Supporting Information File

**Revised**

**Allenediazonium Ions and their Protonation Chemistry: A DFT Study**

Rodrigo O. M. A. de Souza\(^a\), Pierre M. Esteves\(^a,\)*, Kenneth K. Laali\(^b,\)*

\(^a\) Institute of Chemistry, Universidade Federal do Rio de Janeiro, Brazil
\(^b\) Department of Chemistry, Kent State University Kent, Ohio, USA

**List of Captions**

**Figure S1:** Optimized structures for protonated allenediazonium cation C, with selected geometric parameters, CHelpg charges \((q)\) and GIAO-NMR chemical shifts.

**Figure S2:** Optimized structures for protonated allenediazonium cation D, with selected geometric parameters, CHelpg charges \((q)\) and GIAO-NMR chemical shifts.

**Figure S3:** Optimized structures for protonated allenediazonium cation E, with selected geometric parameters, CHelpg charges \((q)\) and GIAO-NMR chemical shifts.

**Figure S4:** Optimized structures for protonated allenediazonium cation G, with selected geometric parameters, CHelpg charges \((q)\) and GIAO-NMR chemical shifts.

**Figure S5:** Optimized structures for protonated allenediazonium cation I, with selected geometric parameters, CHelpg charges \((q)\) and GIAO-NMR chemical shifts.

**Figure S6:** Optimized structures for protonated allenediazonium cation J, with selected geometric parameters, CHelpg charges \((q)\) and GIAO-NMR chemical shifts.

**Figure S7:** Optimized structures for protonated allenediazonium cation K, with selected geometric parameters, CHelpg charges \((q)\) and GIAO-NMR chemical shifts.
Figure S1. Optimized structures for protonated allenediazonium cation C, with selected geometric parameters, CHelpg charges ($q$) and GIAO-NMR chemical shifts.
**Figure S2:** Optimized structures for protonated allenediazonium cation D, with selected geometric parameters, CHelpg charges \((q)\) and GIAO-NMR chemical shifts.

![Diagram of optimized structures for protonated allenediazonium cation D with selected geometric parameters, CHelpg charges \((q)\) and GIAO-NMR chemical shifts.](image)
Figure S3: Optimized structures for protonated allenediazonium cation E, with selected geometric parameters, CHelpg charges ($q$) and GIAO-NMR chemical shifts.
**Figure S4.** Optimized structures for protonated allenediazonium cation G, with selected geometric parameters, CHelpG charges ($q$) and GIAO-NMR chemical shifts.
**Figure S5:** Optimized structures for protonated allenediazonium cation I, with selected geometric parameters, CHelpg charges ($q$) and GIAO-NMR chemical shifts.
**Figure S6.** Optimized structures for protonated allenediazonium cation J, with selected geometric parameters, CHelpg charges ($q$) and GIAO-NMR chemical shifts.
Figure S7. Optimized structures for protonated allenediazonium cation $\mathbf{K}$, with selected geometric parameters, CHelpg charges ($q$) and GIAO-NMR chemical shifts.