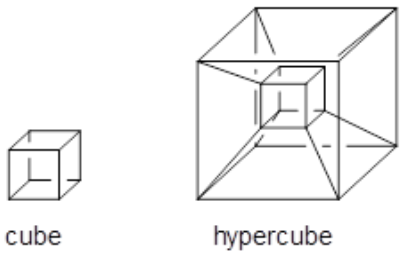
HYPERCUBANE

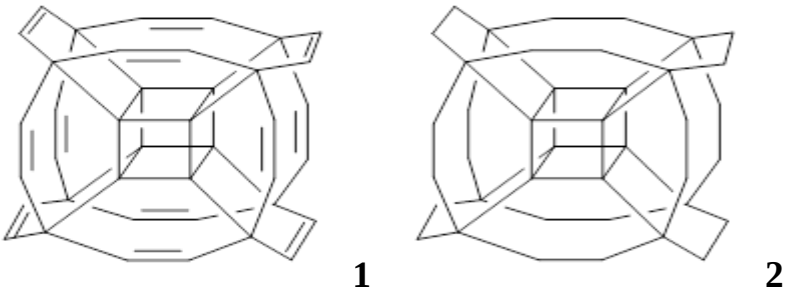
Three-dimensional objects can be projected into four-dimensional objects. So for example a cube can be projected into a hypercube, as in Scheme 1.

Scheme 1.



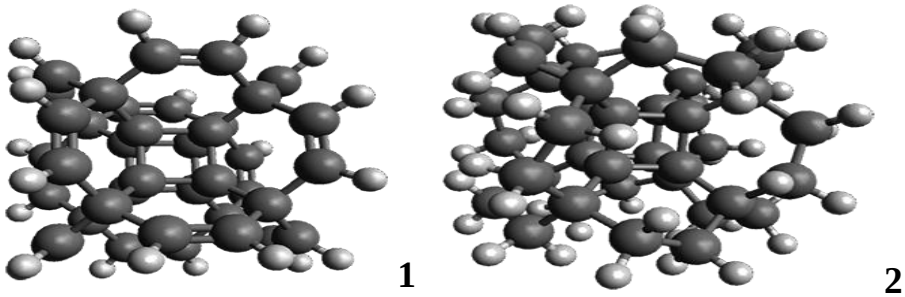
Pichierri proposes a hydrocarbon analogue of the hypercube. The critical decision is the connecting bridge between the outer (exploded) carbons. This distance is too long to be a single carbon-carbon bond. Pichierri opts to use ethynyl bridges, to give the hypercube **1**.[1]

Now, unfortunately he does not supply *any* supporting materials. So I have reoptimized this $O_h$geometry at B3LYP/6-31G(d), and show this structure in Figure 1. Pichierri does not report much beyond the geometry of **1** and the perfluoronated analogue. One interesting property that might be of interest is the ring strain energy of **1**, which I will not take up here.



1 **2**

But a question I will take up is just what bridges might serve to create the hydrocarbon hypercube. A more fundamental choice might be ethanyl bridges, to create **2**. However, the O_h conformer of **2**has 13 imaginary frequencies at B3LYP/6-31G(d). Lowering the symmetry to D_3 give a structure that has only real frequencies, and it's shown in Figure 1. An interesting exercise is to ponder other choices of bridges, which I will leave for the reader.



1 **2**

Figure 1. B3LYP/6-31G(d) optimized structures of **1** and **2**.

As always, be sure to click on the image to enable Jmol for interactive viewing of these interesting structures!

Source: http://comporgchem.com/blog/?p=3372