THE CONFORMATIONS OF PROTEINOGENIC AMINO ACID GLUTAMINE: MORE ACCURACY IS URGENTLY NEEDED IN THEORETICAL CALCULATIONS

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Glutamine is α-amino acid that is used in the biosynthesis of proteins. The large flexibility of the molecule has several potential conformational candidates. Among them, the three most stable isomers have been characterized both using a laser ablation chirped pulse Fourier-transform microwave spectrometer (LA-CP-FTMW) and a laser ablation molecular-beam Fourier-transform microwave spectrometer (LA-MB-FTMW).[a,b] Two of the conformers can be determined using the spectroscopic constants provided by the theoretical methods. On the other hand, the third conformer is not reproduced by conventional theoretical methods and one should use some tricks to characterize the conformer's structure. In addition, even the slightest different prediction in the site position of the nitrogen atoms makes the conformer's spectroscopic characterization very challenging because the nuclear quadrupole coupling interactions depend critically on the electronic environment, position and orientation of the ^{14}N nuclei. In this work we show several important conclusions: first, we present the three conformers of glutamine detected in gas phase; second, we highlight that more accurate theoretical methods are needed and that glutamine can be used as a test to benchmark the calculations; finally, we propose one trick to help the scientific community when the calculations are not sufficient to predict the structure and how to deal with the complicated hyperfine structure with no starting grounds.

[a] S. Mata, I. Peña, C. Cabezas, J. C. López and J. L. Alonso, J. Mol. Spectrosc., 2012, 280, 91–96.

[b] J. L. Alonso and J. C. López, in Gas-Phase IR Spectroscopy and Structure of Biological Molecules, eds. A. M. Rijs and J. Oomens, Topics in., 2015, vol. 364, pp. 335–402.