

A high-resolution database for the vibration-rotation spectrum of acetylene (0 – 8022 cm⁻¹)

B. Amyay,^a A. Fayt,^b M. Herman,^a R. Georges,^c and J. Vander Auwera^a

^a Service de Chimie Quantique et Photophysique, CP 160/09
Université Libre de Bruxelles, 50 av. Roosevelt, B-1050 Brussels, Belgium
bamyay@ulb.ac.be, mherman@ulb.ac.be, jauwera@ulb.ac.be

^b Laboratoire de Spectroscopie Moléculaire, Université Catholique de Louvain,
2 Chemin du Cyclotron, bte L7.01.07, B-1348 Louvain-La-Neuve, Belgium
andre.fayt@uclouvain.be

^c Institut de Physique de Rennes, Astrochimie Expérimentale UMR 6251 CNRS
Université de Rennes 1 Bât. 11C, Campus de Beaulieu 35042 Rennes Cedex, France
robert.georges@univ-rennes1.fr

We have built an effective Hamiltonian capable of reproducing all published vibration-rotation lines in ¹²C₂H₂ accessing levels up to 8900 cm⁻¹, within three times their stated experimental standard deviation [1]. It was applied to predict IVR dynamics including rotational degrees of freedom [2] and to calculate partition function and other thermodynamical quantities up to 2,000 K with previously unmatched accuracy [3]. We have now exploited the predictive power of this Hamiltonian to build a database providing line positions and intensities for ¹²C₂H₂ from the FIR ($v_5 - v_4$) through the MIR (v_5 , $v_4 + v_5$, $v_2 - v_5$, v_3) to the NIR ($v_1 + v_3$) spectral ranges. The ¹²C₂H₂ database, named FASE for Femto-, Astro-, Spectro-Ethyne, will be presented and discussed.

- [1] B. Amyay, M. Herman, A. Fayt, A. Campargue, S. Kassi, *J. Mol. Spectrosc.* **2011**, 267, 80.
- [2] D.S. Perry, J. Martens, B. Amyay, M. Herman, *Mol. Phys.* **2012**, 110, 2687.
- [3] B. Amyay, A. Fayt, M. Herman, *J. Chem. Phys.* **2011**, 135, 234305/1.