ELECTRON SPIN-TORSION AND SPIN-ROTATION EFFECTS IN THE OPEN-SHELL CH_3CO RADICAL[1]

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Although open-shell molecules displaying a fine interaction and non-rigid molecules displaying a large amplitude motion have been the subject of numerous spectroscopic investigations, fewer results are available about molecules displaying *both* a fine interaction and a large amplitude motion. A non-exhaustive list of such species include the open shell CH_2, CH_2OH, and Na_3 species displaying[2] respectively a large amplitude bending, torsion, and pseudorotation. The acetyl radical CH_3CO is a benchmark molecule for this subclass of molecules as it presents a low barrier internal rotation of its methyl group and a fine interaction. In the first spectroscopic investigation of the radical,[3] a few low J, $K_a = 0$ transitions were measured in its microwave spectrum and a new theoretical model was developed to model its spectrum.

In this poster, new measurements carried out in the submillimeter wave spectrum of CH_3CO will be presented. More than 300 transitions have been assigned up to $N = 22$ and $K_a = 5$ in the ground torsional state for both A and E torsional species and for both F_1 and F_2 electron spin-rotation components. Based on a newly developed theoretical approach, a line frequency analysis has been carried out and line frequencies were reproduced with a unitless standard deviation of 1.2.

The analysis shows that two effects, ignored in the pioneering approach of Hirota *et al.*,[3] are quite important. These are the electron spin-torsion coupling, described by a term in $p_\alpha S_z$, where p_α is the momentum conjugated to the torsional angle α, and a dependence of the electron spin-rotation coupling tensor on this torsional angle. In the poster the new measurements will be presented and the spectroscopic parameters will be reported. These include the usual torsion-rotation parameters A, B, C, D_{ab}, ρ, and V_3, and the new fine interaction-torsion parameters.

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[2]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

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