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C  -0.15873  0.17979  1.61858
C  -0.09651  1.56445  1.52116
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SCF Done: \( E(\text{RM06}) = -1978.91268275 \) A.U. after 19 cycles

4a (Hückel [36] \( \text{C}^2 \text{T}^{0,10,25,30} \))

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C  -5.23045 -4.05323 -0.19933
C  -3.87399 -3.91427 -0.01533
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SCF Done: E(RM06) = -1978.41818064  A.U. after 17 cycles

4b (Hückel [36]^2+7Φ[C,E,F,H])

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C  3.33493800  5.18653500  -0.39621000
C  2.02891000  5.57492400  -0.37827500
C  0.86456500  4.76214700  -0.19518100
N  -0.31925900  5.34248500  -0.06810600
C  -1.21743500  4.31284900  0.12954900
C  -2.55979900  4.55526000  0.27687800
C  -3.49949900  3.55663100  0.65623300
C  -3.30350300  2.40741800  1.42913000
C  -4.50839100  1.71279800  1.47689300
C  -5.45434900  2.43479700  0.73363900
C  -6.80603900  2.07884100  0.40832000
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SCF Done: E(RM06) = -1978.36842618  A.U. after 7 cycles

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SCF Done:  E(RM06) =  -1978.40266700  A.U. after  7 cycles

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SCF Done: E(RM06) = -1978.37780916 A.U. after 7 cycles

4f (Möbius [36]^{1}J^{RCF})

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C  8.35484  1.16523  -0.98657  
C  7.61095  2.16428  -1.50577  
C  6.22271  1.84401  -1.18692  
C  5.15562  2.71355  -1.46242  
C  3.82154  2.44767  -1.19676  
N  2.81414  3.38742  -1.21675  
C  1.6126  2.82487  -0.84728  
C  0.44756  3.53859  -0.63257  
C  -0.7948  2.9464  -0.35265  
C  -1.29504  1.64637  -0.6369  
C  -2.56749  1.55249  -0.12977  
C  -2.89591  2.79061  0.48849  
C  -3.99139  3.20447  1.24232  
C  -5.14765  2.5022  1.55155  
N  -5.54265  1.27603  1.07485  
C  -6.76638  0.94876  1.59626  
C  -7.51861  -0.14915  1.1802  
C  -7.14167  -1.05178  0.19261  
C  -8.09009  -1.9148  -0.49238  
C  -7.41602  -2.45704  -1.52954  
C  -6.04508  -1.99125  -1.40105  
C  -5.00882  -2.42458  -2.23846  
C  -3.65555  -2.33717  -1.97028  
N  -3.0972  -1.90954  -0.7888  
C  -1.73212  -2.10888  -0.80144  
C  -0.91984  -1.91676  0.30652  
C  0.48249  -2.00518  0.31236  
C  1.4322  -1.9283  -0.74335  
C  2.69193  -2.02566  -0.20168  
C  2.56416  -2.17734  1.20473  
C  3.5373  -2.47157  2.16457  
C  4.90717  -2.30765  2.00421  
N  5.51493  -1.51538  1.05813  
C  6.87502  -1.61631  1.1712  
C  7.77295  -0.82381  0.45337  
N  6.12647  0.67914  -0.5094  
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C  1.88027  1.43397  -0.61827  
N  -1.80424  3.61154  0.29149  
C  -6.16266  2.94076  2.45599  
C  -7.14369  1.98874  2.49302  
N  -5.89222  -1.13969  -0.35794  
C  -2.5782  -2.78502  -2.79627  

75
SCF Done: E(RM06) = -1978.42150412  A.U. after 7 cycles

4g (Twisted-Hückel [36]+T20\gamma)

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C  6.51797  3.34541  -1.1295
C  5.30091  3.72498  -1.60204
C  4.38285  2.62706  -1.41824
C  3.03161  2.59233  -1.75845
C  2.22585  1.45551  -1.71363
N  0.86114  1.49875  -1.76206
C  0.30839  0.22012  -1.683
C  -1.04353  0.00815  -1.63452
C  -1.74085  -1.21867  -1.4971
C  -1.32802  -2.56827  -1.45017
C  -2.46065  -3.35521  -1.31703
C  -3.57691  -2.50003  -1.25357
C  -4.94538  -2.83311  -1.1339
C  -5.97827  -1.95883  -0.88806
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4h (Twisted-Hückel [36]22-2T2(6))
SCF Done: E(RM06) = -1978.42701832  A.U. after 20 cycles

4i (Twisted-Hückel [36]2−T2′ex)

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| C      | 5.44302700 | 3.57405400 | -0.22358200 |
| C      | 4.21801000 | 4.16940200 | -0.46687400 |
| C      | 3.28322100 | 3.13905500 | -0.69104600 |
| C      | 1.93691300 | 3.22653400 | -1.09867300 |
| C      | 1.11227700 | 2.16036700 | -1.37511200 |
| N      | 1.49845900 | 0.83169300 | -1.28840600 |
| C      | 0.41071300 | 0.13455600 | -1.61793800 |
| C      | 0.44774400 | -1.29248800 | -1.70675600 |
| C      | -0.60920200 | -2.14104000 | -1.57891800 |
| C      | -0.60358800 | -3.55995500 | -1.81055600 |
| C      | -1.83699500 | -4.04448800 | -1.53127000 |
| C      | -2.66927700 | -2.95410200 | -1.09005300 |
| C      | -3.98562800 | -3.10117500 | -0.69885400 |
| C      | -4.94012400 | -2.14124200 | -0.34576900 |
| N      | -4.77684600 | -0.78080000 | -0.28205400 |
| C      | -6.01240800 | -0.17896800 | -0.00449600 |
| C      | -6.23231500 | 1.16681300 | 0.14765900 |
| C      | -5.25966100 | 2.17659900 | 0.27404300 |
| C      | -5.44301400 | 3.57402300 | 0.22360300 |
| C      | -4.21798000 | 4.16932100 | 0.46692700 |
| C      | -3.28322900 | 3.13893600 | 0.69108700 |
| C      | -1.93693200 | 3.22637400 | 1.09876800 |
| C      | -1.11230800 | 2.16020400 | 1.37524400 |
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H 4.05318100 -0.28572300 0.78874500

SCF Done: E(RM06) = -1978.42096839  A.U. after 19 cycles

5a (Hückel [38])2+705.1025,30)

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C 8.95199 -0.9007 -0.48497
C 9.0548 0.47109 -0.4561
C 7.78807 1.00613 -0.11962
C 7.38795 2.32803 0.04415
C 6.06244 2.75176 0.12227
C 5.53482 3.99784 0.54698
C 4.16363 3.9412 0.46967
C 3.79182 2.6678 -0.04059
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C 1.28395 2.55404 -0.17141
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SCF Done: $E(\text{RM06}) = -1979.63837571$ A.U. after 8 cycles

$5b$ (Hückel [38]$^2\! T\pi^B,C,F,H$)

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SCF Done: \( E(RM06) = -1979.628777659 \) A.U. after 7 cycles

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5g (Twisted-Hückel [38]²1T₂\(\Delta\))

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5h (Twisted-Hückel [38]^2*72c.0)

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SCF Done: E(RM06) = -1979.64484814  A.U. after 7 cycles

Si (Twisted-Hückel [38]±2T_{2u})

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C  -4.33735  -3.84487  -2.05618
C  -3.31436  -2.92795  -1.70149
C  -1.95092  -3.06393  -1.90768
C  -0.97632  -2.07643  -1.77017
C   0.42953  -2.24083  -1.71439
C   1.00415  -0.99903  -1.57573
C  -0.02353  -0.01971  -1.5692
C  -0.00932  1.37188  -1.52206
C   1.07841  2.22825  -1.40293
C   1.02778  3.64692  -1.37862
C   2.31103  4.12744  -1.28283
C   3.19381  3.02176  -1.21852
C   4.58101  3.03067  -1.18805
C   5.4293  1.95511  -0.94648
N   5.04573  0.72585  -0.40235
C   6.18134  -0.06152  -0.23212
C   6.27049  -1.30328  0.38867
C   5.30301  -2.09146  0.99195
C   5.53779  -3.33213  1.64327
C   4.3374  -3.84491  2.05611
C   3.3144  -2.92801  1.70144
C   1.95095  -3.06401  1.90765
C   0.97633  -2.07653  1.77017
C  -0.42951  -2.24095  1.71441
C  -1.00415  -0.99916  1.57576
C   0.02352  -0.01981  1.56924
C   0.00929  1.37177  1.52211
C  -1.07843  2.22815  1.403
C  -1.02778  3.64682  1.3787
C  -2.31103  4.12736  1.28291
C  -3.19382  3.02169  1.21858
C  -4.58102  3.03063  1.18808
C  -5.42932  1.95508  0.94648
N  -5.04574  0.72582  0.40234
C  -6.18135  -0.06154  0.23208
C  -6.2705  -1.30329  -0.38873
N  -3.93751  -1.83521  -1.09222
N   2.40692  1.86935  -1.23441
N  -1.21905  -0.72299  -1.64346
C   6.81933  1.88543  -1.19756
N   1.21905  -0.72308  1.64349
C   7.26945  0.65518  -0.78861
N   3.93751  -1.83527  1.09216
N  -2.40695  1.86927  1.23447
C  -6.81935  1.8854  1.19753
C  -7.26947  0.65515  0.78857
H  -6.52101  -3.76375  -1.78393
H  -4.16611  -4.76703  -2.59722
H   0.93391  -3.19864  -1.75354
H   2.06759  -0.80782  -1.49816
H   0.11069 4.22078 -1.43998
H   2.62735 5.16237 -1.24519
H   7.39317 2.67332 -1.66909
H   8.27728 0.26576 -0.86154
H   6.52106 -3.76375 1.78384
H   4.16619 -4.76707 2.59714
H  -0.93388 -3.19877 1.75355
H  -2.0676  -0.80797 1.49819
H  -0.11069 4.22067 1.44009
H  -2.62733 5.16233 1.24528
H  -7.39319 2.67328 1.66907
H  -8.2773  0.26574 0.86148
H  -3.44123 -1.31223 -0.38083
H   2.78621 1.01463 -1.62095
H   3.44122 -1.31230 0.38077
H  -2.78626 1.01455 1.62098
H  -5.06276 3.98255 1.39915
H  -7.27543 -1.71886 -0.42026
H   1.60535 -4.04679 2.21903
H  -1.60529 -4.04669 -2.21906
H   5.06275  3.98259 -1.39913
H  -0.97351  1.87682 -1.58885
H   0.97348  1.87671  1.58891
H   7.27543 -1.71884  0.42019
H  -2.08003  -0.29718 -1.96339
H   2.08001  -0.29726  1.96341
H   4.27462  0.69307  0.25392
H  -4.27462  0.69304 -0.25392

SCF Done:  E(RM06) =  -1979.65223320  A.U. after 18 cycles