The norbornyl cation has been a source of controversy for decades. Just what is the nature of this cation? Should one consider it a classical cation A or of some non-classical character B? A recent computational study adds further fuel to this fire.\(^1\)

The B3LYP/6-311G(d,p) structure of the norbornyl cation is shown in Figure 1, and this structure is little changed when reoptimized at PBE1PBE/6-311G(d,p) or CCSD/6-311G(d,p). Application of the topological method (sometimes referred to as atoms-in-molecules or AIM) reveals a bond path network that resembles the bicyclo[3.2.0]heptyl cation C. The C\(_1\)-C\(_2\) distance is 1.75 Å and a bond path does connect these two atoms, though the density at the bond critical point is only 60% the value at the other C-C bonds in the compound.
There is no bond path connecting C\textsubscript{1} to C\textsubscript{3} that would close up a three-member ring. The C\textsubscript{1}-C\textsubscript{3} distance is 1.955 Å. So, the non-classical structure is not a proper description of this unusual species.

**Figure 1.** B3LYP/6-311G(d,p) optimized structure of the norbornyl cation.

Source: [http://comporgchem.com/blog/?p=52](http://comporgchem.com/blog/?p=52)