PROBLEMS, PROBLEMS, PROBLEMS: THE LONG JOURNEY OF PHENYL ACETATE

LYNN FERRES, WOLFGANG STAHL[a], *Institute for Physical Chemistry, RWTH Aachen University, Aachen, Germany*; LUCA EVANGELISTI, ASSIMO MARIS, SONIA MELANDRI, WALTHER CAMINATI, *Dipartimento di Chimica G. Ciamician, Università di Bologna, Bologna, Italy*; HA VINH LAM NGUYEN, *Université Paris-Est Créteil et Université de Paris, Laboratoire Interuniversitaire des systèmes atmosphériques (LISA), CNRS UMR7583, Creteil, France*.

The rotational spectrum of phenyl acetate, $CH_3COOC_6H_5$, was measured using a free jet absorption millimeterwave spectrometer in the range from 60 to 78 GHz and two pulsed jet Fourier transform microwave spectrometers covering a total frequency range from 2 to 26.5 GHz. The features of two coupled large amplitude motions, the methyl group internal rotation and the skeletal torsion tunneling of the CH_3CO group with respect to the phenyl ring C_6H_5 (tilted of about 70°), characterize the spectrum. The vibrational ground state splits into four widely spaced sublevels, labeled as A0, E0, A1, and E1, each of them with its set of rotational transitions, and with additional interstate transitions. A global fit of the line frequencies of the four sublevels leads to the determination of 40 spectroscopic parameters, including the $\Delta E_{A0/A1}$ and $\Delta E_{E0/E1}$ vibrational splittings of about 36.4 GHz and 34.0 GHz, respectively. These parameters were used to deduce the V_3 barrier to methyl internal rotation (about 136 cm^{-1}) and the skeletal torsion B_2 barrier to orthogonality of the two planes (about 68 cm^{-1}).

[a]Deceased.