

INSTRUMENTAL AND THEORETICAL INVESTIGATION TOWARDS A GLOBAL VIBRATION–ROTATION MODEL IN 4–ATOM SPECIES: $^{12}\text{C}_2\text{HD}$ AND $^{13}\text{C}^{12}\text{CH}_2$

M. HERMAN, C. DEPIESSE, D. HURTMANS, S. KASSI, S. ROBERT, J. VANDER AUWERA, *Service de Chimie Quantique et Photophysique C. P. 160/09, Université Libre de Bruxelles, 50 Avenue F. D. Roosevelt, B–1050 Brussels, Belgium*; G. DI LONARDO, L. FUSINA, F. TAMASSIA, *Dipartimento di Chimica Fisica e Inorganica, Università di Bologna, Viale Risorgimento 4, I–40136 Bologna, Italy*; A. FAYT, *Laboratoire de Spectroscopie Moléculaire, Université Catholique de Louvain, Louvain-la-Neuve, Belgium*.

We used an experimental set-up built in Brussels connecting an Ar^+ pumped, home-made Sa:Ti laser cavity to a commercial high resolution Fourier transform spectrometer Bruker IFS120HR,^a to perform ultra sensitive (ICLAS) molecular absorption spectroscopy in the near infrared range in both $^{12}\text{C}_2\text{HD}$ and $^{13}\text{C}^{12}\text{CH}_2$. We also recorded new conventional FT data in Bologna and Brussels. They are being analyzed and the results are gathered with literature information on additional vibrational energy states in both acetylene isotopologues separately. We are first attempting to perform global modeling of the vibrational energy pattern by defining adequate polyad interaction schemes and will then turn on to global vibration-rotation modeling, using a dedicated computer program package developed in Louvain.^b We shall report on the latest results.

^aD. Hurtmans, S. Kassi, C. Depiesse and M. Herman, *Mol. Phys.* **100** (2002) 3507–3511; S. Kassi, C. Depiesse, M. Herman and D. Hurtmans, *Mol. Phys.* **101** (2003) 1155–1163.

^bC. Vigouroux, A. Fayt, A. Guarnieri, A. Huckauf, H. Bürger, D. Lentz and D. Prugschat, *J. Mol. Spectrosc.* **202** (2002) 1–18; A. Fayt, C. Vigouroux, F. Willaert, L. Margules, L. F. Constantin, J. Demaison, G. Pawelke, El Bachir Mkadmi and H. Bürger, *J. Mol. Struct.*, in press.