

AIP

The Journal of Chemical Physics

HOME

BROWSE

MORE ▼

[Home](#) > [The Journal of Chemical Physics](#) > [Volume 143, Issue 14](#) > [10.1063/1.4932603](#)

< PREV

NEXT >



No Access

Submitted: 23 July 2015

Accepted: 25 September 2015

Published Online: 13 October 2015

Electronic excitation of furfural as probed by high-resolution vacuum ultraviolet spectroscopy, electron energy loss spectroscopy, and *ab initio* calculations

J. Chem. Phys. **143**, 144308 (2015); <https://doi.org/10.1063/1.4932603> PDF

F. Ferreira da Silva¹, E. Lange¹, P. Limão-Vieira^{1,2, a)}, N. C. Jones³, S. V. Hoffmann³, M.-J. Hubin-Franskin⁴,  J. Delwiche⁴, M. J. Brunger^{2,5, a)},  R. F. C. Neves^{2,6,7}, M. C. A. Lopes⁶, E. M. de Oliveira⁸, R. F. da Costa^{8,9}, M. T. do N. Varella¹⁰,  M. H. F. Bettega¹¹,  F. Blanco¹², G. García¹³,  M. A. P. Lima^{8, a)}, and  D. B. Jones²

[View Affiliations](#)

[View Contributors](#)



Topics ▾

ABSTRACT

The electronic spectroscopy of isolated furfural (2-furaldehyde) in the gas phase has been investigated using high-resolution photoabsorption spectroscopy in the 3.5–10.8 eV energy-range, with absolute cross section measurements derived. Electron energy loss spectra are also measured over a range of kinematical conditions. Those energy loss spectra are used to derive differential cross sections and in turn generalised oscillator strengths. These experiments are supported by *ab initio* calculations in order to assign the excited states of the neutral molecule. The good agreement between the theoretical results and the measurements allows us to provide the first quantitative assignment of the electronic state spectroscopy of furfural over an extended energy range.

Acknowledgments

F.F.S. and P.L.V. acknowledge the Portuguese Foundation for Science and Technology (FCT-MEC) through Grant Nos. SFRH/BPD/68979/2010 and SFRH/BSAB/105792/2014, respectively, the research Grant Nos.



 PDF

acknowledges his Visiting Research Fellow position at Flinders University, Adelaide, South Australia. The Patrimoine of the University of Liège, the Fonds National de la Recherche Scientifique, and the Fonds de la Recherche Fondamentale Collective of Belgium have also supported this research. E.L. and R.F.C.N. thank CNPq (Brazil) and the Science Without Borders Programme for opportunities to study abroad. The authors wish to acknowledge the beam time at the ISA synchrotron at Aarhus University, Denmark. The research leading to these results has received funding from the European Community's Seventh Framework Programme (Grant No. FP7/2007-2013) CALIPSO under Grant Agreement No. 312284. D.B.J. thanks the Australian Research Council for financial support provided through a Discovery Early Career Research Award. M.J.B. also thanks the Australian Research Council for some financial support, while M.J.B. and M.C.A.L. acknowledge the Brazilian agencies CNPq and FAPEMIG for financial support. F.B. and G.G. acknowledge partial financial support from the Spanish Ministry MINECO (Project No. FIS2012-31230) and the EU COST Action No. CM1301 (CELINA). Finally, R.F.C., M.T.do N.V., M.H.F.B., and M.A.P.L. acknowledge support from the Brazilian agency CNPq.

REFERENCES

1. A. S. Mamman, J.-M. Lee, Y.-C. Kim, I. T. Hwang, N.-J. Park, Y. K. Hwang, J.-S. Chang, and J.-S. Hwang, *Biofuels, Bioprod. Biorefin.* **2**, 438 (2008). <https://doi.org/10.1002/bbb.95>, [Google Scholar](#), [Crossref](#)



Chem. A **103**, 858 (1999). <https://doi.org/10.1021/jp983883d>,

[Google Scholar](#), [Crossref](#)

3. A. J. Ragauskas, C. K. Williams, B. H. Davison, G. Britovsek, J. Cairney, C. A. Eckert, W. J. Frederick, J. P. Hallett, D. J. Leak, C. L. Liotta, J. R. Mielenz, R. Murphy, R. Templer, and T. Tschaplinski, *Science* **311**, 484 (2006). <https://doi.org/10.1126/science.1114736>, [Google Scholar](#), [Crossref](#)
-

4. H. Gomez Bernal, L. Bernazzani, and A. M. Raspolli Galletti, *Green Chem.* **16**, 3734 (2014). <https://doi.org/10.1039/c4gc00450g>, [Google Scholar](#), [Crossref](#)
-

5. J.-P. Lange, E. van der Heide, J. van Buijtenen, and R. Price, *ChemSusChem* **5**, 150 (2012). <https://doi.org/10.1002/cssc.201100648>, [Google Scholar](#), [Crossref](#)
-

6. J. D. Keating, C. Panganiban, and S. D. Mansfield, *Biotechnol. Bioeng.* **93**, 1196 (2006). <https://doi.org/10.1002/bit.20838>, [Google Scholar](#), [Crossref](#)
-

7. P. Pienkos and M. Zhang, *Cellulose* **16**, 743 (2009). <https://doi.org/10.1007/s10570-009-9309-x>, [Google Scholar](#), [Crossref](#)
-

8. L. D. Schmidt and P. J. Dauenhauer, *Nature* **447**, 914 (2007). <https://doi.org/10.1038/447914a>, [Google Scholar](#), [Crossref](#)
-



Process. Polym. **10**, 670 (2013).

<https://doi.org/10.1002/ppap.201200158>, [Google Scholar](#), [Crossref](#)

10. N. Schultz-Jensen, F. Leipold, H. Bindslev, and A. Thomsen, Appl. Biochem. Biotechnol. **163**, 558 (2011).

<https://doi.org/10.1007/s12010-010-9062-5>, [Google Scholar](#), [Crossref](#)

11. J. S. Bak, J. K. Ko, Y. H. Han, B. C. Lee, I.-G. Choi, and K. H. Kim, Bioresour. Technol. **100**, 1285 (2009).

<https://doi.org/10.1016/j.biortech.2008.09.010>, [Google Scholar](#), [Crossref](#)

12. A. W. Khan, J. P. Labrie, and J. McKeown, Biotechnol. Bioeng. **28**, 1449 (1986). <https://doi.org/10.1002/bit.260280921>, [Google Scholar](#), [Crossref](#)
-

13. R. F. da Costa, E. M. de Oliveira, M. H. F. Bettega, M. T. d. N. Varella, D. B. Jones, M. J. Brunger, F. Blanco, R. Colmenares, P. Limão-Vieira, G. García, and M. A. P. Lima, J. Chem. Phys. **142**, 104304 (2015).

<https://doi.org/10.1063/1.4913824>, [Google Scholar](#), [Scitation](#), [ISI](#)

14. R. F. C. Neves, D. B. Jones, M. C. A. Lopes, K. L. Nixon, G. B. da Silva, H. V. Duque, E. M. de Oliveira, R. F. da Costa, M. T. d. N. Varella, M. H. F. Bettega, M. A. P. Lima, K. Ratnavelu, G. García, and M. J. Brunger, J. Chem. Phys. **142**, 104305 (2015). <https://doi.org/10.1063/1.4913825>,

[Google Scholar](#), [Scitation](#), [ISI](#)



15. D. B. Jones, G. B. da Silva, R. F. C. Neves, H. V. Duque, L. Chiari, E. M. de Oliveira, M. C. A. Lopes, R. F. da Costa, M. T. d. N. Varella, M. H. F. Bettega, M. A. P. Lima, and M. J. Brunger, *J. Chem. Phys.* **141**, 074314 (2014). <https://doi.org/10.1063/1.4893116>, [Google Scholar](#), [Scitation](#), [ISI](#)
-
16. D. B. Jones, E. Ali, K. L. Nixon, P. Limão-Vieira, M.-J. Hubin-Franskin, J. Delwiche, C. G. Ning, J. Colgan, A. Murray, D. H. Madison, and M. J. Brunger, "Electron- and photon-impact ionization of furfural," *J. Chem. Phys.* (submitted). [Google Scholar](#)
-
17. A. D. Walsh, *Trans. Faraday Soc.* **42**, 62 (1946).
<https://doi.org/10.1039/tf9464200062>, [Google Scholar](#), [Crossref](#)
-
18. V. Santhamma, *Proc. Natl. Acad. Sci., India, Sect. A* **22**, 256 (1956).
[Google Scholar](#)
-
19. J. E. Purvis, *J. Chem. Soc.* **97**, 1648 (1910).
<https://doi.org/10.1039/ct9109701648>, [Google Scholar](#), [Crossref](#)
-
20. A. Gandini, P. A. Hackett, and R. A. Back, *Can. J. Chem.* **54**, 3089 (1976). <https://doi.org/10.1139/v76-440>, [Google Scholar](#), [Crossref](#)
-
21. R. Zwarich and I. Rabinowitz, *J. Chem. Phys.* **63**, 4565 (1975).
<https://doi.org/10.1063/1.431265>, [Google Scholar](#), [Scitation](#)
-
22. R. F. da Costa, M. H. F. Bettega, M. A. P. Lima, M. C. A. Lopes, L. R. Hargreaves, G. Serna, and M. A. Khakoo, *Phys. Rev. A* **85**, 062706



, [Crossref](#)

-
23. A. Giuliani, J. Delwiche, S. V. Hoffmann, P. Limão-Vieira, N. J. Mason, and M.-J. Hubin-Franskin, *J. Chem. Phys.* **119**, 3670 (2003).
<https://doi.org/10.1063/1.1590960>, [Google Scholar](#), [Scitation](#), [ISI](#)
-
24. A. Giuliani, I. C. Walker, J. Delwiche, S. V. Hoffmann, C. Kech, P. Limão-Vieira, N. J. Mason, and M.-J. Hubin-Franskin, *J. Chem. Phys.* **120**, 10972 (2004). <https://doi.org/10.1063/1.1738642>, [Google Scholar](#), [Scitation](#)
-
25. A. Giuliani, I. C. Walker, J. Delwiche, S. V. Hoffmann, P. Limao-Vieira, N. J. Mason, B. Heyne, M. Hoebeke, and M. J. Hubin-Franskin, *J. Chem. Phys.* **119**, 7282 (2003). <https://doi.org/10.1063/1.1603733>, [Google Scholar](#), [Scitation](#), [ISI](#)
-
26. F. Kossoski and M. H. F. Bettega, *J. Chem. Phys.* **138**, 234311 (2013).
<https://doi.org/10.1063/1.4811218>, [Google Scholar](#), [Scitation](#), [ISI](#)
-
27. I. C. Walker, M. H. Palmer, J. Delwiche, S. V. Hoffmann, P. Limão-Vieira, N. J. Mason, M. F. Guest, M.-J. Hubin-Franskin, J. Heinesch, and A. Giuliani, *Chem. Phys.* **297**, 289 (2004).
<https://doi.org/10.1016/j.chemphys.2003.10.012>, [Google Scholar](#), [Crossref](#)
-
28. R. A. Motiyenko, E. A. Alekseev, S. F. Dyubko, and F. J. Lovas, *J. Mol. Spectrosc.* **240**, 93 (2006). <https://doi.org/10.1016/j.jms.2006.09.003>



29. F. A. Miller, W. G. Fateley, and R. E. Witkowski, *Spectrochim. Acta, Part A* **23**, 891 (1967). [https://doi.org/10.1016/0584-8539\(67\)80016-3](https://doi.org/10.1016/0584-8539(67)80016-3), [Google Scholar](#), [Crossref](#)
-
30. M. Rogojerov, G. Keresztury, and B. Jordanov, *Spectrochim. Acta, Part A* **61**, 1661 (2005). <https://doi.org/10.1016/j.saa.2004.11.043>, [Google Scholar](#), [Crossref](#)
-
31. A. Gandini, J. M. Parsons, and R. A. Back, *Can. J. Chem.* **54**, 3095 (1976). <https://doi.org/10.1139/v76-441>, [Google Scholar](#), [Crossref](#)
-
32. D. Klapstein, C. D. MacPherson, and R. T. O'Brien, *Can. J. Chem.* **68**, 747 (1990). <https://doi.org/10.1139/v90-118>, [Google Scholar](#), [Crossref](#)
-
33. S. Eden, P. Limão-Vieira, S. V. Hoffmann, and N. J. Mason, *Chem. Phys.* **323**, 313 (2006). <https://doi.org/10.1016/j.chemphys.2005.09.040>, [Google Scholar](#), [Crossref](#)
-
34. M. H. Palmer, T. Ridley, S. V. Hoffmann, N. C. Jones, M. Coreno, M. de Simone, C. Grazioli, M. Biczysko, A. Baiardi, and P. Limão-Vieira, *J. Chem. Phys.* **142**, 134302 (2015). <https://doi.org/10.1063/1.4916121>, [Google Scholar](#), [Scitation](#), [ISI](#)
-
35. M. J. Brunger and P. J. O. Teubner, *Phys. Rev. A* **41**, 1413 (1990). <https://doi.org/10.1103/PhysRevA.41.1413>, [Google Scholar](#), [Crossref](#)



36. S. J. Cavanagh and B. Lohmann, J. Phys. B: At., Mol. Opt. Phys. **32**, L261 (1999). <https://doi.org/10.1088/0953-4075/32/12/102>, [Google Scholar](#), [Crossref](#)
-
37. F. Blanco and G. García, J. Phys. B: At., Mol. Opt. Phys. **42**, 145203 (2009). <https://doi.org/10.1088/0953-4075/42/14/145203>, [Google Scholar](#), [Crossref](#)
-
38. F. Blanco and G. García, Phys. Lett. A **330**, 230 (2004). <https://doi.org/10.1016/j.physleta.2004.07.027>, [Google Scholar](#), [Crossref](#)
-
39. R. F. da Costa, M. A. P. Lima, M. H. F. Bettega, E. M. de Oliveira, M. T. d. N. Varella, G. Garcia, D. B. Jones, and M. J. Brunger, “Elastic electron collisions with furfural: an investigation on the behavior of the cross sections under the influence of multichannel coupling effects” (unpublished). [Google Scholar](#)
-
40. P. Palihawadana, J. Sullivan, M. Brunger, C. Winstead, V. McKoy, G. Garcia, F. Blanco, and S. Buckman, Phys. Rev. A **84**, 062702 (2011). <https://doi.org/10.1103/PhysRevA.84.062702>, [Google Scholar](#), [Crossref](#)
-
41. L. R. Hargreaves, J. R. Brunton, A. Prajapati, M. Hoshino, F. Blanco, G. Garcia, S. J. Buckman, and M. J. Brunger, J. Phys. B: At., Mol. Opt. Phys. **44**, 045207 (2011). <https://doi.org/10.1088/0953-4075/44/4/045207>, [Google Scholar](#), [Crossref](#)



42. H. Kato, T. Asahina, H. Masui, M. Hoshino, H. Tanaka, H. Cho, O. Ingolfsson, F. Blanco, G. Garcia, S. J. Buckman, and M. J. Brunger, J. Chem. Phys. **132**, 074309 (2010). <https://doi.org/10.1063/1.3319761>, [Google Scholar](#), [Scitation](#)
-
43. E. N. Lassettre, J. Chem. Phys. **43**, 4479 (1965). <https://doi.org/10.1063/1.1696720>, [Google Scholar](#), [Scitation](#), [ISI](#)
-
44. A. R. P. Rau and U. Fano, Phys. Rev. **162**, 68 (1967). <https://doi.org/10.1103/PhysRev.162.68>, [Google Scholar](#), [Crossref](#)
-
45. L. Vriens, Phys. Rev. **160**, 100 (1967). <https://doi.org/10.1103/PhysRev.160.100>, [Google Scholar](#), [Crossref](#)
-
46. B. R. Lewis, Phys. Rev. A **78**, 026701 (2008). <https://doi.org/10.1103/PhysRevA.78.026701>, [Google Scholar](#), [Crossref](#)
-
47. H. Kawahara, H. Kato, M. Hoshino, H. Tanaka, and M. J. Brunger, Phys. Rev. A **77**, 012713 (2008). <https://doi.org/10.1103/PhysRevA.77.012713>, [Google Scholar](#), [Crossref](#)
-
48. H. Kawahara, D. Suzuki, H. Kato, M. Hoshino, H. Tanaka, O. Ingolfsson, L. Campbell, and M. J. Brunger, J. Chem. Phys. **131**, 114307 (2009). <https://doi.org/10.1063/1.3230150>, [Google Scholar](#), [Scitation](#), [ISI](#)



49. H. Kato, M. Hoshino, H. Tanaka, P. Limão-Vieira, O. Ingolfsson, L. Campbell, and M. J. Brunger, *J. Chem. Phys.* **134**, 134308 (2011).
<https://doi.org/10.1063/1.3575497>, [Google Scholar](#), [Scitation](#), [ISI](#)
-
50. M. W. Schmidt, K. K. Baldridge, J. A. Boatz, S. T. Elbert, M. S. Gordon, J. H. Jensen, S. Koseki, N. Matsunaga, K. A. Nguyen, S. Su, T. L. Windus, M. Dupuis, and J. A. Montgomery, *J. Comput. Chem.* **14**, 1347 (1993). <https://doi.org/10.1002/jcc.540141112>, [Google Scholar](#), [Crossref](#)
-
51. K. K. Baldridge, V. Jonas, and A. D. Bain, *J. Chem. Phys.* **113**, 7519 (2000). <https://doi.org/10.1063/1.1313790>, [Google Scholar](#), [Scitation](#)
-
52. R. Bauernschmitt and R. Ahlrichs, *Chem. Phys. Lett.* **256**, 454 (1996).
[https://doi.org/10.1016/0009-2614\(96\)00440-X](https://doi.org/10.1016/0009-2614(96)00440-X), [Google Scholar](#), [Crossref](#)
-
53. M. E. Casida, *J. Mol. Struct.: THEOCHEM* **914**, 3 (2009).
<https://doi.org/10.1016/j.theochem.2009.08.018>, [Google Scholar](#), [Crossref](#)
-
54. M. J. Frisch *et al.*, gaussian 09, Revision B.01, Gaussian, Inc., Wallington, CT, USA, 2010. [Google Scholar](#)
-
55. I. Colmenar, S. González, E. Jiménez, P. Martín, S. Salgado, B. Cabañas, and J. Albaladejo, *Atmos. Environ.* **103**, 1 (2015).
<https://doi.org/10.1016/j.atmosenv.2014.12.022>, [Google Scholar](#), [Crossref](#)

[Crossref](#)

56. Ed. C. Sándorfy, *The Role of Rydberg States in Spectroscopy and Photochemistry* (Kluwer Academic Publishers, Netherlands, 1999).
[Google Scholar](#), [Crossref](#)
-
57. S. Eden, P. Limão-Vieira, S. V. Hoffmann, and N. J. Mason, *Chem. Phys.* **331**, 232 (2007).
<https://doi.org/10.1016/j.chemphys.2006.10.021>, [Google Scholar](#),
[Crossref](#)
-
58. W. B. DeMore, S. P. Sander, D. M. Golden, R. F. Hampson, M. J. Kurylo, C. J. Howard, A. R. Ravishankara, C. E. Kolb, and M. J. Molina, *Chemical Kinetics and Photochemical Data for Use in Stratospheric Modelling*, Evaluation No. 12 (JPL Publication 97-4, 1997).
[Google Scholar](#)
-
59. P. Limão Vieira, S. Eden, P. A. Kendall, N. J. Mason, and S. V. Hoffmann, *Chem. Phys. Lett.* **364**, 535 (2002).
[https://doi.org/10.1016/S0009-2614\(02\)01304-0](https://doi.org/10.1016/S0009-2614(02)01304-0), [Google Scholar](#),
[Crossref](#)
-
60. R. F. da Costa, M. T. d. N. Varella, M. H. F. Bettega, and M. A. P. Lima, *Eur. Phys. J. D* **69**, 159 (2015).
<https://doi.org/10.1140/epjd/e2015-60192-6>, [Google Scholar](#),
[Crossref](#)
-

© 2015 AIP Publishing LLC.



[Submit Today!](#)

APL Materials

SPECIAL TOPIC: Design, Material, Function, and Fabrication of Metamaterials

Resources

[AUTHOR](#)[LIBRARIAN](#)[ADVERTISER](#)

General Information

[ABOUT](#)[CONTACT](#)[HELP](#)[PRIVACY POLICY](#)[TERMS OF USE](#)[FOLLOW AIP PUBLISHING:](#)

© 2022 AIP Publishing LLC

[↓ PDF](#)

