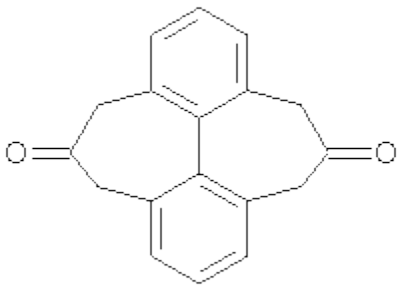
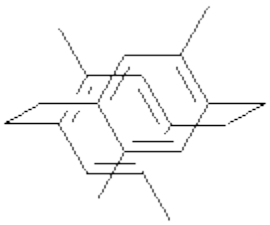
CD OF HIGH-SYMMETRY MOLECULES

I have written a number of blog posts that deal with the computation of optical activity. Trindle and Altun have now reported TD-DFT computations of circular dichroism of high-symmetry molecules.[1] They employ either B3LYP (with a variety of basis sets, the largest being 6-311++G(2d,2p)) and SOAP/ATZP. For a number of the high symmetry molecules (two examples are shown in Figure 1), the two methods differ a bit in their predictions of the first excited state, with SOAP typically predicting a red shift relative to the B3LYP. However, both methods general give the same sign of the CD signals and their line shapes are similar.



1



2

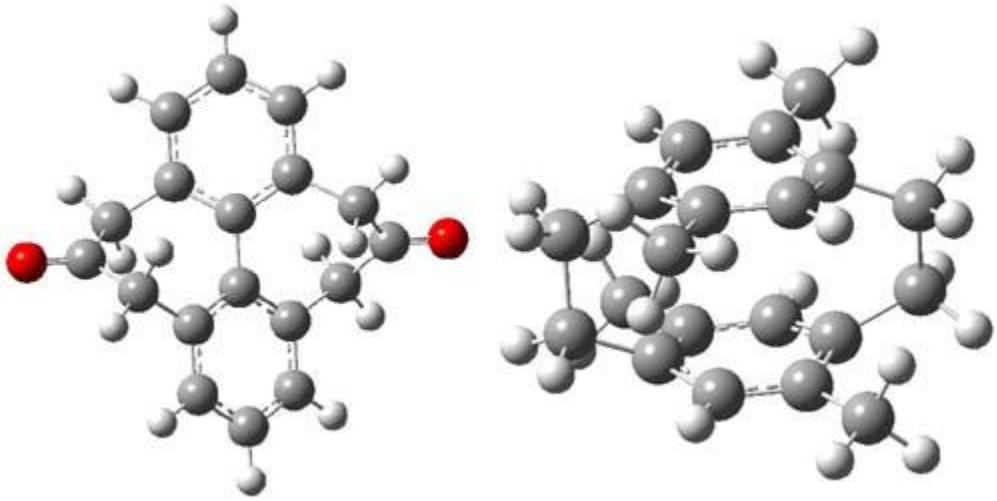


Figure 1. B3LYP/6-31G(d) optimized structures of **1** and **2** (again due to incomplete supporting materials, I reoptimized these structures)

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