ETHYL CATION

The structure of the simple, fundamental ethyl cation has finally been ascertained. Computational studies had long suggested the non-classical structure **1** for this cation. The classical structure **2** is a transition state for scrambling the protons. The MP2/6-311G(2d,p) geometries of both structures are shown in Figure 1.

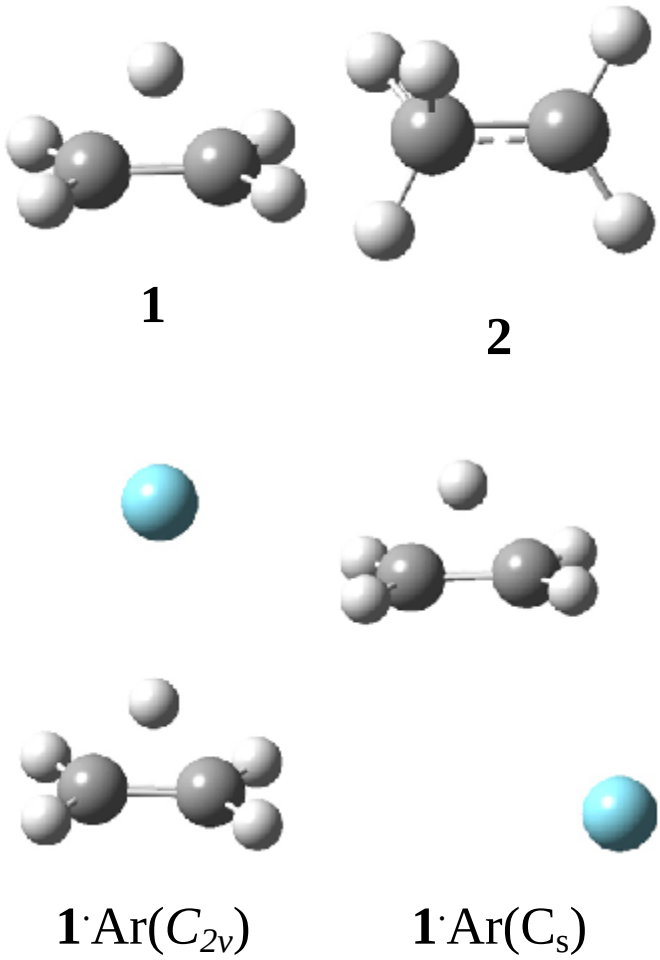

Figure 1. MP2/6-311G(2d,f) structures of **1**, **2**, **1**·Ar(C_{2v}) and **1**·Ar(C_s).

Dopfer[1] has now obtained IR spectrum of ethyl cation by single-photon IR photodissociation spectroscopy through the reaction

$$C_2H_5^+ \cdot Ar + h\nu \rightarrow C_2H_5^+ + Ar$$

Two structures of the ethyl cation associated with Ar were optimized at MP2/6-311G(2df,2pd). (The MP2/6-311G(2d,p) structures are shown in Figure 1.) Both of their computed IR spectra have stretches at nearly identical wavenumbers as for ethyl cation **1** itself. The experimental IR spectra has absorptions at 3317 and 3037 cm^{-1}, very close to the computed frequencies for **1**·Ar(C_{2v}). This provides strong experimental evidence that ethyl cation is in fact a non-classical ion.

Source: http://comporgchem.com/blog/?p=60