The Conformational Landscape of Bioactive Serinol

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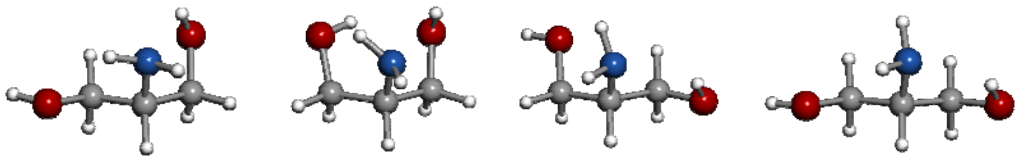
The rotational spectrum of the bioactive amino alcohol serinol CH_2OH-$CH(NH_2)$-CH_2OH has been investigated using chirped-pulsed Fourier transform microwave spectroscopy in combination with laser ablation [1]. Four different conformations have been identified and their rotational and ^{14}N quadrupole constants have been determined. The higher-energy conformer detected presents a tunnelling motion of the hydrogen atoms of the functional groups similar to that observed in glycerol [2]. In all observed conformers several hydrogen bonds are established between the two hydroxyl groups and the amino groups in a chain or circular arrangement. Interestingly, the most abundant conformer is stabilised by O-H···N and N-H··O hydrogen bonds forming a chain rather than a cycle.



[1] S. Mata, I. Peña, C. Cabezas, J. C. López, J. L. Alonso, *J. Mol. Spectrosc.* **2012**, *280*, 91.
[2] V. V. Ilyushin, R.A. Motiyenko, F.J. Lovas, D.F. Plusquellic, *J. Mol. Spectrosc.* **2008**, *251*, 129.