University of Groningen

Intermediate level structure, quantum beats, and nuclear spin effects in the electronic relaxation of the 1B3u ($n\pi^*$) state of pyrazine

van der Meer, Barend J. ; Jonkman, Harry Th.; ter Horst, Gerard M. ; Kommandeur, Jan

Published in:
The Journal of Chemical Physics

DOI:
[10.1063/1.443185](https://doi.org/10.1063/1.443185)

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
1982

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

van der Meer, B. J., Jonkman, H. T., ter Horst, G. M., & Kommandeur, J. (1982). Intermediate level structure, quantum beats, and nuclear spin effects in the electronic relaxation of the 1B3u ($n\pi^*$) state of pyrazine. *The Journal of Chemical Physics*, 76(4), 2099-2100. <https://doi.org/10.1063/1.443185>

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

interesting challenges remain for theoretical and experimental investigators alike. The existence of a concentration threshold for the effect^{9,15} needs to be addressed theoretically. Experimentally, the determination of the exact concentration threshold is made difficult by the weak Raman signals obtained for very dilute solution. Mirone's remark that the splitting is a smooth function of the dielectric constant needs to be verified by *measuring* the concentration dependent dielectric constant, since this property is not necessarily proportional to the volume fraction,¹⁷ as was assumed in Refs. 2 and 9. And finally, in conjunction with the development of more refined theoretical methods taking local order into account, experiments which vary density and temperature independently also need to be performed.

Support for this research by the Petroleum Research Fund of the American Chemical Society, and by an M. J. Murdock Charitable Trust Grant of Research Corporation, is gratefully acknowledged.

- ¹P. Mirone, J. Chem. Phys. **77**, 2704 (1982).
- ²J. McHale, J. Chem. Phys. **75**, 30 (1981).
- ³C. H. Wang and J. McHale, J. Chem. Phys. **72**, 4039 (1980).
- ⁴C. J. F. Böttcher, *Theory of Electric Polarization* (Elsevier, Amsterdam, 1952).
- ⁵E. L. Pollock, B. J. Alder, and L. R. Pratt, Proc. Natl. Acad. Sci. USA **77**, 49 (1980).
- ⁶T. Keyes, Chem. Phys. Lett. **76**, 369 (1980).
- ⁷L. Onsager, J. Am. Chem. Soc. **58**, 1486 (1936).
- ⁸H. Fröhlich, *Theory of Dielectrics* (Oxford, London, 1958).
- ⁹P. Mirone and G. Fini, J. Chem. Phys. **71**, 2241 (1979).
- ¹⁰J. G. Kirkwood, J. Chem. Phys. **7**, 911 (1939).
- ¹¹G. Nienhuis and J. M. Deutch, J. Chem. Phys. **56**, 1819 (1972); **55**, 4213 (1971).
- ¹²G. N. Patey and J. P. Valleau, J. Chem. Phys. **61**, 534 (1974).
- ¹³L. Verlet and J. -J. Weis, Mol. Phys. **28**, 665 (1974).
- ¹⁴G. D. Mahan, Phys. Rev. **153**, 983 (1967).
- ¹⁵M. Kamoun and P. Mirone, Chem. Phys. Lett. **75**, 287 (1980).
- ¹⁶G. Fini and P. Mirone, Spectrochim. Acta A **32**, 625 (1976).
- ¹⁷F. Franks and D. J. G. Ives, Q. Rev. Chem. Soc. London **20**, 1 (1965).

ERRATA

Erratum: Intermediate level structure, quantum beats, and nuclear spin effects in the electronic relaxation of the $^1B_{3u}(n\pi^*)$ state of pyrazine [J. Chem. Phys. **76**, 2099 (1982)]

Barend J. van der Meer, Harry Th. Jonkman, Gerard M. ter Horst, and Jan Kommandeur

Laboratory for Physical Chemistry, University of Groningen, Nyenborgh 16, 9749 AG Groningen, The Netherlands

The structure in the spectra of pyrazine and pyrimidine shown in Fig. 1 of our paper has recently been shown to be due to the mode structure of the laser used. It should, therefore, not be viewed as "intermediate level structure."

All other conclusions of our paper remain unaffected.