Is NMR the Tool to Characterize the Structure of C20 Isomers?

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Abstract

We investigate the feasibility of using nuclear magnetic resonance (NMR) chemical shift calculations as a tool to provide structural information for C20 fullerene type molecules. NMR chemical shifts are extremely sensitive to the local chemical environment of an atom, reflecting unambiguously its bond lengths and angles as well as its hybridization. Thus, they can distinguish between the different isomers that are candidates for the ground state of this molecule. We calculate the NMR shifts for several C20 isomers and show that NMR constitutes a potential tool to discriminate and identify experimentally a particular C20 molecular conformation, and also the level of theory which best describes the experimental structure.