Conformational dynamics of substituted N-acetyl-N-phenylbenzylamines. 1H-DNMR and AM1-MO study

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Activation parameters for the rotation around the methylene-nitrogen single bond found in a series of four 2,2'-disubstituted N-acetyl-N-phenylbenzylamines, dissolved in DMSO-d6, were measured employing the temperature dependence of the 1H-NMR spectrum lineshape between 340 and 400 K. The results are : (I) 2 - [N-acetyl -N- (2-acetamidophenyl) aminomethyl]phenylacetate AG-=79.9±2.0 kJ/mol (370K), AH'=96.2±6.0 kJ/mol and AS'=+45±20 J/Kmol; (II) 2 [N - acetyl - N - (2-acetyloxybenzyl)amino]benzylacetate AG'=82.0±2.0 kJ/mol (370K), AH-=79.1±6.0 kcal/mol and AS'=-8±20 J/Kmol; (III) 2 - [N - Acetyl - N - (2nitrobenzyl)amino]benzylacetate AG'=80.8±2.0 kJ/mol (380K), AH=60.7±6.0 kcal/mol and AS=-53±20 J/Kmol; (IV) 2-[N-Acetyl-N-(2-acetyloxybenzyl)amino]phenylacetate AG-=77.0±2.0 kJ/mol (370K), AH'=65.3±6.0 kJ/mol and AS'=-32±20 J/Kmol. Substitution at positions 2 and 2' with bulky groups appears to be essential to freeze the gauche structure at room temperature and consequently, the main cont