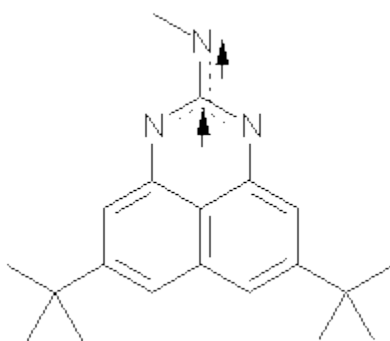


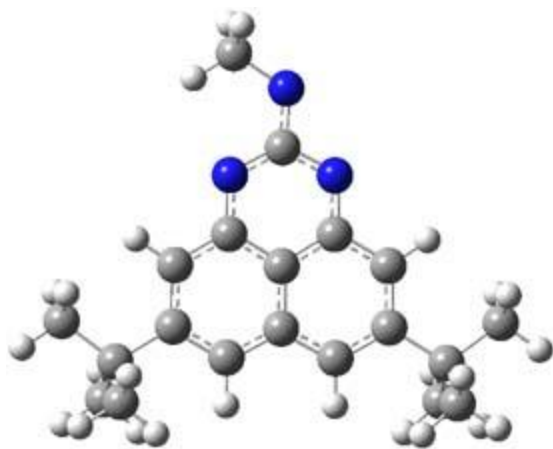
NON-KEKULE TRIplet DIRADICAL

I missed this when it came out, but Quast, Sander and Borden have made the very interesting non-Kekule diradical **1**.¹



³**1**

The EPR spectra shows the characteristic six-line signal, with zero-field splitting parameters consistent with related triplet diradicals. The Curie-Weiss plot is linear from 4.6 to 22.9 K. These data suggest a triplet ground state. CASSCF(14,14)/6-31G* computations indicate that the triplet lies 8.5 kcal mol⁻¹ below the singlet. The optimized triplet geometry is shown in Figure 1. The triplet ground state is consistent with the Borden-Davidson rules for radicals.²



³1

Figure 1. CASSCF(14,14)/6-31G* optimized structure of triplet **1**.

Source: <http://comporgchem.com/blog/?p=119>