ANALYSIS OF THE OPEN-SHELL CH_3CO RADICAL: INTERNAL ROTATION, SPIN-ROTATION, AND HYPERFINE STRUCTURE[a]

OLIVIER PIRALI, ROSEMONDE CHAHBAZIAN, MARIE-ALINE MARTIN-DRUMEL, L. H. COUDERT, *Institut des Sciences Moléculaires d'Orsay, Université Paris Saclay, CNRS, Orsay, France*; LUYAO ZOU, R. A. MOTIYENKO, L. MARGULÈS, *UMR 8523 - PhLAM - Physique des Lasers Atomes et Molécules, University of Lille, CNRS, F-59000 Lille, France*.

Although many non-rigid open-shell molecules can be spectroscopically accounted for without a dedicated approach, a subclass of these requires specific theoretical treatments. Such is the case of the CH_2 and CH_2OH radicals and of the Na_3 trimer for which new approaches were setup to model a large amplitude motion together with the electron spin-rotation coupling.[b] The acetyl radical CH_3CO is a benchmark molecule for this subclass of molecules as it presents a low barrier torsional motion and fine interaction. This radical was first studied some time ago[c] and a new theoretical model was developed to analyze its spectroscopic data. Unfortunately, only a few low-J transitions could be measured then.

An analysis of the new submillimeter wave transitions recorded at the ISMO and PhLAM laboratories for the CH_3CO radical will be presented. The theoretical approach developed parallels that of Hirota *et al.*[c] It relies on an effective torsion-rotation Hamiltonian[d] to which the spin-rotation and hyperfine couplings[e] are added.

The results of preliminary line frequency analyses will be presented. Values for the torsion-rotation Hamiltonian parameters A, B, C, D_{ab}, and ρ were obtained from a data set consisting of 143 rotation-torsion transitions split by spin-rotation and hyperfine couplings. The electron spin-rotation coupling tensor components were also determined.

[a]Supported by the Programme National PCMI of CNRS/INSU with INC/INP co-funded by CEA and CNES

[b]Ohashi, Tsuura, Hougen, Ernst, and Rakowsky, *J. Mol. Spec.* **184** (1997) 22; Coudert, *J. Chem. Phys.* **153** (2020) 144115; and Coudert, Chitarra, Spaniol, Loison, Martin-Drumel, and Pirali, *J. Chem. Phys.* **156** (2022) 244301

[c]Hirota, Mizoguchi, Ohsima, Katoh, Sumiyoshi, and Endo, *Mol. Phys.* **105** (2007) 455

[d]Nakagawa, Tsunekawa, and Hojima, *J. Mol. Spec.* **126** (1987) 329

[e]Brown and Sears, *J. Mol. Spec.* **75** (1979) 111; and Coudert, Gutlé, Huet, Grabow, and Levshakov, *J. Chem. Phys.* **143** (2015) 044304