Determining conformational preferences by NMR of simple molecules

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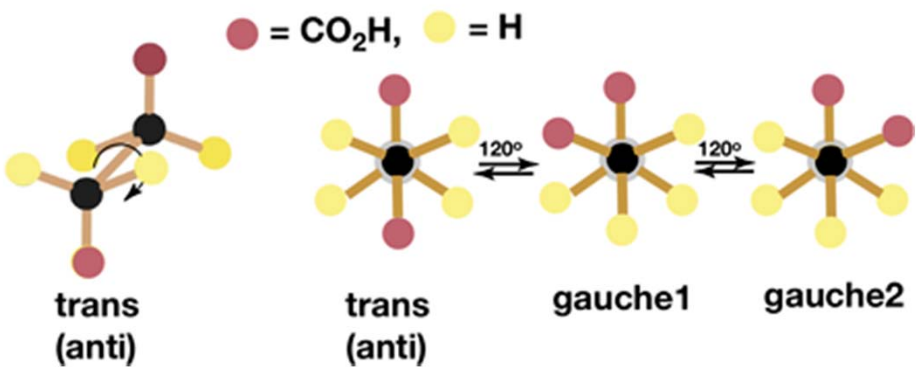
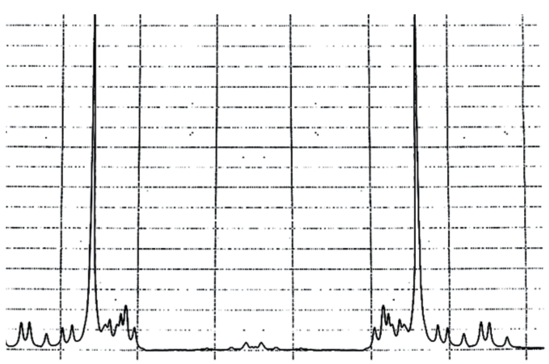
Conformers of simple organic molecules such as succinic acid, $HO_2C-CH_2-CH_2-CO_2H$ undergo rotation about their central CH_2-CH_2 bond with incredible speed, millions to billions times per second and yet we often speak of these rapidly rotating molecules of favoring particular spatial arrangements, "conformations", as though they could be separated and treated as stable entities. How can we measure the preferences for each of the different conformers despite the enormity of their speeds of rotation? First, what are conformers and how rotation turns one into the other. Representations follow of the conformations as chemists have made models of them using simple ball-and-stick for more than 125 years. On the far left, is a psuedo-three-dimensional, so-called "sawhorse" drawing showing an oblique view of what we call the trans conformer with a curved arrow showing where rotation occurs about the central *C-C* bond. The other three drawings are views along the axes of the *C-C* bonds to show how each 120° rotation changes from one conformer to the next.



Gauche1 and gauche2 are not the same structure but actually mirror images, not chemically identical, but equal for us here. As the conformers rotate, they appear to slow down slightly as each comes up in its tur simple idea. conformers behave in accord with this

Hydrogen nuclei in each rotating conformer interact magnetically to produce an averaged NMR spectrum (left). We can then calculate theoretically what each conformer if it were not rotating would contribute to the NMR spectrum and we can analyze the observed spectrum to determine the proportions of each conformer. To understand this, imagine a three-bladed propellor spinning fast, but abruptly stopping for a short. but different intervals at each 120° part of its rotation. If each of the blades is a different color you would see faint averaged images at each 120° stopping point, with the average color determined at each point by the interval of stopping and the intensities and hues of the blade colors.



NMR spectrum of hydrogens of succinic acid

of the stopping intervals and color intensities