

1-Benzyl-1,2,3,4-tetrahydroisoquinolines. ¹H NMR conformational studies and rotational barriers

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The conformational preferences of a series of 1-benzyl-1,2,3,4- tetrahydroisoquinolines (norlaudanosine and coclaurine analogues) were investigated with the aid of their ¹H NMR spectra and NOESY experiments, coupled with ab initio theoretical studies to estimate energy barriers among the various stable conformers of these systems. The secondary amines prefer an extended conformation, while the N-alkylated derivatives prefer a semi-folded one, with considerable freedom to exchange between both forms. A third, folded conformation, although not much higher in energy, is relatively inaccessible.