HIGH RESOLUTION ROTATIONAL SPECTROSCOPY OF A FLEXIBLE CYCLIC ETHER

F. GÁMEZ AND B. MARTÍNEZ-HAYA, *Departamento de Sistemas Físicos, Químicos y Naturales, Universidad Pablo de Olavide, 41013 Seville, Spain*; S. BLANCO, J. C. LÓPEZ, J. L. ALONSO, *Grupo de Espectroscopía Molecular (GEM). Edificio Quifima. Laboratorios de Espectroscopía y Bioespectroscopía. Parque Científico. Universidad de Valladolid, 47011 Valladolid. (Spain).*

Crown ethers stand as one cornerstone molecular class in host-guest Supramolecular Chemistry and constitute building blocks for a broad range of modern materials. We report here the first high resolution rotational study of a crown ether: 1,4,7,10,13-pentaoxacyclopentadecane (15-crown-5 ether,15c5). Molecular beam Fourier transform microwave spectroscopy[a] has been employed. The liquid sample of 15c5 has been vaporized using heating methods[b]. The considerable size of 15c5 and the broad range of conformations allowed by the flexibility of its backbone pose important challenges to spectroscopy approaches. In fact, the ab-initio computational study for isolated 15c5[c], yields at least six stable conformers with relative free energies within 2 kJ mol^{-1} (167 cm^{-1}). Nevertheless, in this investigation it has been possible to identify and characterize in detail one stable rotamer of the 15c5 molecule and to challenge different quantum methods for the accurate description of this system. The results pave the ground for an extensive description of the conformational landscape of 15c5 and related cyclic ethers in the near term.

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