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Department of Chemistry and Applied Chemistry: W J Orville-Thomas, Emeritus Professor of Physical Chemistry

WJOT/ND

19 October 1992

Professor M.W.Evans,
Dept. of Physics,
University of North Carolina,
Charlotte,
NC 28223,
U.S.A.

Dear Myron,

Thank you for your letter of 6 October 1992. I agree that it would be a nice gesture to publish a volume to mark the retirement of Alun Price. Provided that he raises no objections then I would support such a venture.

Unfortunately, I have just been deposed as editor of MOLLIQ and replaced, against my wishes, by Jack Yarwood. Fortunately, my old friend and colleague

Professor Henryk Ratajczak,
Institute of Chemistry,
University of Wroclaw,
ul Joliot Curie 14,
50-383 Wroclaw,
POLAND,

remains as editor and I would like you to give him as much support as you have given me in the past. I shall send a copy of this letter to put him in the picture and it would be appreciated if you would liaise directly with him.

My abrupt dismissal as editor by Dr.Julian Pitt, of Elsevier, a new broom, gave me quite a shock since there had been virtually no discussion of my retirement and I thought that they were waiting for recommendations as to possible replacements from myself. In the event it was not to be. I got a letter from Pitt telling that as from 31 October 1992 the MOLLIQ operation would be transferred to Yarwood in Durham. Naturally, their treatment of me has hurt but I do hope that you will not allow this to influence you in any way since my endeavours now will be to support Henryk as senior editor of MOLLIQ and to give him all the help I can, since from the financial point of view, the small amount of money he gets for editing MOLLIQ is of vital importance to him.

I was glad to read in a previous letter that you are settling in well at UNC. It is a campus that I know well since I spent over a year at Duke University.

With very best regards,

Yours sincerely,

UNC CHARLOTTE
The University of North Carolina at Charlotte
Charlotte, N.C. 28223

Department of Physics
704/547-2536
FAX 704/547-3160

7 June, 1993

Prof. Dr. Henryk Ratajczak,
Editor, "The Journal of Molecular Liquids",
Institute of Chemistry,
University of Wroclaw,
ul Joliot-Curie 14,
50-383 Wroclaw,
POLAND,

Subjects:

1) Editor of "Journal of Molecular Liquids": Analysis & Recommendations
2) Status of Two of My Manuscripts (MSS)
3) Scientific Rebuttal - in Appendix

References: Dr. Yarwood's Letter of 24th May, 1993.
MSS: "Theory of the Optical Faraday Effect";
MSS: "The Control of Light Self Squeezing with the Intensity Dependent Optical Faraday Effect in Liquids."

Dear Prof. Ratajczak,

On the inside back cover of JML it is stated that authors are requested to submit manuscripts to one of the Editors, and I was pleased to submit the above MSS to you lately. To my surprise, I have received the enclosed letter from Dr. Yarwood, who appears to have interceded and to have rejected them. As you can see, Dr. Yarwood, who refers to himself now as "Editor in Chief" is openly hostile.

The previous editor, Prof. W. J. Orville-Thomas, known as "Orville" to his colleagues throughout the profession, has been replaced by Dr. Yarwood, but without consultation of the Board. I am sure that Messrs. Elsevier appointed Dr Yarwood with the best of intentions, probably after being approached privately by Dr Yarwood himself, and my letter implies no criticism of the Publishers or any member of staff of Elsevier. However, I believe that the Board

Therefore I believe that the Board should assess candidature according to some guidelines, for example past contributions to the journal of a candidate, and the qualifications of that candidate. A Vita from each candidate is surely a minimum requirement. The Board has seen nothing of your credentials at all. The manner of your appointment has no discernible element of democracy or meritocracy. Indeed, the appointment appears to have been the personal, no doubt well intentioned, but at the same time ill-judged, decision of ONE inexperienced member of staff at Elsevier. Orville-Thomas' own letter of intent, with recommendations for candidature, was ignored in the most lamentable fashion. The distinguished members of the Editorial Board were likewise swept aside, and the self-engineered appointment pressed ahead full steam. Now we find that Henryk Ratajczak, a distinguished Senior Editor disappears overnight, and my mail to him is returned to me by you, the self styled editor in chief.

I hope that the silent majority on the Board will voice opinion on these acts, which appear to me to be shaded with ill-balanced judgement. This is a regrettable way to treat Prof. Orville-Thomas, a kindly man whose services to science have been recognised by the international community of scientists. Among these awards are two Gold Medals and two degrees Honoris Causa. He has been EUCMOS Chairman for many years, has lectured in some fifty countries, has produced fourteen books and over two hundred papers. Above all, he has edited over **two hundred volumes** of scientific papers. You have edited no journal. He is professor emeritus in the University of Salford. His services to science and to mankind are manifest. His opinion and mine are that you are not the best candidate. You must take count, surely, of the opinion of your own Ph. D. advisor and former teacher.

Are the Members of the Board to be treated as distinguished fellow scientists or ignored? When candidature for a position in academia is assessed, the decision is not made by the candidate himself, as in your case, but through the combined opinion of experienced assessors. I will now proceed to obtain the opinion of all Board Members on your appointment, a procedure in which you chose yourself to be editor. No other candidates were even aware that the process was going on, and none had a chance to apply.

So far the opinions of two Board Members are known. Prof. Orville-Thomas (if he has not been removed arbitrarily) and myself are negative. As soon as Prof. Dr. Ratajczak finds out that he has been removed from the Senior Editorship which the journal advertises him to hold, then I feel that he is likely to be negative. I will now consult other Board Members by mail and ask for their opinions and if they are interested in candidature or in suggesting names.

An objective (statistically valid) assessment of Orville-Thomas' performance can be obtained from any good library in the Journals Ratings of the Science Citation Index. The impact factors of his journals compare well with others in the field over a period of years. The appearance of "The Journal of Molecular Liquids" has been against it, because it is not typeset by Elsevier. This is hardly a criticism of the contributors or editor. Its predecessor journal "Advances in Molecular Relaxation (and Interaction) Processes", started out as typeset, but for some reason Elsevier decided to produce it "camera-ready". My personal contributions to the journal over some twenty years amount to about eighty articles and reviews, all produced camera ready. These have attracted well over one thousand requests for reprints from scholars in many countries. This work (and more like it) was recognised, as you know, by the Meldola Medal and

by members of my former group, and are presumably aware of the above work. Your article is therefore misleading, and I will point this out in detail in a rebuttal.

Reproduction of Artwork from "The Journal of Molecular Liquids."

In the footnote to your figure (5.4.11), page 258 of the abovementioned article you claim to have obtained permission to reproduce a figure from J. Mol. Liq., 36, 237 (1987), a figure which I recognise as having been produced from my theoretical work. I received no request for permission to reproduce this Figure, and I gave no such permission. I do not know whether you requested or received permission from Dr Gareth J. Evans. Tracing this reference, I find it listed in your article as ref. (169a), by **J. Yarwood.** I received no request from you to reproduce my figure in your ref. (169a).

If a comparison is made of your Figure (5.4.11), which you claim as your own, with Figure (6.3.2.14), page 469 of "Molecular Dynamics", by M. W. Evans, G. J. Evans, W. T. Coffey, and P. Grigolini (Wiley Interscience, New York, 1982), it can be seen clearly that curves B, C and D of "your" figure are identical with curves 1, 2 and 4 of the figure by Evans et al. I remember this because it was I who originally computed the curves, and it was I who drew the original figures. My original drawings have been traced and reproduced as if they were taken from ref. (169a) of your article.

In this article, however, it is made to look as if you were the sole author and instigator of this work. In the caption of Fig. (5.4.11) there is no reference to "Molecular Dynamics". The theoretical and experimental work for this figure was carried out at the Edward Davies Chemical Laboratories by Dr Gareth J. Evans and myself, then working in the group of Prof. Mansel Davies. The work was made available to your laboratory and was published in M. W. Evans, G. J. Evans, J. Yarwood, P. L. James, and R. Arndt, Mol. Phys., 38, 699 (1979). I wrote most if not all of this paper myself. You refer obliquely to this paper as your ref. (145), but there is nothing to link the figure you have reproduced with the original work by G. J. Evans and myself. Instead, you refer to your ref. (169a) as the source of your Figure (5.4.11).

You are in fact using data obtained by the same author (G. J. Evans) as you are criticising. These data were not obtained in your laboratory, and are not original to your ref. (169a). The reader is told that ref. (169a) is the source of these data, whereas the real source is work carried out much earlier by G. J. Evans. The source of the theoretical curves is work carried out circa 1977/1978 by myself as British Ramsay Memorial Fellow at Aberystwyth.

At no stage did you ever ask me for permission to reproduce my own work.

Finally, despite having been the originator of several ideas in the far infra red, and depsite being a double medallist of the Royal Society of Chemistry of London, I received no invitation from you to contribute to this volume. I am flattered you think so highly of my work as to go to the trouble of re-drawing it for reproduction.

Sincerely Yours,

Myron Evans.

(Dr. M. W. Evans)

Copied : Interested Colleagues, Messrs. Elsevier.

UNCCHARLOTTE
The University of North Carolina at Charlotte
Charlotte, N.C. 28223

Department of Physics
704/547-2536
FAX 704/547-3160

8 June, 1993,

Chief Executive Officer,
Elsevier Science Publishers,
P.O. Box 211,
1000 AE Amsterdam,
THE NETHERLANDS,

Dear Sir/Madame,

**"By doubting we come to questioning,
and by questioning we perceive the truth."**

In the Europe of 1122, Peter Abelard got into a lot of trouble by asking questions, but we like to think that he improved matters a little in the end. In the hopes of improving matters, I wish to ask a few questions, make a few comments, and suggest a few answers regarding "The Journal of Molecular Liquids".

Questions:

Q1. Has Elsevier given Dr. Yarwood the title of "editor in chief"? (What is Prof. Ratajczak's title - or is he no longer an editor?)

Q2. Are **all** authors now forced to submit their manuscripts to Dr Yarwood? If so, why has the previous policy, giving authors a choice of editor, been changed?

Comments:

C1. In the enclosed copy of my June 7th 1993 letter to Dr. Ratajczak, I've described the ways in which Dr Yarwood's behavior is well outside the accepted norm for editors; see for example the guidelines of the American Physical Society.

C2. I believe Dr. Yarwood, in his May 24th 1993 letter to me, misrepresented my 6/12/92 letter ("Please note that threats of the nature made in your letter of 6/12/92 do nothing to enhance your reputation and will have no effect on editorial decisions this time.") If he copied his letter to anyone - the remark may be construed as an attempts at character assassination. This is a serious matter.

C3. Many of us were disturbed at the way in which Prof. Orville-Thomas was summarily removed as editor of the Journal. The choice of Dr. Yarwood was also a mystery.

Suggestions:

S1. I suggest that Elsevier investigate this matter. A list of the relevant documents I have enclosed is noted below.

S2. I urge you to elect Orville Thomas as Editor Emeritus of the Journal with executive powers as a Senior Editor.

S3. I urge you to replace Dr. Yarwood. In this context, I recommend that you utilize the Editorial Board. Specifically, why not have the Board be involved in the selection process, recommending outstanding Scientists in the subject matter covered by the Journal? (There are in fact several Board Members who are equally, if not better qualified then Dr. Yarwood.)

S4. I suggest that the 'editorial term' should be limited to about two years. In this way, the Journal will continue to be alert and open to new ideas.

Thank you for your time and consideration,
Sincerely Yours,

Myron Evans

Dr. M. W. Evans
Professor, Dept. of Physics

List of Enclosures:

1. Dr. Yarwood's May 24, 1993 letter to me.
2. My June 7, 1993 letter to Prof. Dr. Henryk Ratajczak.
3. Orville-Thomas' October 19, 1992 letter to me.
4. My November 18th, 1992 letter to Orville-Thomas.
5. Orville-Thomas' November 24, 1992 letter to me.
6. My December 6th letter to Dr. Yarwood.

M. W. Evans, Ph.D., D.Sc.

Professor of Physics,
Department of Physics,
University of North Carolina,
Charlotte,
NC 28223,
U.S.A.

14 June, 1993,

Dr. J. Yarwood,
Chemistry Department,
University of Durham,
South Road, Durham, DH1 3LE,
Great Britain,

Dear Dr. Yarwood,

On p. 222 of a volume "Spectroscopy and Relaxation of Molecular Liquids", which you edited in 1991 for Elsevier you claim to have checked the far infra red peaks work of Dr Gareth J. Evans, to which you refer in refs. 76 to 78. A sample of your checking spectrum is given in Fig. (5.3.12), in which you estimate an uncertainty of 10 to 20 wavenumbers. You claim that the measured absorption spectrum was in good agreement with "the indirect measurements of the same study", presumably refraction interferograms.

You conclude that if discrete features were present in the FIR spectrum of liquid acetonitrile they must be less intense than the levels implied by the random uncertainties in the measurements. These levels, you claim, were significantly less than the levels in the earlier studies, presumably by G. J. Evans.

GJE and I know about these remarks only because the volume was sent to me for review, you appear not to have given either of us a chance to see your remarks, and did not communicate with us prior to publication. We were not even aware that the work was taking place. I will shortly prepare a formal paper rebutting your remarks, which should have been sent to us in preprint form. The uncertainty in your spectra means that they were too noisy for any conclusion to be drawn. The spectra by GJE are of higher quality and less noisy.

In respect of theory of far infra red peaks, you do not refer to the key paper by Coffey, Corcoran and myself, which produced the Evans peaks theoretically:

"On the Existence of Far infra red Absorption Peaks in the Complex Polarisability of the Itinerant Oscillator Model of Polar Fluids." by W. T. Coffey, P. Corcoran and M. W. Evans, "Molecular Physics", 61(1), 15-22 (1987).

You do, however, refer to other papers by these authors in the Proceedings of the Royal Society of London and "Chemical Physics Letters". You also refer to many other papers

by members of my former group, and are presumably aware of the above work. Your article is therefore misleading, and I will point this out in detail in a rebuttal.

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Myron Evans.

(Dr. M. W. Evans)

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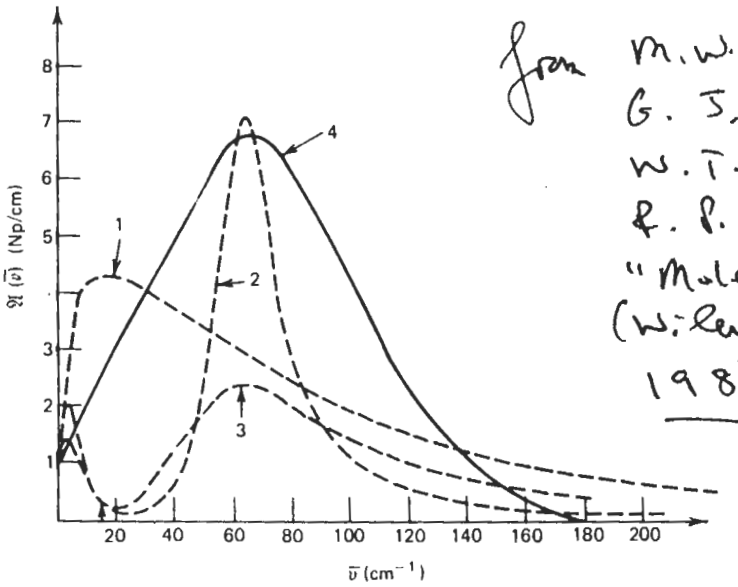


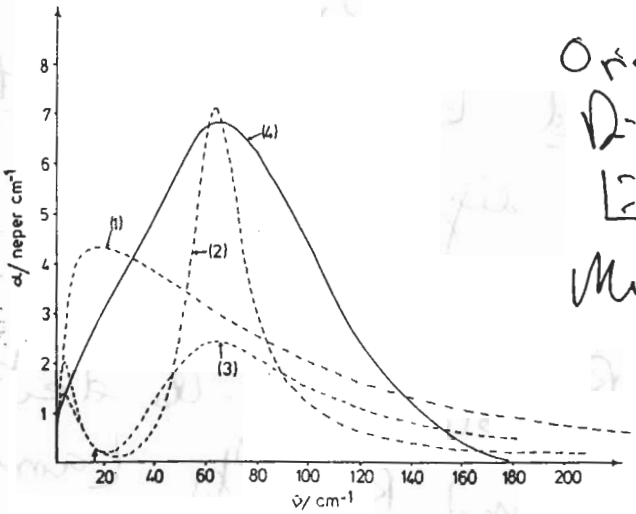
from M.W. Evans, G. J. Evans, W. T. Coffey, P. P. Grigolini, "Molecular Dynamics" (Wiley, New York, 1982)

Figure 6.3.2.14 Comparison of experimental and theoretical results for CH_3CN in CCl_4 (0.02 mole fraction at 318°K). Solid line, observed data. 1, Symmetrical top itinerant oscillator model with $I_1 = 10I_2$, $\beta_2 = 5$ THz. 2, Symmetrical top itinerant oscillator model with $I_1 = 10I_2$, $\beta_2 = 15$ THz. 3, Binary collision model for comparison with $\beta_1 = 20$ THz. (Note that this zero-order Mori truncation is unable to shift the frequency of maximum absorption to observed experimental frequencies. The itinerant oscillator model, on the other hand, produces two distinct peaks corresponding to the low and high frequency absorptions but is unable to produce one continuous profile matching the experimental observation.)

factor $\epsilon''(\omega)/\omega$, the short time details are concealed and resolved only with the most careful intensity control.

The models we use should be restricted to those that successfully describe the short time details of the motion. The rotational diffusion model used to calculate NMR correlation times is unacceptable because it obscures these features, giving artificial experimental correlation times.

The intercomparison of results from different experiments for this molecule proves inconsistent. In his review of the data available, Griffiths (1973) concludes t the best values for the $l = 1$ and $l = 2$ correlation times $\tau_{1R}(\perp)$ and $\tau_{2R}(\perp)$ are 3.3 and 1.1 psec, respectively, at 298°K, which (conveniently) is exactly the ratio expected for rotational diffusion. There is evidence, however (Chapter 12), that both these values may be incorrect. The τ_{1R} value is obtained from microwave data on the liquid and includes the effects of cross correlations but still has a large uncertainty associated with it. Data on τ_{2R} obtained from more recent measurements on ν_2 and ν_3 modes of CH_3CN suggest a value nearer 1.4 psec at 298°K. This lack of agreement may be a consequence of the strongly oriented local structure of



Original Diagram, Evans et al., Mol. Phys., (1979), vol. 38.

Comparison of observed and predicted data for CH_3CN in CCl_4 (0·02 mole fraction, 318 K). Curve (1), Binary collision (J diffusion) model first-order truncation, $\beta_1 = 20$ THz; Curve (2), Symmetric top itinerant oscillator model $I_1 = I_2$, $\beta_1 = 5$ THz; Curve (3), same with $\beta_2 = 15$ THz; Curve (4), observed data.

generalized since the collisions are elastic and infinitely short. The r.m.s. torque is again undefined.

In previous studies on highly polar molecules [8 (b), 17 (b, d)] the symmetric oscillator model produces a far-infra-red spectral distribution (figure 4) which is too narrow even for large values of the molecule–annulus friction parameter β_1 (figure 4). It is clear that fixing β_1 at $kT\tau_D/I_2$ (where τ_D is the inverse frequency of the loss peak) and varying β_2 does little to improve the situation ($I_1 = 10I_2$ as one would expect [17 (b)]). Furthermore, the dipole–dipole coupling interpretation of equation (7) is not considered to be realistic since solutions since such coupling should have been largely removed.

Figure 5 shows the results of comparing our observed data at 318 K with the second-order approximants of the Mori continued fraction (for example, equations (4) and (5)). It is seen that second- and successive-order continued fraction approximants of the orientational autocorrelation function, $C_u(t)$, first used by Evans *et al.* [32] seem a little more realistic than models (1) and (2) which are respectively the zeroth- and first-order approximants to the continued fraction representation of the angular momentum autocorrelation function. Since we approached these model calculations in several ways, it is worth outlining the methods used.

First we had some difficulty in fitting our data to equation (8) since complex refractive index data were not available [14 (a)]. Initially we therefore fitted $\alpha(\omega)$ data to an expression [23 (c, f), 14 (a)] which is independent of ϵ_∞:

$$\alpha(\omega) = \sqrt{(2)}\epsilon''(\omega)\omega/c[(\epsilon'(\omega)^2 + \epsilon''(\omega)^2)^{1/2} + \epsilon'(\omega)]^{1/2}, \qquad (13)$$

($\epsilon_0 - \epsilon_\infty$) was fixed at the observed value (table 1). This equation gives