JET-COOLED MID-INFRARED LASER SPECTROSCOPY OF CENTROSYMMETRIC TWO-RING PAHS

PIERRE ASSELIN, SATHAPANA CHAWANANON, *CNRS, De la Molécule aux Nano-Objets: Réactivité, Interactions, Spectroscopies, MONARIS, Sorbonne Université , PARIS, France*; MANUEL GOUBET, *UMR 8523 - PhLAM - Physique des Lasers Atomes et Molécules, University of Lille, CNRS, F-59000 Lille, France*; OLIVIER PIRALI, *Institut des Sciences Moléculaires d'Orsay, Université Paris Saclay, CNRS, Orsay, France*.

The recent detection of cyano naphthalenes within TMC-1 using radioastronomy[a] provided the first unambiguous confirmation of the interstellar PAH's hypothesis. In the mid-infrared (IR) domain, the launch of the James Webb Space Telescope opens exciting perspectives to collect information about polycyclic aromatic compounds. In this context, high resolution (HR) IR studies' enabling to resolve the rotational structure of vibrational bands of large aromatic species mainly used synchrotron-based Fourier Transform (FT) spectroscopy coupled to room temperature long path cells but the spectral analysis of such recordings remains very challenging. Nowadays, very few set-ups combining HR IR spectroscopy to the supersonic jet technique were developed to target low volatile PAH compounds[b].

A tunable mid-IR quantum cascade laser spectrometer coupled to a pulsed supersonic jet (SPIRALES set-up) recently implemented allows to record the rotationally resolved spectra of large molecules at low temperatures. We report the jet-cooled rovibrational IR study of three centrosymmetric two-ring PAH molecules: naphthalene, 1,5-naphthyridine and biphenyl in both regions of in plane ring C-H bending and C-C ring stretching vibrations, enabling to extract reliable spectroscopic parameters both in ground and excited vibrational states. Comparison between experiment and quantum chemistry calculations give confidence in the predictive power of corrected calculated rotational parameters. Last, experimental inertial defects of naphthalene and 1,5-naphthyridine complemented by similar two-ring and larger species agree well with an extended Oka's empirical formula developed for estimating the inertial defects of aromatic ring compounds.

---

[a] B.A. Mc Guire, R.A. Loomis, A. M. Burkhardt, K.L. K. Lee, C. N. Shingledecker, S. B. Charnley, I. R. Cooke, M. A. Cordiner, E. Herbst, S. Kalenskii, M. A. Siebert, E. R. Willis, C. Xue, A. J. Remijan, and M. C. Mc Carthy, Science, 371, 1265 (2021)

[b] B. E. Brumfield, J. T. Stewart and B. J. McCall, J. Phys. Chem. Lett 3, 1985 (2012) O. Pirali, M. Goubet, T. Huet, R. Georges, P. Soulard, P. Asselin, J. Courbe, P. Roy and M. Vervloet, PCCP. 15, 10141 (2013)