Colloquium Spectroscopicum Internationale XLI & I Latin American Meeting on LIBS

BOOK OF ABSTRACTS

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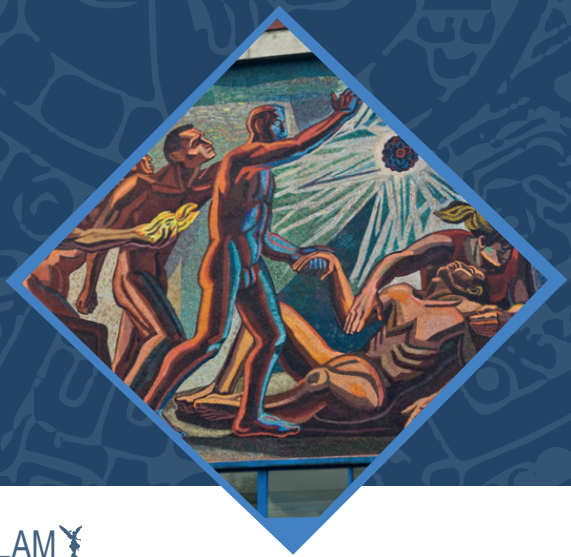

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National and Autonomous University of Mexico

Mexico City, June 9 – 14, 2019

www.csi2019mexico.com

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Modeling of the torsional spectra of the methanediol molecule to the complete basis set

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Uladzimir U. Sapeshka [a], Alex E. Malevich [b], Andrey A. Ostyakov [b], George A. Pitsevich [b], Alexander A. Kamnev [c]

[a] *University of Illinois at Chicago, Chicago, IL, USA*

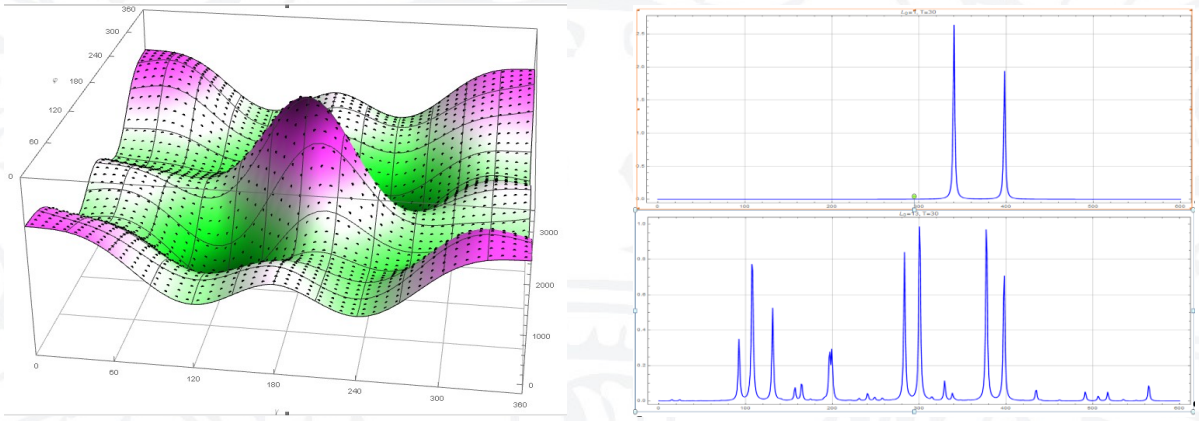
[b] *Belarusian State University, Minsk, Belarus*

[c] *Institute of Biochemistry and Physiology of Plants and Microorganisms, Russian Academy of Sciences, Saratov, Russia*

Email: aakamnev@ibppm.ru; a.a.kamnev@mail.ru

Keywords: internal rotation, PES, torsional spectra, conformations, complete basis set (CBS).

The methanediol molecule (MD) is a subject of intensive search in the interstellar space [1]. A number of papers present calculations of the geometry and IR spectrum of the molecule, but the internal rotation of the two OH groups has not yet been analyzed. In this paper, the 2D PES for the MD molecule was calculated in the 1) MP2 / cc-pVQZ and 2) MP2 / cc-pVTZ approximations. The kinematic parameters were determined using the Wilson vector formalism. Using the data of energy calculations performed within these two approximations, at each point, extrapolation of energy values to the complete basis set (CBS) limit was performed. The values of the torsional energy levels were determined using the DVR method. Fig. 1a shows the 2D PES for the MD molecule.



a) b)

Figure 1. Calculated 2D PES for the torsional motion of the OH groups in the MD molecule indicating the grid nodes where potential energies were calculated (a), and torsional spectra (up to 600 cm^{-1}) of the molecule for configurations with global (upper spectrum) and local (lower spectrum) energy minima at T = 30 K (b).

Fig. 1b shows the torsional spectra of the MD molecule calculated in the CBS limit in configurations with the antiparallel (upper spectrum of Fig. 1b) and parallel (lower spectrum of Fig. 1b) orientations of the hydroxyl groups at a temperature of 30 K. For the first time, the frequency of tunneling in the ground state was determined for the MD molecule, the value of which was found to be 63301 Hz.

References:

[1] C. Barrientos, P. Redondo, H. Martinez, A. Largo, Computational prediction of the spectroscopic parameters of methanediol, an elusive molecule for interstellar detection, Astrophys. J. 784(2) (2014) 132 (7 pp.). https://iopscience.iop.org/article/10.1088/0004-637X/784/2/132.