Table S1: Electronic energies, Zero-Point Vibrational Energies, Thermal Energies, Entropies and relative free energies for species calculated at B3LYP/LANL2DZ for structures described in Figures 3 and 7. Italicized relative free energy values are in kcal mol\(^{-1}\) while values in parentheses are in kJ mol\(^{-1}\).

<table>
<thead>
<tr>
<th>Structure</th>
<th>Electronic energy (Hartrees)</th>
<th>ZPE (kcal mol(^{-1}))</th>
<th>(H_{298}^o - H_0^o) (kcal mol(^{-1}))</th>
<th>Entropy (cal mol(^{-1}) K(^{-1}))</th>
<th>Relative free energy at 298 K</th>
</tr>
</thead>
<tbody>
<tr>
<td>1A</td>
<td>-1639.2886242</td>
<td>312.6</td>
<td>19.6</td>
<td>196.8</td>
<td>0.0 (0.0)</td>
</tr>
<tr>
<td>TS(_{(1A\rightarrow1B)})</td>
<td>-1639.2026501</td>
<td>309.3</td>
<td>20.5</td>
<td>207.5</td>
<td>48.3 (202.1)</td>
</tr>
<tr>
<td>1B</td>
<td>-1639.2708451</td>
<td>312.4</td>
<td>20.5</td>
<td>207.6</td>
<td>8.7 (36.4)</td>
</tr>
<tr>
<td>TS(_{(1B\rightarrow1C)})</td>
<td>-1639.2497207</td>
<td>311.1</td>
<td>20.5</td>
<td>206.8</td>
<td>20.8 (87.0)</td>
</tr>
<tr>
<td>1C</td>
<td>-1639.2682279</td>
<td>312.3</td>
<td>20.5</td>
<td>206.6</td>
<td>10.4 (43.5)</td>
</tr>
<tr>
<td>TS(_{(1C\rightarrow2A)})</td>
<td>-1639.1456481</td>
<td>307.1</td>
<td>20.9</td>
<td>210.0</td>
<td>81.6 (341.4)</td>
</tr>
<tr>
<td>2A</td>
<td>-1639.2843606</td>
<td>311.4</td>
<td>21.4</td>
<td>218.1</td>
<td>-3.1 (-13.0)</td>
</tr>
<tr>
<td>2B + CO(_2)</td>
<td>-1639.288777</td>
<td>312.0</td>
<td>20.5</td>
<td>235.1</td>
<td>-11.3 (-47.3)</td>
</tr>
<tr>
<td>TS(_{(2B\rightarrow3A)}) + CO(_2)</td>
<td>-1639.232367</td>
<td>309.8</td>
<td>20.6</td>
<td>241.0</td>
<td>20.3 (84.9)</td>
</tr>
<tr>
<td>3A + CO(_2)</td>
<td>-1639.262436</td>
<td>310.4</td>
<td>20.9</td>
<td>244.4</td>
<td>1.3 (5.4)</td>
</tr>
<tr>
<td>TS(_{(3A\rightarrow4A)}) + CO(_2) + HCOOH</td>
<td>-1639.101313</td>
<td>305.2</td>
<td>21.1</td>
<td>283.6</td>
<td>85.6 (358.2)</td>
</tr>
<tr>
<td>4A + CO(_2) + HCOOH</td>
<td>-1639.229491</td>
<td>307.3</td>
<td>21.7</td>
<td>256.1</td>
<td>7.2 (30.1)</td>
</tr>
</tbody>
</table>