THE AMINO ALCOHOL PROLINOL: A ROTATIONAL STUDY

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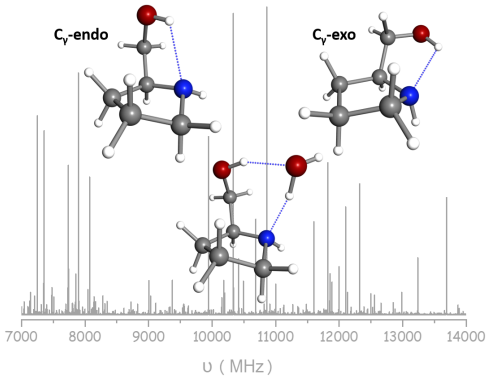

The amino alcohol prolinol is a reduction product of the chiral amino acid proline, which is widely used as a chiral auxiliary in noted reactions. Up to date, only IR data for prolinol is available.[a] Here, we report the first high-resolution microwave study of this system. Two endo-like and exo-like conformations stabilized by strong intramolecular hydrogen bonds O-H···N have been detected in the supersonic expansion of our CP-FTMW technique.[b,c] These structures have been successfully identified by comparison of the experimental rotational and ^{14}N nuclear quadrupole coupling constants with those predicted theoretically. Given the high sensitivity reached in our experiment, the seven monosubstituted species of ^{13}C, ^{15}N and ^{18}O have also been observed in their natural abundance for both conformers, and the corresponding r$_s$ substitution structure has been derived. The monohydrate of the most abundant endo form has also been detected. The water interacts simultaneously, acting as a proton donor to the imine nitrogen atom and accepting a proton from the hydroxyl group. This configuration benefits from two intermolecular hydrogen bonds, OH···O and O-H···N, closing a six-membered ring configuration. These first results pave the way for future studies on the chiral recognition of prolinol.

[a] J.J. Lee, S. Hesse, M.A. Suhm. *Journal of Molecular Structure*, **2010**, 976, 397–404

[b] I. Uriarte, C. Pérez, E. Caballero-Mancebo, F. J. Basterretxea, A. Lesarri, J. A. Fernández and E. J. Cocinero, *Chem. - A Eur. J.*, **2017**, 23, 7156

[c] C. Calabrese, W. Li, G. Prampolini, L. Evangelisti, I. Uriarte, I. Cacelli, S. Melandri,and E. J. Cocinero, *Angew.Chem.*, **2019**, 131,8525–8530