

Combined Use of 2-D NMR Correlation Experiments, GIAO DFT ¹³C Chemical Shifts and 1-D NOESY Methods in Regioisomeric and Conformational Structure Determination of Cyclophanes in Solution

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Abstract

The combined application of two-dimensional nuclear magnetic resonance (2-D NMR) correlation experiments and gauge-including atomic orbital (GIAO) ¹³C NMR chemical shift calculations allowed reliable and simple determination of regioisomeric structure of heterocyclic substituents on the calix[4]arene lower rim. Moreover, the 1-D double pulsed field gradient nuclear Overhauser effect technique allows quick and efficient measurement of small nuclear Overhauser effects and, in doing so, establishes a 3-D structure of calix[4]arene simply and unequivocally. In general, these methods may find application in the regio- and stereoisomeric structure determination of complicated macrocyclic compounds. © 2011 Springer-Verlag.

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