ROTATIONAL SPECTROSCOPY OF SUPRAMOLECULAR SYNTHONS: HYPERFINE ANALYSIS OF TETRACYANOCYCLOPROPANE−THF COMPLEXES FORMED VIA TETREL BONDS

NUNO M. CAMPOS, RITA J. C. ROQUE, ELISA M. BRÁS, *CFisUC, Department of Physics, University of Coimbra, Coimbra, Portugal*; TIDDO J. MOOIBROEK, *Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, Amsterdam, The Netherlands*; MELANIE SCHNELL, *FS-SMP, Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany*; SÉRGIO R. DOMINGOS, *CFisUC, Department of Physics, University of Coimbra, Coimbra, Portugal*.

1,1,2,2-Tetracyanocyclopropane (TCCP) and its derivatives can serve as synthetically accessible and versatile synthons [1]. The four cyano groups create an electron-poor region in the center of the $(NC)_2C$-$C(CN)_2$ fragment, which can interact with an electron-rich partner, like the lone pair of tetrahydrofuran (THF), through tetrel bonds with the sp^3 hybridized carbons [2]. Microwave spectroscopy, when combined with quantum chemistry calculations, can be a useful tool to study these interactions. However, the presence of four nitrogen atoms turns the analysis of the rotational spectrum into a much more difficult task. While the splitting pattern due to the quadrupolar electric field of a single nucleus is normally easy to resolve, each additional nuclei increases its complexity considerably. We will present and discuss our analysis of the broadband rotational spectra of 3,3-dimethyl-TCCP and 3,3-diethyl-TCCP and their complexes with THF, obtained from full and partial fits including nuclear quadrupole interactions. These results illustrate both the potential and limitations of broadband experiments in accurately determining information from hyperfine splitting.

References:

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