Supplemental materials

S.I. Table I: Cartesian Coordinates (in Angstroms) for Geometry Optimized 1-Chloro-1,2,2-trifluorocyclobutane in the Standard Orientation.

<table>
<thead>
<tr>
<th>Atomic Center</th>
<th>Equatorial</th>
<th>Axial</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>X</td>
<td>Y</td>
</tr>
<tr>
<td>C1</td>
<td>0.429470</td>
<td>0.392727</td>
</tr>
<tr>
<td>C2</td>
<td>-0.114700</td>
<td>1.335313</td>
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<tr>
<td>C3</td>
<td>-1.550721</td>
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<td>F11</td>
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<tr>
<td>F12</td>
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S.I. Table II. Cartesian Coordinates (in Angstroms) for Geometry Optimized Trans 1,2-Dichlorohexacyclobutane in the Standard Orientation.

<table>
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<tr>
<th>Atomic Center</th>
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<tbody>
<tr>
<td></td>
<td>X</td>
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<tr>
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Parameterizations of F3 and F6

S.I. Table III. Cartesian Coordinates (in Angstroms) for Geometry Optimized Cis 1,2-Dichlorohexacyclobutane in the Standard Orientation.

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