

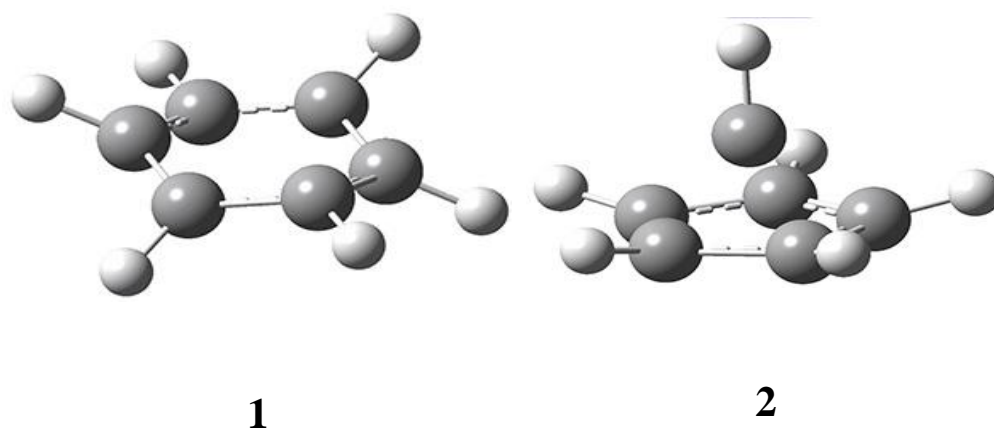
# STRUCTURE OF BENZENE DICATION

Benzene is certainly one of the most iconic chemical compounds – its planar hexagonal structure is represented often in popular images involving chemists, and its alternating single and double bonds the source of one of chemistry's most mythic stories: Kekule's dream of a snake biting its own tail. So while the structure of benzene is well-worn territory, what of the structure of the benzene dication? Jasik, Gerlich and Rithova probe that question using a combined experimental and computational approach.<sup>1</sup>

The experiment involves generation of the benzene dication at low temperature and complexed to helium. Then, using infrared predissociation spectroscopy (IRPD), they obtained a spectrum that suggested two different structures.

Next, employing MP2/aug-cc-pVTZ computations, they identified a number of possible geometries, and the two lowest energy singlet

dications have the geometries shown in Figure 1. The first structure (**1**) has a six member ring, but the molecule is no longer planar. Lying a bit lower in energy is **2**, having a pentagonal pyramid form. The combination of the computed IR spectra of each of these two structures matches up extremely well with the experimental spectrum.



**Figure 1.** MP2/aug-cc-pVTZ geometries of benzene dication **1** and **2**.

Source: <http://comporgchem.com/blog/?p=3046>