The Structure of *N*-Acetylprolinamide in the Solid State and in the Gasphase. A Remarkable Lattice Effect as the Result of a Competition Between Inter- and Intramolecular Hydrogen Bonds of Different Strengths

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In the solid state, the conformation of *N*-actetylprolinamide is stabilized by two intermolecular O···H bridges and one intramolecular N···H hydrogen bond. According to quantum chemical *ab initio* calculations with the 6-31+G* basis set at the one-determinant level, the intramolecular N···H bond is not strong enough to maintain the solid-state molecular conformation the gas phase. The conformational changes predominantly consist in a rotation of the amide group about its C-C bond to the proline ring, resulting in a *cis*-like conformation which is stabilized by a presumably stronger intramolecular O···H bond between one hydrogen atom of the NH_2 group and the carbonyl oxygen of the acetyl subsituent bonded to the nitrogen atom of the five-membered ring.

These confirmational changes cause a reduction of the molecular dipole moment by about 50%, indicating that the conformation in solution might be strongly solvent dependent.

While both the MINDO/3 and the MNDO method in their standard parametrizations fail to reproduce the *ab initio* results, the lattice effect is reproduced at least qualitatively with the PM3 as well as with the AM1 method.

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