THE SOLEIL VIEW ON PROTOTYPICAL ORGANIC NITRILES: SELECTED VIBRATIONAL MODES OF ETHYL CYANIDE, C_2H_5CN, AND SPECTROSCOPIC ANALYSIS USING AN AUTOMATED SPECTRAL ASSIGNMENT PROCEDURE (ASAP)

CHRISTIAN ENDRES, PAOLA CASELLI, *The Center for Astrochemical Studies, Max-Planck-Institut für extraterrestrische Physik, Garching, Germany*; MARIE-ALINE MARTIN-DRUMEL, MICHAEL C McCARTHY, *Atomic and Molecular Physics, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, USA*; OLIVIER PIRALI, *AILES beamline, Synchrotron SOLEIL, Saint Aubin, France*; NADINE WEHRES, STEPHAN SCHLEMMER, SVEN THORWIRTH, *I. Physikalisches Institut, Universität zu Köln, Köln, Germany*.

Vibrational spectra of small organic nitriles, propionitrile and n-butyronitrile, have been investigated at high spectral resolution at the French national synchroton facility SOLEIL using Fourier-transform far-infrared spectroscopy (< 700 cm^{-1}). The *Automated Spectral Assignment Procedure* (ASAP)[a] has been used for line assignement and accurate determination of rotational level energies, in particular, of the ν_{20}=1 and the ν_{12}=1 states of propionitrile. The analysis does not only confirm the applicability of the ASAP in the treatment of (dense) high-resolution infrared spectra but also reveals some of its limitations which will be discussed in some detail.

[a]M. A. Martin-Drumel, C. P. Endres, O. Zingsheim, T. Salomon, J. van Wijngaarden, O. Pirali, S. Gruet, F. Lewen, S. Schlemmer, M. C. McCarthy, and S. Thorwirth 2015, J. Mol. Spectrosc. 315, 72