

A ROTATIONAL STUDY OF 1-SUBSTITUTED BARBARALONES

MAURO MATO, (*ICIQ*), *Institute of Chemical Research of Catalonia*, Tarragona, Spain; MIGUEL SANZ NOVO, IKER LEÓN, *Grupo de Espectroscopia Molecular, Lab. de Espectroscopia y Bioespectroscopia, Unidad Asociada CSIC, Universidad de Valladolid, Valladolid, Spain*; ELENA R. ALONSO, *Departamento de Química Física, Universidad del País Vasco (UPV-EHU), Bilbao, Spain*; ANTONIO M ECHAVARREN, (*ICIQ*), *Institute of Chemical Research of Catalonia*, Tarragona, Spain; JOSÉ L. ALONSO, *Grupo de Espectroscopia Molecular, Lab. de Espectroscopia y Bioespectroscopia, Unidad Asociada CSIC, Universidad de Valladolid, Valladolid, Spain*.

The phenomena of valence tautomerism consists in a particular intramolecular process involving just one reactive species where an intramolecular bond migrates raising to a sometimes different, but not always, molecular structure. In this context, barbaralones, widely well-known fluxional molecules, have been deeply ingrained in the understanding of the phenomena of valence tautomerism. They can undergo low energy [3, 3]-sigmatropic process, where the number of constitutional isomers depends on the presence and chemical nature of any possible substituent that induces isomerization restrictions. We have laser-ablated 1-(4-tert-Butyl)phenyl)tricyclo[3.3.1.0^{2,8}]nona-3,6-dien-9-one, a large fluxional molecule that is central to the understanding of the phenomena of valence tautomerism, and one conformer has been characterized using chirped-pulse Fourier transform microwave LA-CP-FTMW spectroscopy. This precise structural data should be useful in future studies as a reference point in the characterization of new fluxional molecules.

- **Acknowledgments:** The authors thank the financial fundings from Ministerio de Ciencia e Innovacion (CTQ2016-76393-P and PID2019-111396GB-I00), Junta de Castilla y Leon (VA077U16 and VA244P20) and European Research Council under the European Union's Seventh Framework Programme (FP/2007-2013) / ERC-2013-SyG, Grant Agreement n. 610256 NANOCOSMOS, are gratefully acknowledged. E.R.A. acknowledges MINECO for a Juan de la Cierva postdoctoral fellowship and the Fundación Biofísica Bizkaia (Spain). M.S.N. acknowledges funding from the Spanish "Ministerio de Ciencia, Innovación y Universidades" under predoctoral FPU Grant (FPU17/02987).