

ANALYSIS OF THE SPECTRUM OF ETHYLENE IN THE 800–1500 CM⁻¹ REGION USING TENSORIAL FORMALISM: FREQUENCIES AND INTENSITIES

M. ROTGER, V. BOUDON, *Laboratoire de Physique de l'Université de Bourgogne, UMR CNRS 5027, 9, av. Alain Savary, B.P. 47870, F-21078 Dijon Cedex, France*; A. FAYT, *Molecular spectroscopy laboratory, Université Catholique de Louvain, Chemin du Cyclotron 2, B-1348 Louvain-La-Neuve, Belgium*; 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*.

Recently, we have presented a tensorial formalism^{a,b} adapted to the spectroscopy of X₂Y₄ molecules. It is based on formalisms already developed in Dijon for spherical-top molecules^c as well as on the work of Sartakov^d. This approach has the advantages to allow a systematic development of rovibrational interactions and to make global analyses easier to perform. We have used this tool to perform a re-analysis of the $\nu_{10}/\nu_7/\nu_4/\nu_{12}$ tetrad both in frequencies and intensities in the 800–1500 cm⁻¹ region. We have used 8943 infrared data in the $\nu_{10}/\nu_7/\nu_4$ region from W. E. Blass' atlas^e completed by 5420 more recent data in the same range^f (207 of these having a precision of a few 10⁻⁶ cm⁻¹) and by 1138 data in the ν_{12} region from a spectrum recorded in Brussels. We obtain a global reduced RMS of 0.54 for line positions, which is comparable to the result of Ref. *f*. Concerning line intensities, we used 10657 data from Blass' atlas and 25 high-precision diode laser data^g. We obtain a 11.6 % RMS in this case.

^aW. Raballand, M. Rotger, V. Boudon and M. Loëte, *J. Mol. Spectrosc.* **217**, 239–248 (2003).

^bCh. Wenger, W. Raballand, M. Rotger and V. Boudon, *J. Quant. Spectrosc. Radiat. Transfer* **95**, 521–538 (2005).

^cV. Boudon, J.-P. Champion, T. Gabard, M. Loëte, F. Michelot, G. Pierre, M. Rotger, Ch. Wenger and M. Rey, *J. Mol. Spectrosc.* **228**, 620–634 (2004).

^dB. G. Sartakov, J. Oomens, J. Reuss and A. Fayt, *J. Mol. Spectrosc.* **185** 31–47 (1997).

^eW. E. Blass, J. J. Hillman, A. Fayt, S. J. Daunt, L. R. Senesac, A. C. Ewing, L. W. Jennings, J. S. Hager, S. L. Mahan, D. C. Reuter and M. Sirota, *J. Quant. Spectrosc. Radiat. Transfer* **71**, 47–60 (2001).

^fF. Willaert, J. Demaison, L. Margulès, H. Mäder, H. Spahn, T. Giesen and A. Fayt, *Mol. Phys.* **104**, 273–292 (2006).

^gJ. Walrand, M. Lengelé, Gh. Blanquet and M. Lepère, *Spectrochim. Acta A* **59** 421–426 (2003).