N-METHYL INVERSION IN PSEUDO-PELLETIERINE

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We have previously conducted rotational studies of several tropanes, [a,b,c] since this bicyclic structural motif forms the core of different alkaloids of pharmaceutical interest. Now we report on the conformational properties and molecular structure of pseudo-pelletierine (9-methyl-9-azabicyclo[3.3.1]nonan-3-one), probed in a jet expansion with Fourier-transform microwave spectroscopy. Pseudo-pelletierine is an azabicycle with two fused six-membered rings, where the *N*-methyl group can produce inverting axial o equatorial conformations. The two conformations were detected in the rotational spectrum, recorded in the region 6-18 GHz. Unlike tropinone and *N*-methylpiperidone, where the most stable conformer is equatorial, the axial species was found dominant for pseudo-pelletierine. All monosubstituted isotopic species (^{13}C, ^{15}N and ^{18}O) were identified for the axial conformer, leading to an accurate determination of the effective and substitution structures. An estimation of conformational populations was derived from relative intensities. The experimental results will be compared with *ab initio* (MP2) and DFT (M06-2X, B3LYP) calculations.

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