Electronic Supplementary Material for Organic & Biomolecular Chemistry

Supporting Information

Triflic Acid-Catalyzed Adamantylation of Aromatics in [BMIM][OTf] Ionic Liquid; Synthetic Scope and Mechanistic Insight[+]

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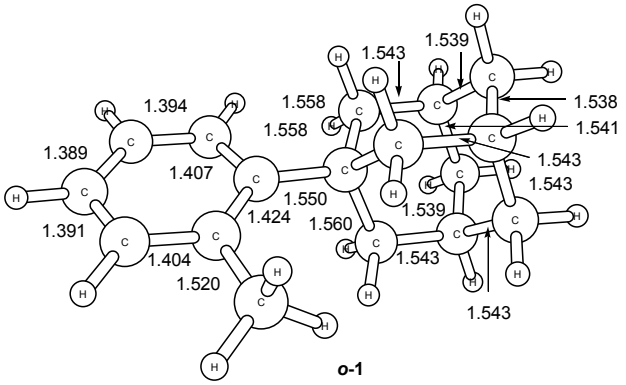
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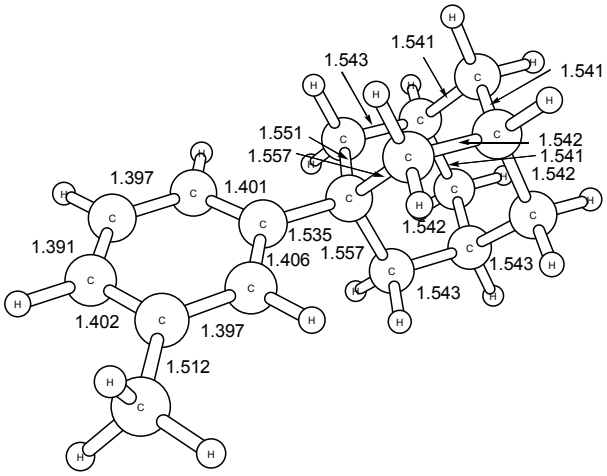
1.543

***o*-1**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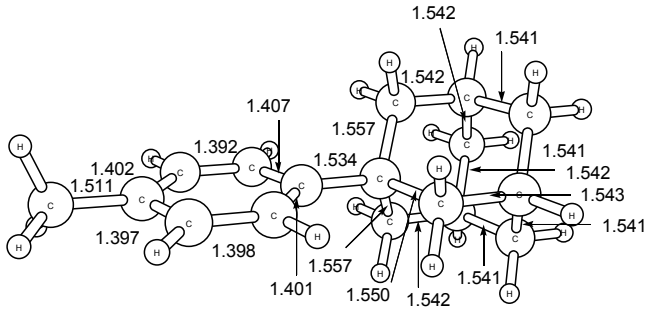
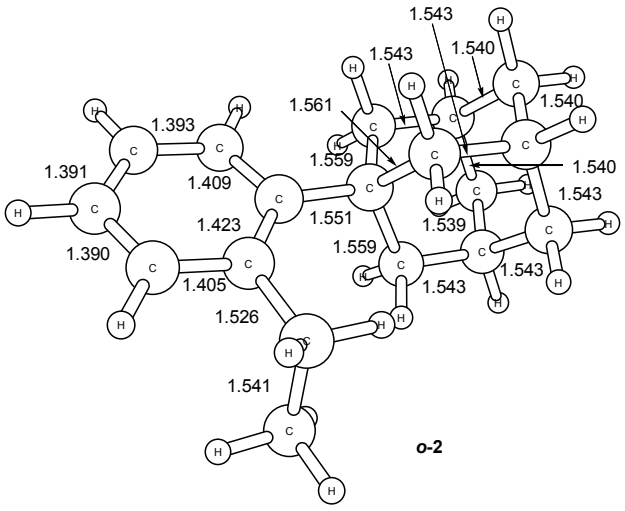
1.512

***m*-1**

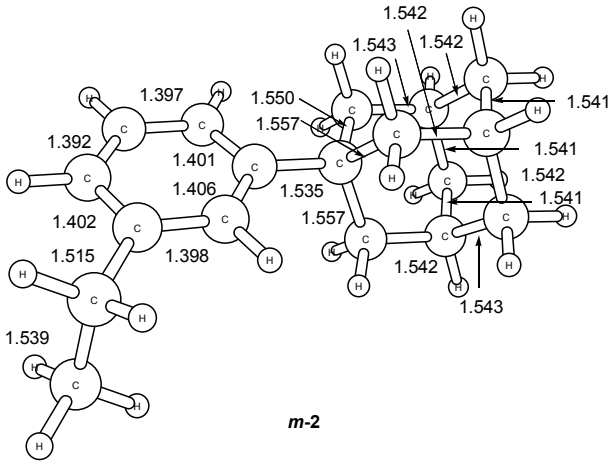


p-**1**

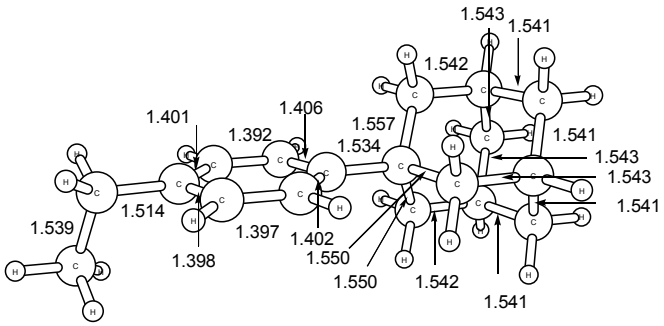
Fig S1. B3LYP/6-31G(d) optimized geometries and bond lengths, Å, fo*r* ***o*-1**, ***m*-1**, ***p*-1**, ***o*-2**, ***m*-2**, ***p*-2**, ***o*-3**, ***p*-3**, ***m*-3**, ***o*-1H$^+$**, ***m*-1H$^+$**, ***p*-1H$^+$**, ***o*-2H$^+$**, ***m*-2H$^+$**, ***p*-2H$^+$**, ***o*-3H$^+$**, ***p*-3H$^+$**, ***m*-3H$^+$**, **4H$^+$** and **5H$^+$**.



o-**2**

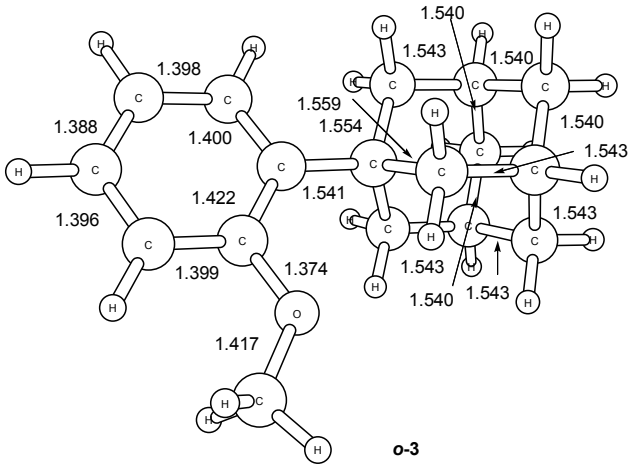


m-**2**

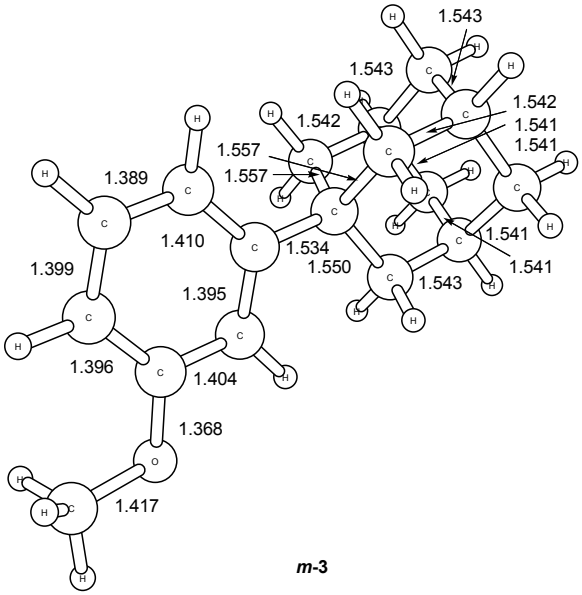


p-**2**

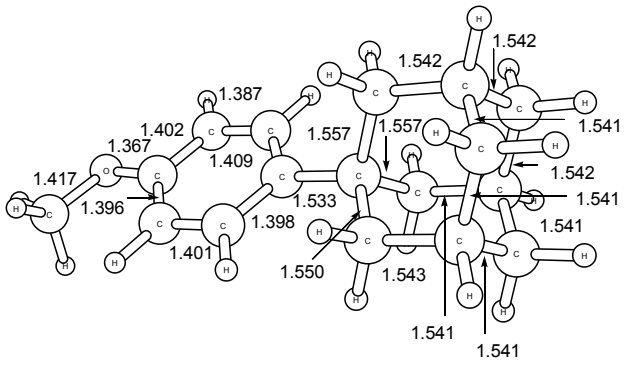
Fig S1 (continued).



o-**3**

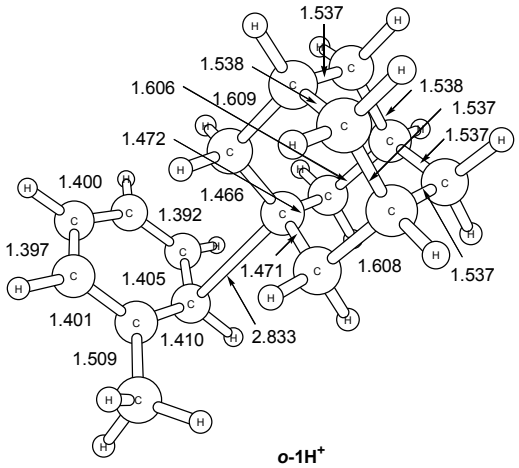


m-**3**

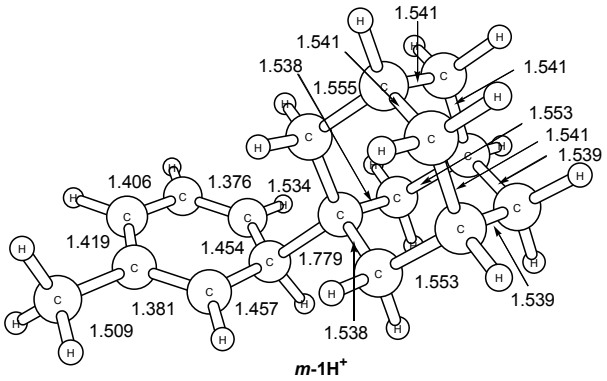


p-**3**

Fig S1 (continued).



o-**1H**$^+$



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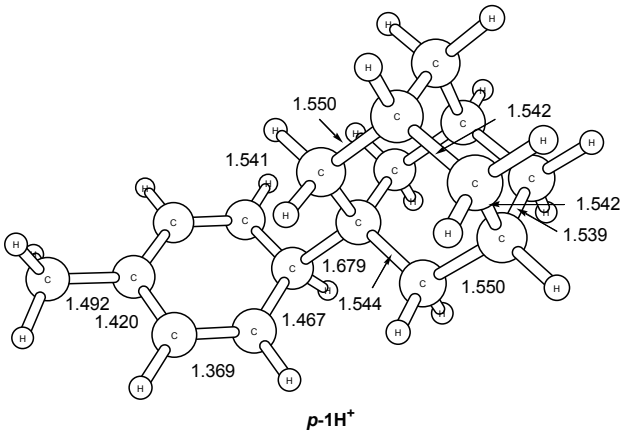
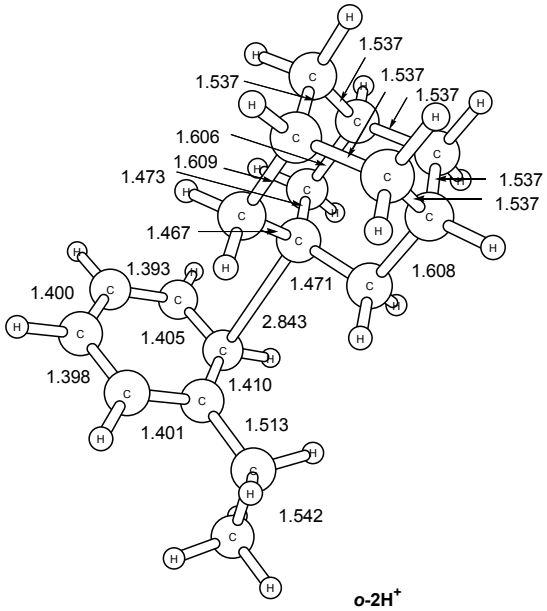
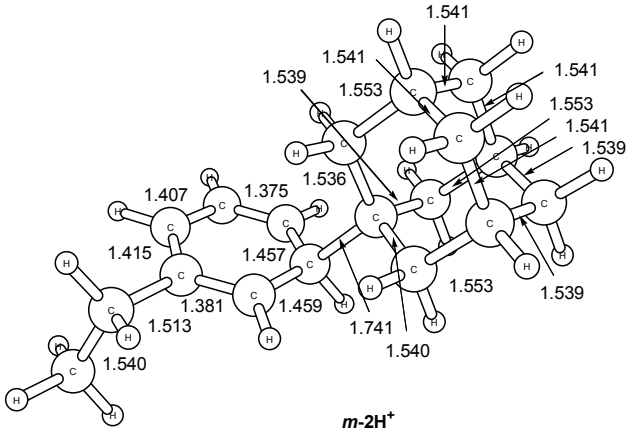


p-1H$^+$

Fig S1 (continued).



o-2H$^+$



m-2H$^+$

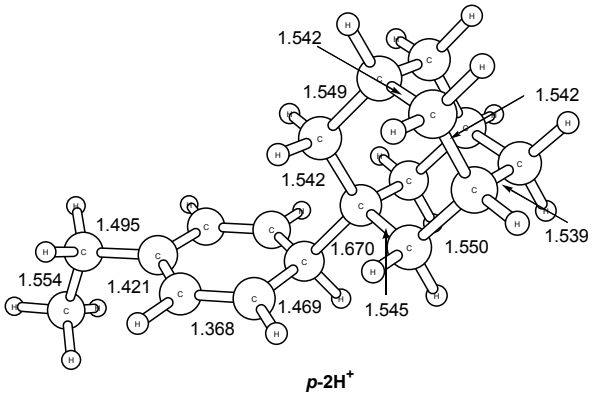
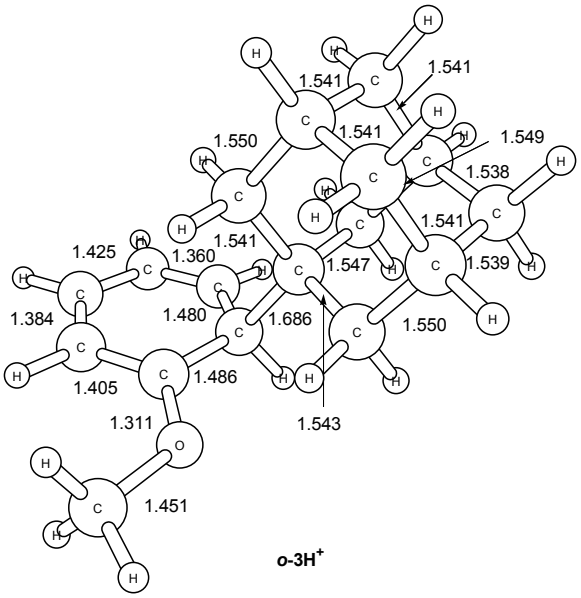
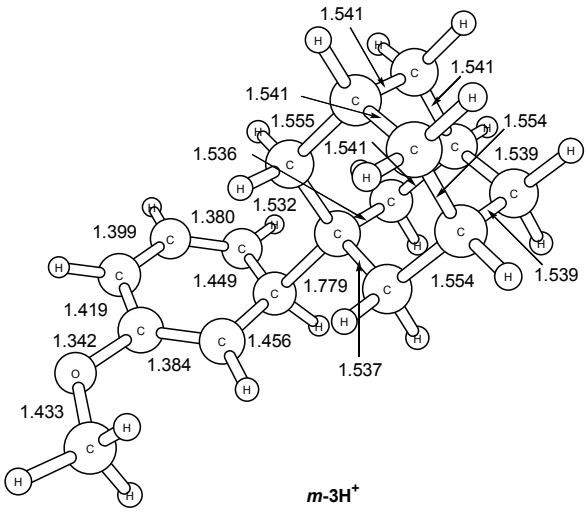


Fig S1 (continued).





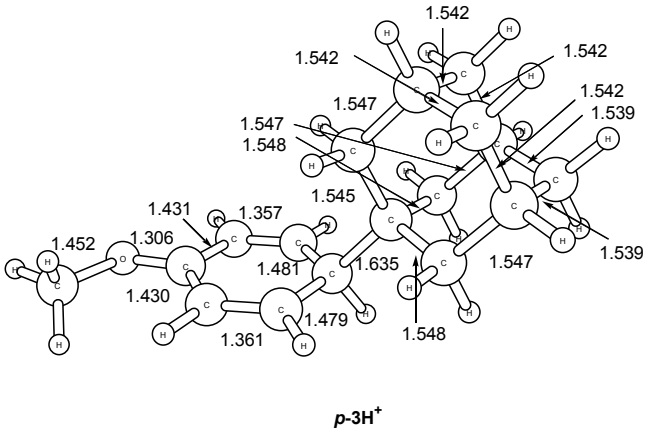
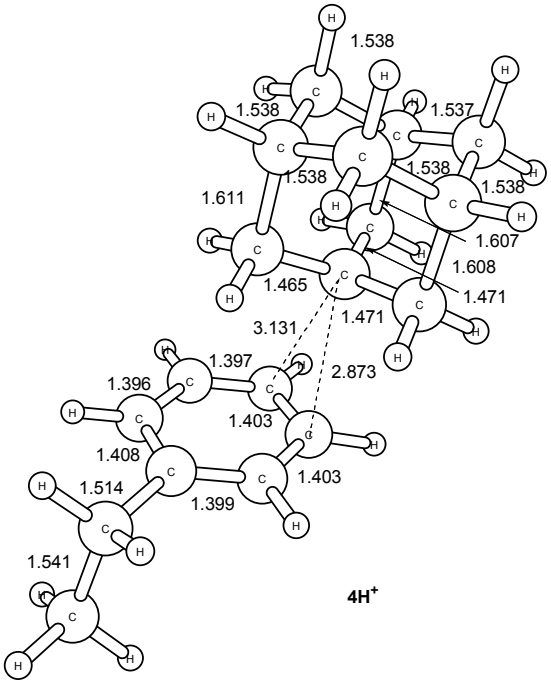
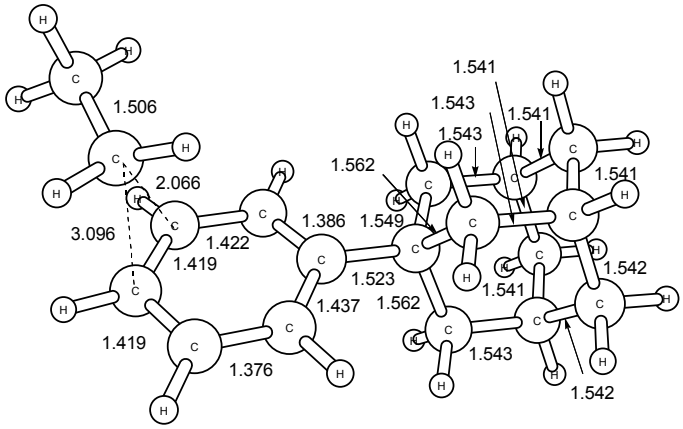


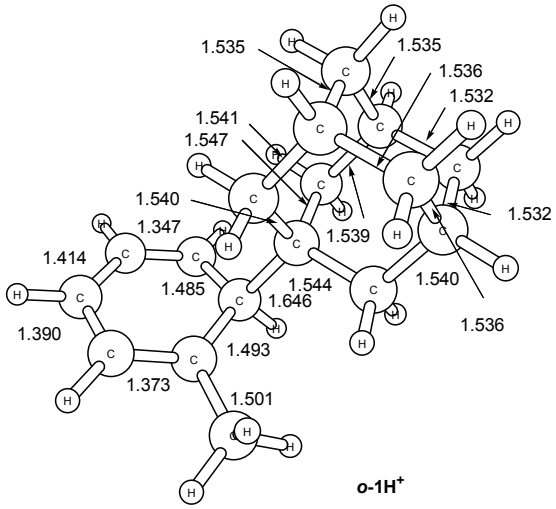
Fig S1 (continued).



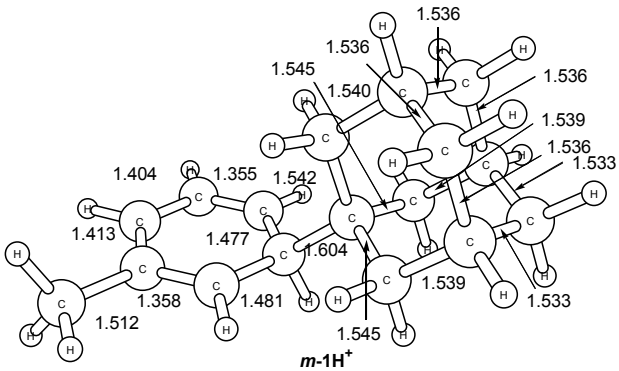


5H$^+$

Fig S1 (continued).



***o*-1H$^+$**



***m*-1H$^+$**

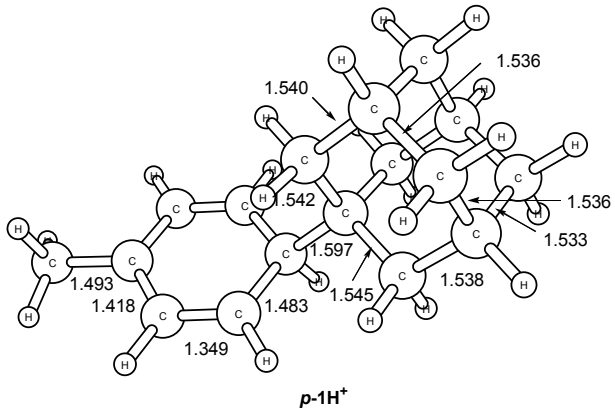
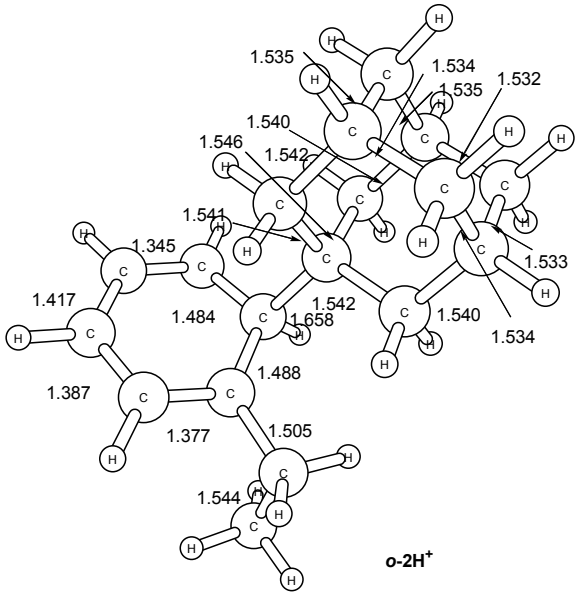
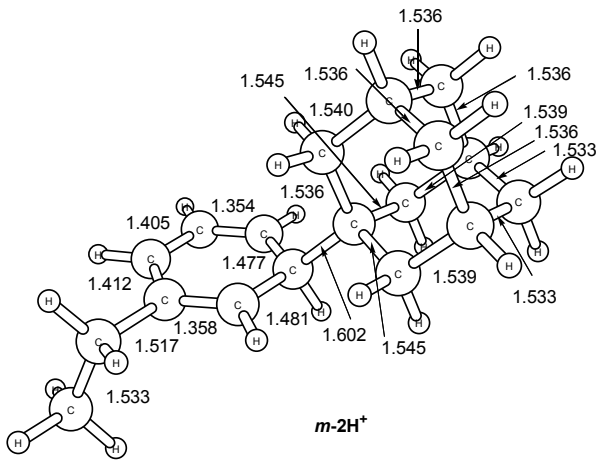
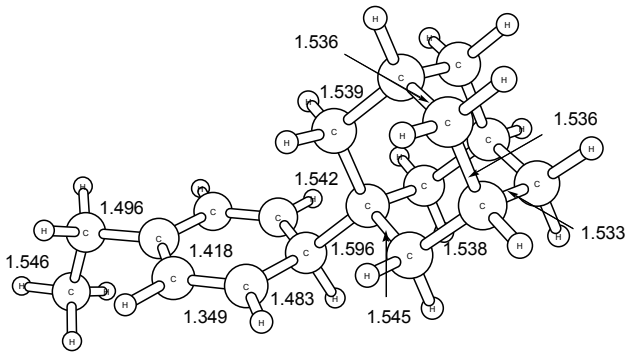


Fig S2. HF/6-31G(d) optimized geometries and bond lengths, Å, for ***o*-1H**$^+$, ***m*-1H**$^+$, ***p*-1H**$^+$, ***o*-2H**$^+$, ***m*-2H**$^+$, and ***p*-2H**$^+$.







p-2H$^+$

Fig S2 (continued).