Some other higher energy structures of (9eG:1mT)H⁺ along with their enthalpies and 298 K Gibbs energies relative to GN7_GN7-TO4_TN3-GO6 and computed IR spectra (black trace) compared to the experimental IRMPD spectrum (grey trace). All energies are presented in kJ mol⁻¹.

Figure S1

GO6_TN3-GN7_GO6-TO2
Δ_{rel}H = 20.4
Δ_{rel}G = 20.0

TO2_TO2-GO6_TN3-GN7
Δ_{rel}H = 17.4
Δ_{rel}G = 20.7

GN7_GN1-TO2_TN3-GO6
Δ_{rel}H = 21.6
Δ_{rel}G = 22.1

GN7_GN1-TN3_GN2-TO4_TO2-GO6
Δ_{rel}H = 23.0
Δ_{rel}G = 32.3

GN3_GN1-TN3_GN2-TO2_TO4-GO6
Δ_{rel}H = 51.9
Δ_{rel}G = 59.8

GN3_GN1-TN3_GN2-TO4_TO2-GO6
Δ_{rel}H = 63.6
Δ_{rel}G = 71.6

GN3_GN1-TO4_TN3-GO6
Δ_{rel}H = 73.1
Δ_{rel}G = 72.1

GN3_GN1-TO2_TN3-GO6
Δ_{rel}H = 86.9
Δ_{rel}G = 84.8
Some other higher energy structures of (9eG:9mA)H⁺ along with their enthalpies and 298 K Gibbs energies relative to AN1_AN1-GO6_AN6-GN7 and computed IR spectra (black trace) compared to the experimental IRMPD spectrum (grey trace). All energies are presented in kJ mol⁻¹.

AN1_AN1-GO6_AN6-GN1
\[ \Delta_{rel} H = 34.2 \]
\[ \Delta_{rel} G = 44.6 \]

AN1_AN1-GN1_AN6-GO6
\[ \Delta_{rel} H = 41.9 \]
\[ \Delta_{rel} G = 46.9 \]

GN7_GN1-AN1_GO6-AN6
\[ \Delta_{rel} H = 50.8 \]
\[ \Delta_{rel} G = 54.0 \]

AN1_AN1-GO6_AN6-GN7
\[ \Delta_{rel} H = 65.2 \]
\[ \Delta_{rel} G = 72.1 \]

AN1_AN1-GO6_AN6-GN1
\[ \Delta_{rel} H = 70.1 \]
\[ \Delta_{rel} G = 75.4 \]

GN7_GN2-AN1_AN6-GN3
\[ \Delta_{rel} H = 78.3 \]
\[ \Delta_{rel} G = 76.0 \]

Figure S2
Some other higher energy structures of (9eG:9mA)H⁺ along with their enthalpies and 298 K Gibbs energies relative to AN1_AN1‐GO6_AN6‐GN7 and computed IR spectra (black trace) compared to the experimental IRMPD spectrum (grey trace). All energies are presented in kJ mol⁻¹.
Some other higher energy structures of (9eG:9eG)H+ along with their enthalpies and 298 K Gibbs energies relative to GN7_GN7-GN7_GC8-GO6 and computed IR spectra (black trace) compared to the experimental IRMPD spectrum (grey trace).

All energies are presented in kJ mol⁻¹.
Some other higher energy structures of (9eG:9eG)H$^+$ along with their enthalpies and 298 K Gibbs energies relative to GN7_GN7-GN7_GC8-GO6 and computed IR spectra (black trace) compared to the experimental IRMPD spectrum (grey trace). All energies are presented in kJ mol$^{-1}$. 

Figure S5
Figure S6. Comparison of the geometries of the lowest energy (9eG:1mT)H⁺ structure, GN7_GN7-TO4_TN3-GO6 computed using B3LYPD3 and M06-2X.
Figure S7. Comparison of the geometries of the two lowest energy (9eG:9mA)H⁺ structures computed using B3LYPD3 and M06-2X.
Figure S8. Comparison of the geometries of the lowest energy (9eG:9eG)H⁺ structure, GN7_GN7-GN7_GC8-GO6, computed using B3LYPD3 and M06-2X.
Figure S9. Comparison of the experimental IRMPD spectrum of (9eG:1mT)H\(^+\) with the lowest energy computed IR spectra using M06-2X/6-31+G(d,p).
Figure S10. Comparison of the experimental IRMPD spectrum of (9eG:9mA)H\(^+\) with the lowest energy computed IR spectra using M06-2X/6-31+G(d,p).
Figure S11. Comparison of the experimental IRMPD spectrum of (9eG:9eG)H⁺ with the lowest energy computed IR spectra using M06-2x/6-31+G(d,p).
Table S1 298K relative enthalpies and Gibbs energies, in kJ mol$^{-1}$, of five lowest energy isomers of (9eG:1mT)H$^+$ by three different computational methods. Relative Gibbs energies are indicated in parentheses.

<table>
<thead>
<tr>
<th>Structures of (9eG:1mT)H$^+$</th>
<th>B3LYP3/6-31+G(d,p)</th>
<th>B3LYP3/6-311+G(3df,3pd) //B3LYP3/6-31+G(d,p)</th>
<th>M06-2X/6-31+G(d,p)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GN7_GN7-TO4_TN3-GO6</td>
<td>0.0 (0.0)</td>
<td>0.0 (0.0)</td>
<td>0.0 (0.0)</td>
</tr>
<tr>
<td>TO4_TO4-GO6_TN3-GN7</td>
<td>2.6 (6.8)</td>
<td>3.4 (7.6)</td>
<td>-3.7 (0.2)</td>
</tr>
<tr>
<td>GN7_GN7-TO2_TN3-GO6</td>
<td>10.7 (9.8)</td>
<td>10.2 (9.3)</td>
<td>9.9 (9.2)</td>
</tr>
<tr>
<td>GN7_GN1-TO4_TN3-GO6</td>
<td>11.6 (13.0)</td>
<td>11.5 (12.9)</td>
<td>13.6 (14.7)</td>
</tr>
<tr>
<td>GN7_GN2-TO2_GN1-TN3-GO6</td>
<td>7.0 (16.5)</td>
<td>7.9 (17.4)</td>
<td>4.8 (13.2)</td>
</tr>
</tbody>
</table>

Table S2 298K relative enthalpies and Gibbs energies, in kJ mol$^{-1}$, of four lowest energy isomers of (9eG:1mA)H$^+$ by three different computational methods. Relative Gibbs energies are indicated in parentheses.

<table>
<thead>
<tr>
<th>Structures of (9eG:1mA)H$^+$</th>
<th>B3LYP3/6-31+G(d,p)</th>
<th>B3LYP3/6-311+G(3df,3pd) //B3LYP3/6-31+G(d,p)</th>
<th>M06-2X/6-31+G(d,p)</th>
</tr>
</thead>
<tbody>
<tr>
<td>AN1_AN1-GO6_AN6-GN7</td>
<td>0.0 (0.0)</td>
<td>0.0 (0.0)</td>
<td>0.0 (0.0)</td>
</tr>
<tr>
<td>AN1_AN1-GN7_AN6-GO6</td>
<td>2.1 (1.1)</td>
<td>3.8 (1.8)</td>
<td>4.5 (2.6)</td>
</tr>
<tr>
<td>AN7_AN7-GO6_AN6-GN7</td>
<td>28.3 (29.3)</td>
<td>28.8 (27.8)</td>
<td>30.7 (31.7)</td>
</tr>
<tr>
<td>AN7_AN7-GN7_AN6-GO6</td>
<td>35.6 (36.7)</td>
<td>34.9 (36.0)</td>
<td>33.2 (35.5)</td>
</tr>
</tbody>
</table>

Table S3 298K relative enthalpies and Gibbs energies, in kJ mol$^{-1}$, of five lowest energy isomers of (9eG:9eG)H$^+$ by three different computational methods. Relative Gibbs energies are indicated in parentheses.

<table>
<thead>
<tr>
<th>Structures of (9eG:9eG)H$^+$</th>
<th>B3LYP3/6-31+G(d,p)</th>
<th>B3LYP3/6-311+G(3df,3pd) //B3LYP3/6-31+G(d,p)</th>
<th>M06-2X/6-31+G(d,p)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GN7_GN7-GN7_GC8-GO6</td>
<td>0.0 (0.0)</td>
<td>0.0 (0.0)</td>
<td>0.0 (0.0)</td>
</tr>
<tr>
<td>GO6_GO6-GN7_GN1/GN2-GO6</td>
<td>4.1 (7.3)</td>
<td>3.2 (6.4)</td>
<td>-0.2 (3.9)</td>
</tr>
<tr>
<td>GN7_GN1-GN7_GN2-GO6</td>
<td>7.1 (12.2)</td>
<td>6.3 (11.5)</td>
<td>10.7 (15.7)</td>
</tr>
<tr>
<td>GN7_GN7-GO6_GC8-GN7</td>
<td>15.9 (14.4)</td>
<td>14.4 (12.8)</td>
<td>15.2 (9.8)</td>
</tr>
<tr>
<td>GN7_GN7-GO6_GO6-GN7</td>
<td>19.5 (21.6)</td>
<td>17.0 (19.0)</td>
<td>16.7 (15.0)</td>
</tr>
</tbody>
</table>