

# Service de Chimie Quantique et Photophysique

## Publications in 2006

1. Ab initio vibrational analysis of hexafluoroethane  $C_2F_6$ , Panchenko Y. N. and De Maré G. R., Russ. J. Struct. Chem., 47 (2006), 232-240.
2. Vibrational spectra and ab initio analysis of tert-butyl, trimethylsilyl, trimethylgermyl and trimethylstannyl derivatives of 3,3-dimethylcyclopropene. VII. 3,3-Dimethyl-1-(trimethylstannyl) cyclopropene, Panchenko Y. N., De Maré G. R., Abramenkov A. V., and de Meijere A., Spectrochim. Acta A, 65 (2006), 351-357.
3. Vibrational spectra and ab initio analysis of tert-butyl, trimethylsilyl, trimethylgermyl and trimethylstannyl derivatives of 3,3-dimethylcyclopropene. VIII. 3,3-Dimethyl-1,2-bis(trimethylstannyl) cyclopropene, Panchenko Y. N., De Maré G. R., Abramenkov A. V., and de Meijere A., Spectrochim. Acta A, 65 (2006), 575-583.
4. Resolved torsional splitting in the  $\nu_{18}$  and  $\nu_{19}$  bands of propene, Lafferty W. J., Flaud J. M., and Herman M., J. Mol. Struct., 780-781 (2006), 65-69.
5. Absolute Line Intensity with FT-ICLAS :  $^{12}C_2H_2$  near  $12800\text{ cm}^{-1}$ , Macko P. and Herman M., Chem. Phys. Lett., 417 (2006), 471-474.
6. Absolute line intensities for carbonyl sulfide from  $827$  to  $2939\text{ cm}^{-1}$ , Vander Auwera J. and Fayt A., J. Mol. Struct., 780-781 (2006), 134-141.
7. Absolute line intensities of  $^{13}C^{16}O_2$  in the  $3090$ - $3920\text{ cm}^{-1}$  region, Vander Auwera J., Claveau C., Teffo J. L., Tashkun S. A., and Perevalov V. I., J. Mol. Spectrosc., 235 (2006), 77-83.
8. The VMFCI Method : a Flexible Tool for Solving the Molecular Vibration Problem, Cassam-Chenai P. and Liévin J., J. Comput. Chem., (2006), 628-640.
9. Ab initio study of the ionization of the DNA bases : ionization potentials and excited states of the cations, Cauët E., Dehareng D., and Liévin J., Journal of Physical Chemistry A, 110 (2006), 9200-9211.
10. Vinylidene-acetylene cation isomerization investigated by large scale *ab initio* calculations, Boyé-Péronne S., Gauyacq D., and Liévin J., J. Chem. Phys., 124 (2006), 214305.
11. The FT absorption spectrum of  $^{13}CH^{12}CH(II)$  : Rotational analysis of the range  $9500$  to  $10000\text{ cm}^{-1}$ , Di Lonardo G., Fusina L., Tamassia F., Fayt A., Robert S., Vander Auwera J., and Herman M., Mol. Phys., 104 (2006), 2617-2625.
12. Spectrum of hot water in the  $2000$ - $4750\text{ cm}^{-1}$  frequency range, Zobov N. F., Shirin S. V., Polyansky O. L., Barber R. J., Tennyson J., Coheur P. F., Bernath P. F., Carleer M., and Colin R., J. Mol. Spectrosc., 237 (2006), 115-122.
13. On the  $X^2S^+$ ,  $A^2P$ , and  $C^2S^+$  states of BeH, BeD, and BeT, Le Roy R. J., Appadoo D. R. T., Colin R., and Bernath P. F., J. Mol. Spectrosc., 236 (2006), 178-188.
14. The  $B^3S^-$  state of the SO radical, Liu C. P., Elliott N. L., Western C. M., Lee Y. P., and Colin R., J. Mol. Spectrosc., 238 (2006), 213-223.

15. The FT Absorption Spectrum of  $^{13}\text{CH}^{12}\text{CH}$  : Rotational Analysis of the vibrational states from 3800 to 6750  $\text{cm}^{-1}$ , Cané E., Fusina L., Tamassia F., Fayt A., Herman M., Robert S., and Vander Auwera J., *Mol. Phys.*, 104 (2006), 515-526.
16. Combined analysis of high sensitivity Fourier transform and ICLAS-VeCSEL absorption spectra of D<sub>2</sub>O between 8800 and 9250  $\text{cm}^{-1}$ , Naumenko O. V., Leshchishina O., Shirin S., Jenouvrier A., Fally S., Vandaele A. C., Bertseva E., and A. Campargue A., *J. Mol. Spectrosc.*, 238(1) (2006), 79-90.
17. The Methylene Saga Continues : Stretching Fundamentals and Zero-Point energy of  $\text{X}^3\text{B}_1\text{CH}_2$ , Czaka G., Furtenbacher T., Szalay V., Czarzar A. G., and Sutcliffe B. T., *J. Mol. Struct.*, 780-781 (2006), 283-294.
18. The idea of a potential energy surface, Sutcliffe B. T., *Mol. Phys.*, 104 (2006), 715-722.
19. Infrared spectra of  $\text{C}_2\text{H}_2$  under jet-cooled and para- $\text{H}_2$  matrix conditions, Lee Y.-C., Venkatesan V., Lee Y.-P., Macko P., Didriche K., and Herman M., *Chem. Phys.*, (submitted for publication).
20. Investigation of the shape of the R(0) absorption line in  $\nu_3$ ,  $\text{N}_2\text{O}$  recorded from an axisymmetric supersonic free jet expansion, Didriche K., Macko P., Herman M., Thiévin J., Benidar A., and Georges R., *JQSRT*, in press (2006),
21. The vibration-rotation energy pattern in acetylene :  $^{13}\text{CH}^{12}\text{CH}$  up to 6750  $\text{cm}^{-1}$ , Fayt A., S. R., Di Lonardo C., Fusina L., Tamassia F., and Herman M., *J. Chem. Phys.*, (submitted for publication).
22. Fantasio : a versatile experimental set-up to investigate jet-cooled molecules, Herman M., Didriche K., Hurtmans D., Kizil B., Macko P., Rizopoulos A., and Van Poucke P., *Mol. Phys.* (in press).
23. The bending vibrations in  $^{12}\text{C}_2\text{H}_2$  : Global vibration-rotation analysis, Robert S., Herman M., Vander Auwera J., Di Lonardo G., Fusina L., Blanquet G., Lepère M., and Fayt A., *Mol. Phys.* (in press).
24. Self-broadening coefficients and absolute line intensities in the  $\nu_4 + \nu_5$  band of acetylene, Lepère M., Blanquet G., Walrand J., Bouanich J. P., Herman M., and Vander Auwera J., *J. Mol. Spectrosc.* (in press).
25. Equilibrium structure of sulfuric acid, Demaison J., Herman M., Liévin J., and Rudolph H. D., *J. Mol. Struct.*, (to be submitted for publication).
26. Perturbation activated transitions in the high resolution infrared spectrum of  $\text{C}_2\text{H}_6$  : rotational constants and torsional splitting in the ground state, Lattanzi F., di Lauro C., Horneman V. M., Herman M., and Vander Auwera J., *Mol. Phys.* (in press),
27. Vibrational spectra and ab initio analysis of tert-butyl, trimethylsilyl, trimethylgermyl, trimethylstannyl and trimethylplumbyl derivatives of 3,3-dimethylcyclopropene. IX. 3,3-Dimethyl-1-(trimethylplumbyl)cyclopropene, De Maré G. R., Panchenko Y. N., and Abramnikov A. V., *Spectrochim. Acta* (in press).
28. Adiabatic Jacobi corrections for  $\text{H}_2^+$  like systems, Czaka G., Czarzar A. G., Szalay V., and Sutcliffe B. T., *J. Chem. Phys.* (accepted).
29. Radical cations of the nucleic bases and radiation damage to DNA : ab initio study, Cauët E. and Liévin J., *Advances in Quantum Chemistry* (in press).