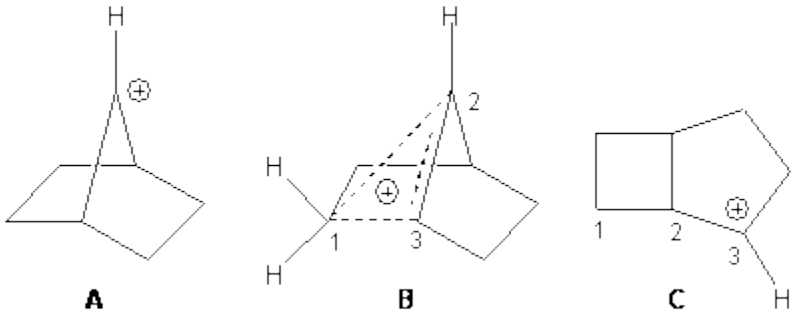
NORBORNYL CATION

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_1 to C_3 that would close up a three-member ring. The C_1-C_3 distance is 1.955 Å. So, the non-classical structure is not a proper description of this unusual species.

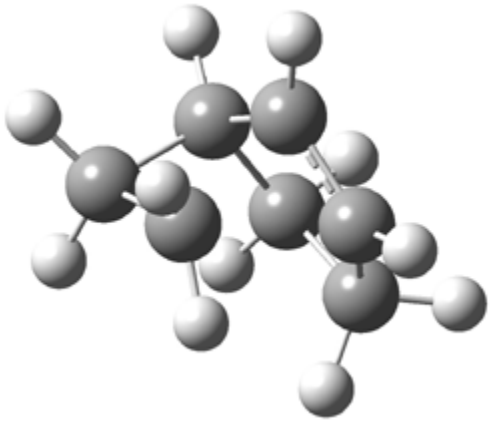


Figure 1. B3LYP/6-311G(d,p) optimized structure of the norbornyl cation.

Source: http://comporgchem.com/blog/?p=52