

## Supporting Information File

*Revised*

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

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#### 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.

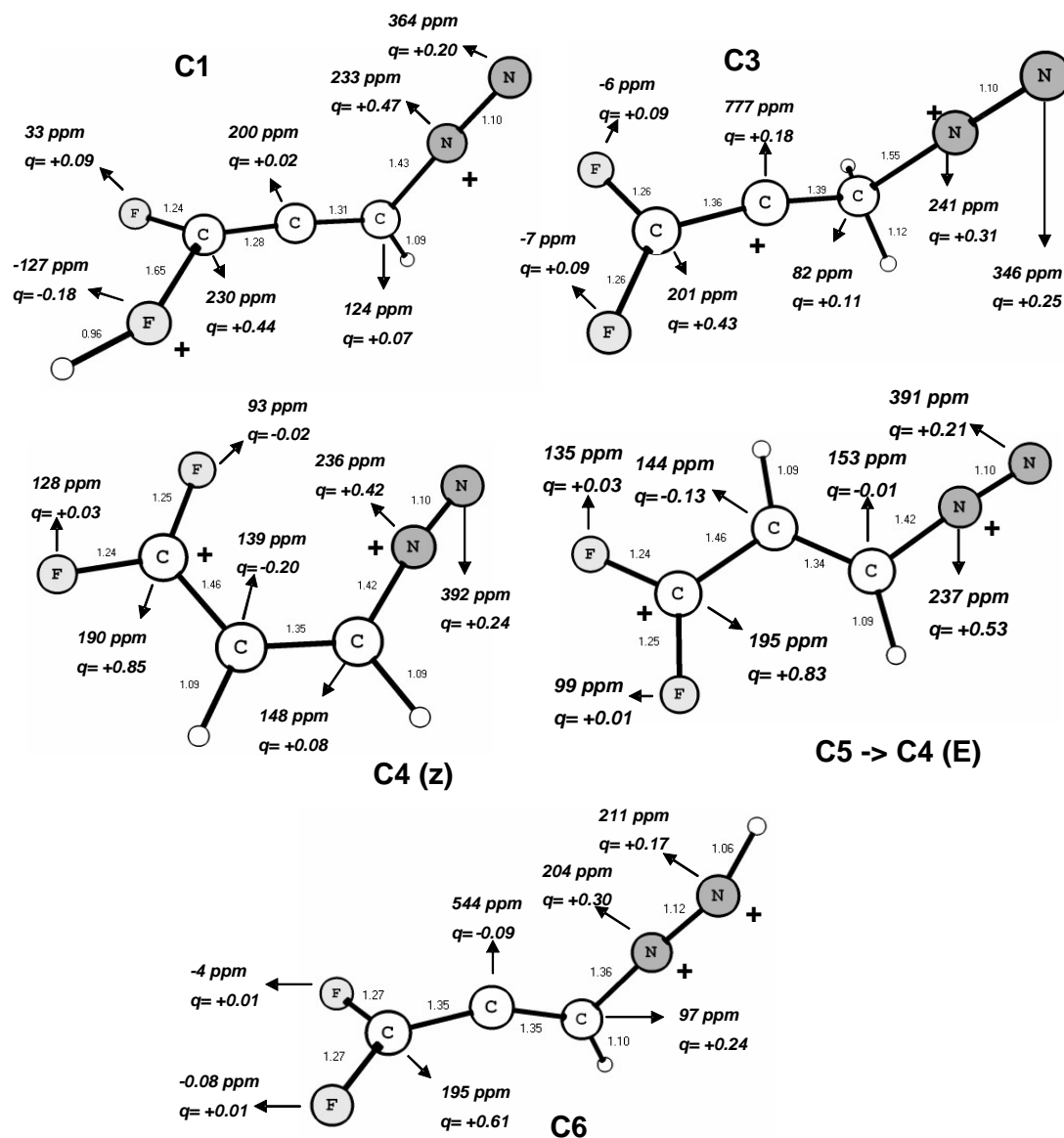
**Figure S4.** Optimized structures for protonated allenediazonium cation **G**, with selected geometric parameters, CHelpg charges ( $q$ ) and GIAO-NMR chemical shifts.

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

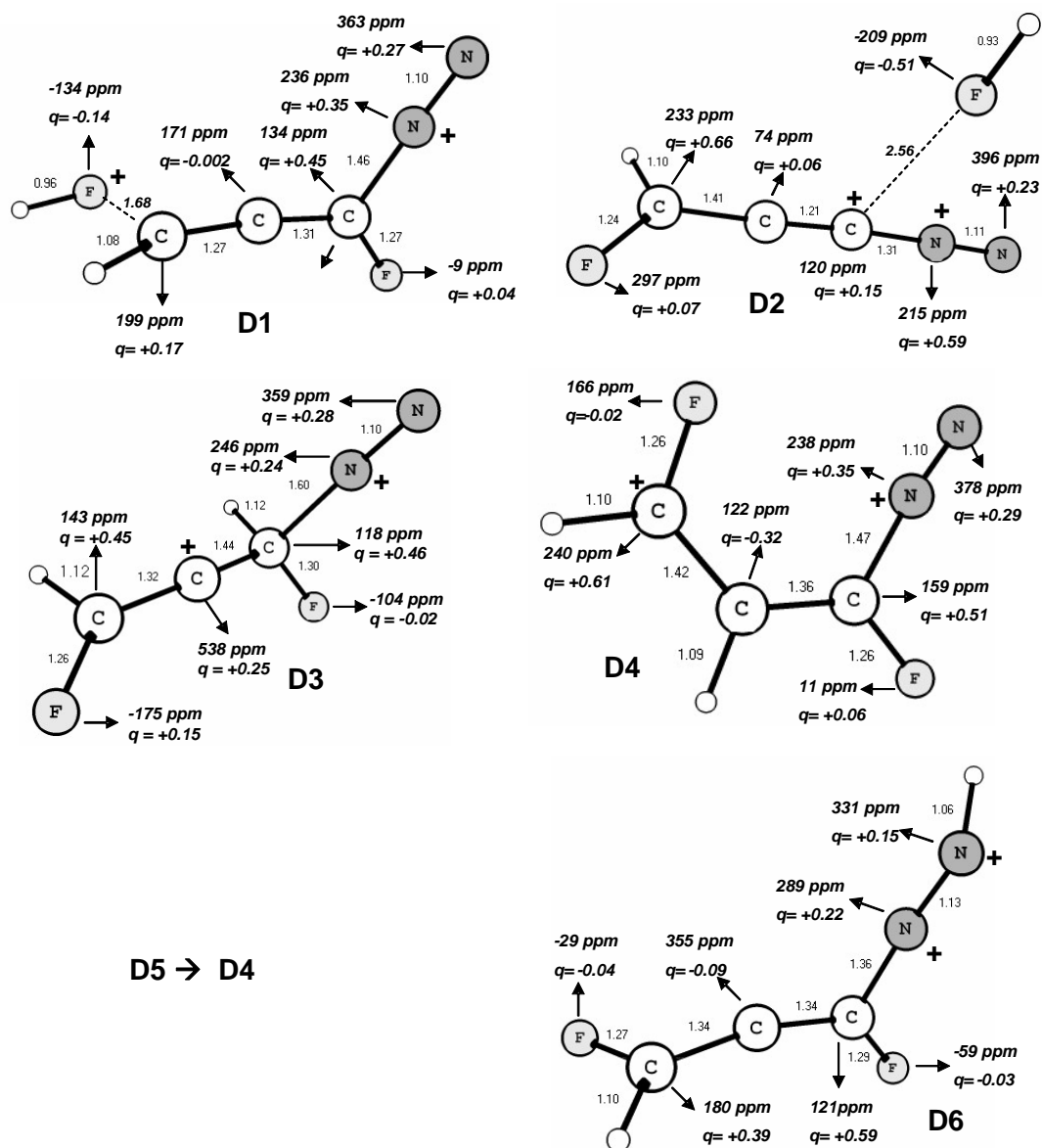
**Figure S6.** Optimized structures for protonated allenediazonium cation **J**, with selected geometric parameters, CHelpg charges ( $q$ ) and GIAO-NMR chemical shifts.

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

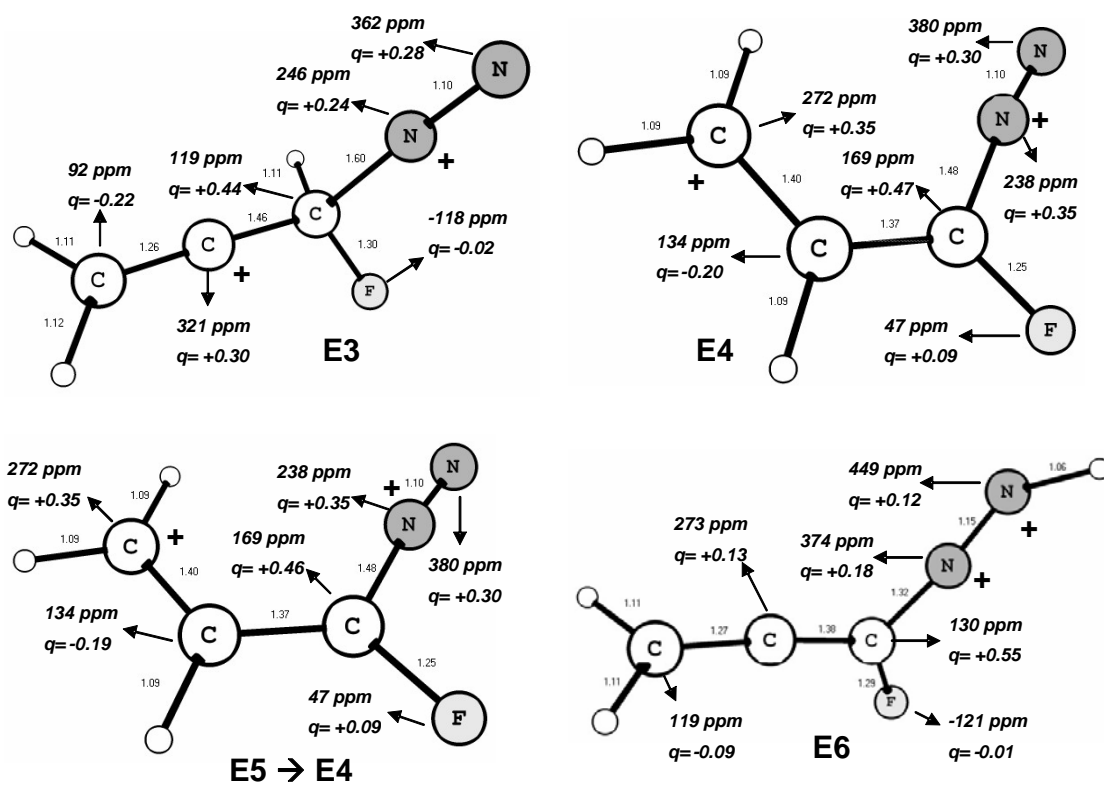
**Figure S1.** Optimized structures for protonated allenediazonium cation **C**, with selected geometric parameters, CHelpg charges ( $q$ ) and GIAO-NMR chemical shifts.



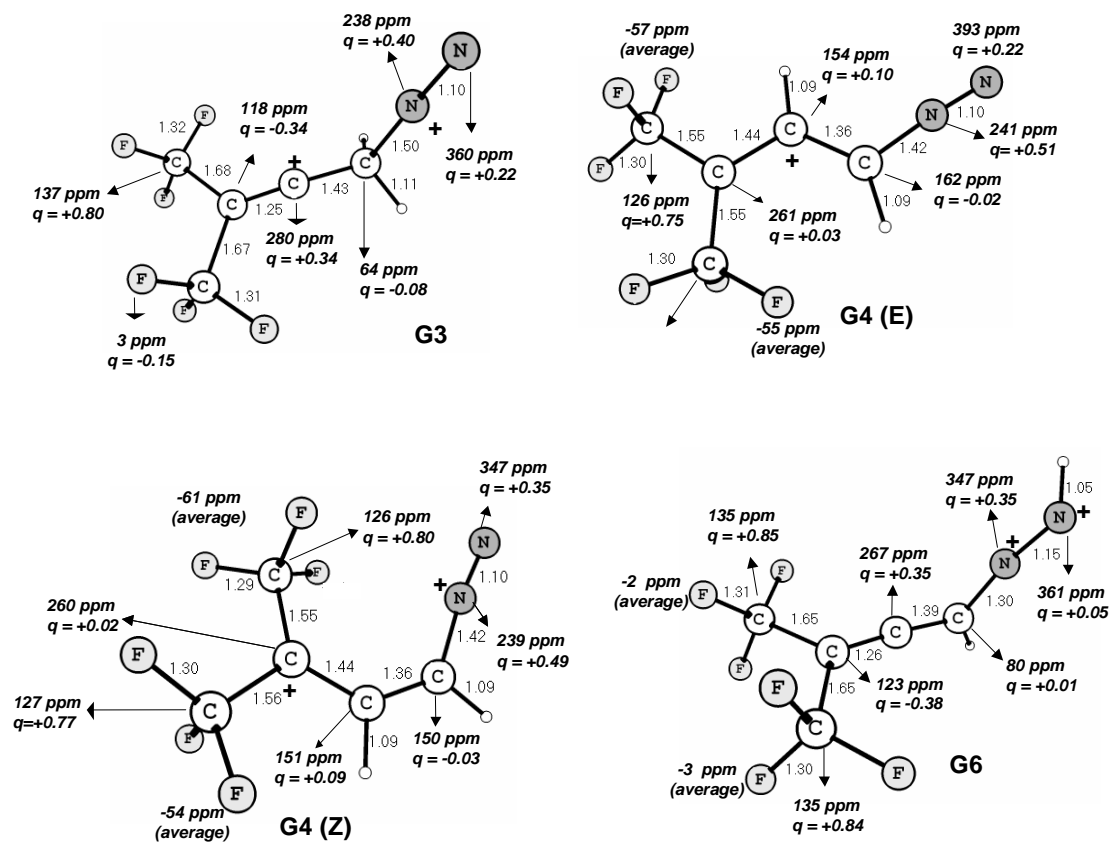
**Figure S2:** Optimized structures for protonated allenediazonium cation **D**, with selected geometric parameters, CHelpg charges ( $q$ ) and GIAO-NMR chemical shifts.



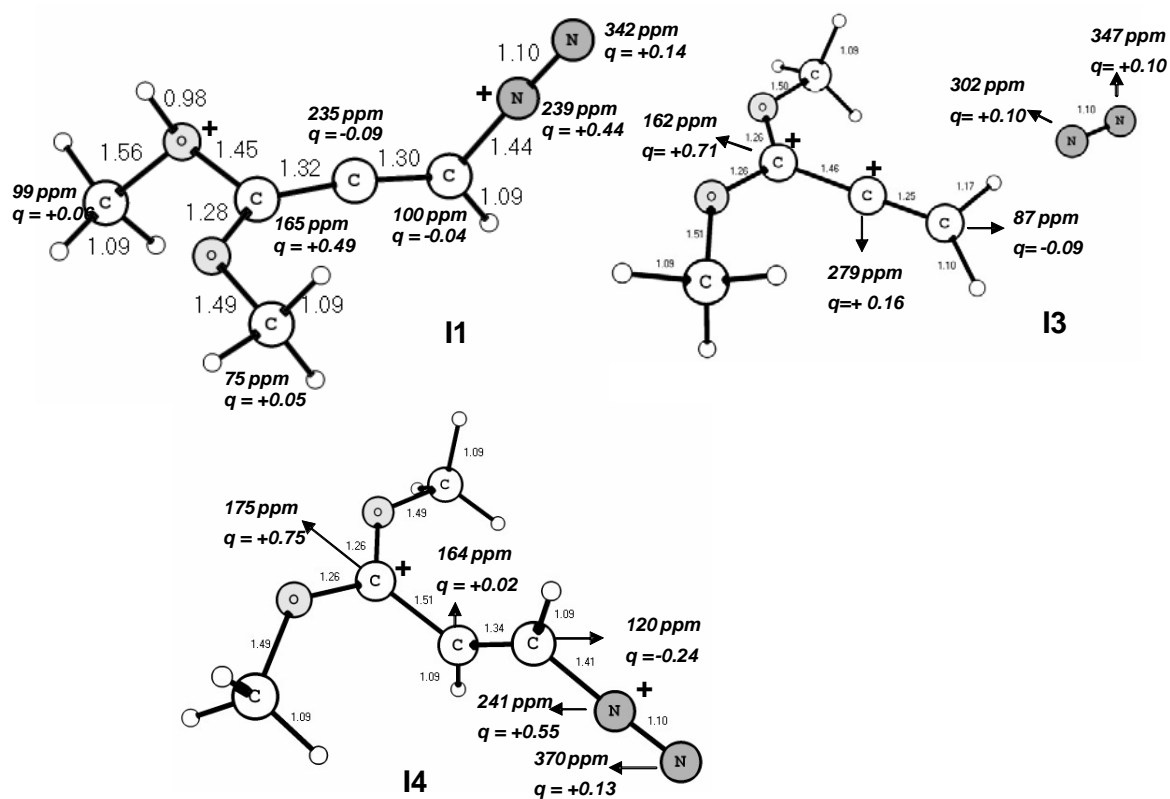
**Figure S3:** Optimized structures for protonated allenediazonium cation **E**, with selected geometric parameters, CHelpg charges ( $q$ ) and GIAO-NMR chemical shifts.



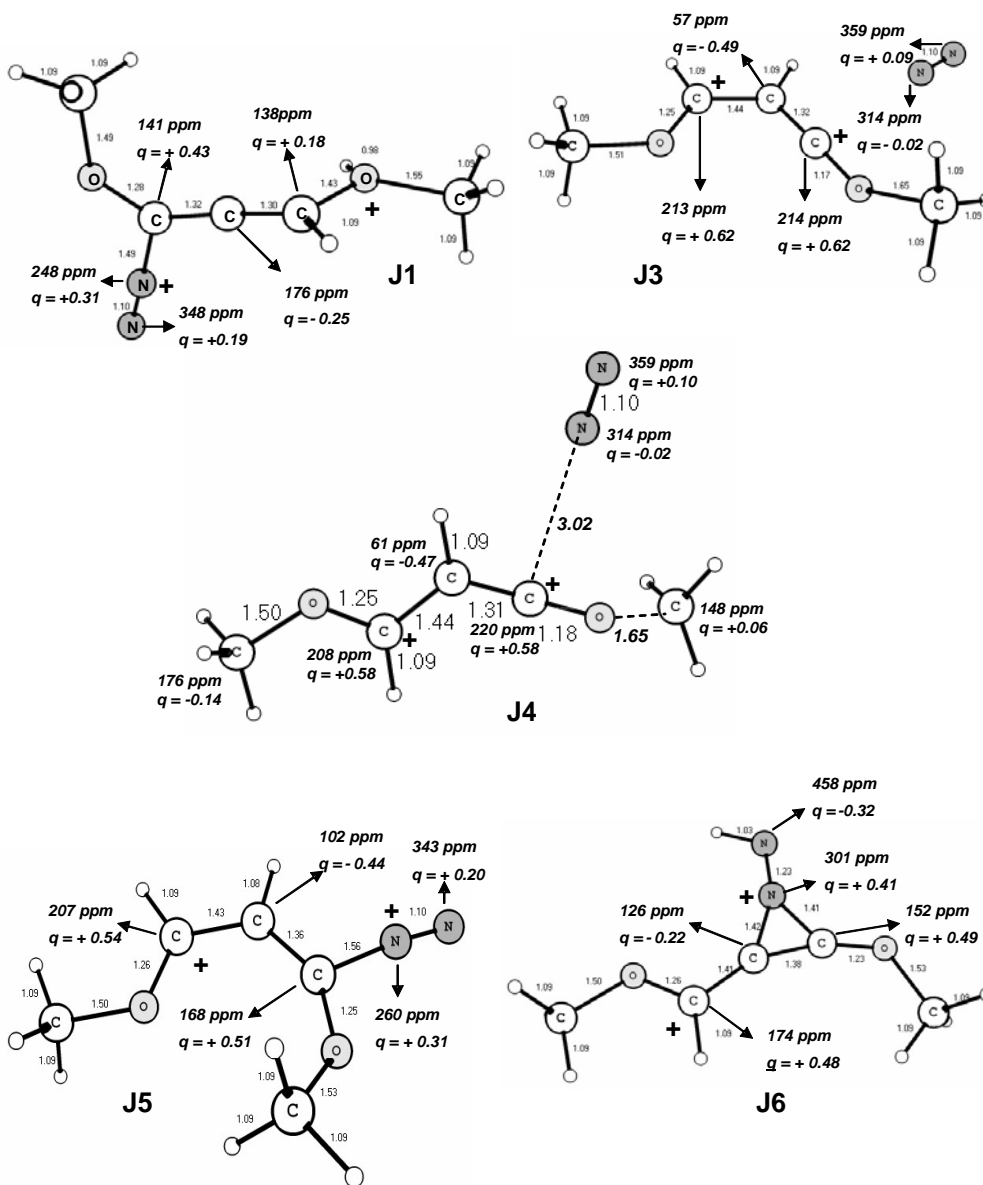
**Figure S4.** Optimized structures for protonated allenediazonium cation **G**, with selected geometric parameters, CHelpg charges ( $q$ ) and GIAO-NMR chemical shifts.



**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.

