EPSC Abstracts
Vol. 8, EPSC2013-494-1, 2013
European Planetary Science Congress 2013

Towards a hot line list for H_2CO: Variational study

A. F. Al-Refaie , S. N. Yurchenko, J. Tennyson and A. Yachmenev
Department of Physics and Astronomy, University College London, London, WC1E 6BT, UK (ahmed.al-refaie.12@ucl.ac.uk)

Abstract

The goal of the ExoMol project [1] is to produce a molecular line list database with spectroscopic data important in characterising atmospheres of (exo)planets and cool stars. Here we introduce formaldehyde (H_2CO) as an addition. Formaldehyde has been detected in interstellar medium. Its spectral characteristics have provided a means of examining the composition of carbon isotopes [2] and to perform densitometry in star forming regions in galaxies [3]. However, there is limited spectral data on formaldehyde at higher vibrational and rotational excitations necessary for modelling high temperature atmospheres of different astronomical bodies such as hot planets and cool stars. As we begin to see the molecule's ever growing involvement in various astrophysical phenomena (that include a recent detection in comets [4]), it makes it vital to have a robust line list over a large range of transitions. This work presents a preliminary ro-vibrational spectra of formaldehyde for elevated temperatures. The line list is computed using the variational ro-vibrational solver TROVE [5] with an empirical potential energy surface [6] and a new *ab initio* dipole moment surface. To reach high rotational excitations required for high temperature applications, large-scale state-of-the-art variational computations were carried out for fully coupled rotational-vibrational problem. Comparison to the experimental spectra is presented.

Acknowledgements

This work was supported by the ERC under Advanced Investigator Project 267219.

References

[1] J. Tennyson and S. N. Yurchenko. Exomol: molecular line lists for exoplanet and other atmospheres. *Monthly Notices of the Royal Astronomical Society*, 425(1):21–33, 2012.

[2] C. Henkel, R. Gusten, and F. F. Gardner. C-12 / c-13 ratios from formaldehyde in the inner galactic disk. *Astronomy and Astrophysics*, 143(1):148–152, 1985.

[3] J. G. Mangum, J. Darling, K. M. Menten, and C. Henkel. Formaldehyde densitometry of starburst galaxies. *Astrophysical Journal*, 673(2):832–846, 2008.

[4] P. D. Feldman, R. E. Lupu, S. R. McCandliss, and H. A. Weaver. The far-ultraviolet spectral signatures of formaldehyde and carbon dioxide in comets. *Astrophysical Journal*, 699(2):1104–1112, 2009.

[5] S. N. Yurchenko, W. Thiel, and P. Jensen. Theoretical rovibrational energies (trove): A robust numerical approach to the calculation of rovibrational energies for polyatomic molecules. *Journal of Molecular Spectroscopy*, 245(2):126–140, 2007.

[6] A. Yachmenev, S. N. Yurchenko, P. Jensen, and W. Thiel. A new "spectroscopic" potential energy surface for formaldehyde in its ground electronic state. *Journal of Chemical Physics*, 134(24):11, 2011.