HAVE YOU PUBLISHED THIS? Disorder in terminal unsaturated five membered heterocyclic rings

Joseph Reibenspies¹

¹Dept. of Chemistry, Texas A & M Univ.

reibenspies@chem.tamu.edu

Terminal unsaturated five membered heterocyclic rings, such as pyrrole, furan and thiophene, found in molecular and extended solids, will often be found to be disordered. The disorder rings are often not modeled as such; rather they are restrained to acceptable parameters. While this is not be a major issue with many journals, is it the acceptable path to follow? This talk will focus on the warning signs of terminal unsaturated five membered heterocyclic ring disorder that can be readily discovered by CIFCHECK and how to model the disorder if found.

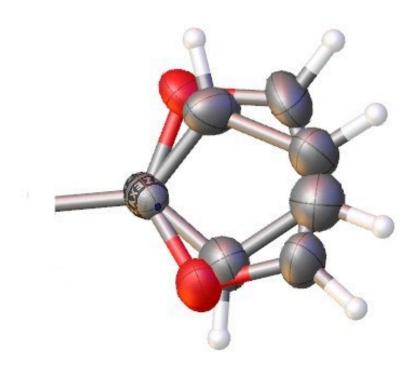


Figure 1