Supporting Information

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

Kenneth K. Laali*, Viorel D. Sarca, Takao Okazaki, Aaron Brock, and Paul Der

Department of Chemistry, Kent State University, Kent, OH 44242, USA

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**Fig S1.** B3LYP/6-31G(d) optimized geometries and bond lengths, Å, for 


**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+.
Fig S1. B3LYP/6-31G(d) optimized geometries and bond lengths, Å, for 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⁺.
Fig S1 (continued).
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**Fig S2.** HF/6-31G(d) optimized geometries and bond lengths, Å, for \( o-1H^+ \), \( m-1H^+ \), \( p-1H^+ \), \( o-2H^+ \), \( m-2H^+ \), and \( p-2H^+ \).
Fig S2 (continued).