This article was downloaded by: [Tomsk State University of Control Systems and Radio]

On: 21 February 2013, At: 11:57

Publisher: Taylor & Francis

Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH,

UK



Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information: http://www.tandfonline.com/loi/gmcl16

Explanation for the Anomalous IR Dielectric Constant of TTF-TCNO

S. Marianer ^a , M. Weger ^a & M. Kaveh ^b

To cite this article: S. Marianer, M. Weger & M. Kaveh (1982): Explanation for the Anomalous IR Dielectric Constant of TTF-TCNQ, Molecular Crystals and Liquid Crystals, 85:1, 147-150

To link to this article: http://dx.doi.org/10.1080/00268948208073640

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: http://www.tandfonline.com/page/terms-and-conditions

This article may be used for research, teaching, and private study purposes. Any substantial or systematic reproduction, redistribution, reselling, loan, sub-licensing, systematic supply, or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae, and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand, or costs or damages

^a Racah Institute of Physics Hebrew University, Jerusalem, Israel

^b Bar Ilan University, Ramat-Gan, Israel Version of record first published: 14 Oct 2011.

whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

Mol. Cryst. Liq. Cryst., 1982, Vol. 85, pp. 147-150 0026-8941/82/8501-0147\$06.50/0
© 1982 Gordon and Breach, Science Publishers, Inc. Printed in the United States of America

(Proceedings of the International Conference on Low-Dimensional Conductors, Boulder, Colorado, August 1981)

EXPLANATION FOR THE ANOMALOUS IR DIELECTRIC CONSTANT OF TTF-TCNQ

S. Marianer, M. Kaveh, and M. Weger Racah Institute of Physics Hebrew University, Jerusalem, Israel.

Received for publication August 31, 1981

The recent data of Tanner et al indicates an anomalous behavior of the dielectric constant ϵ_1 of TTF-TCNQ. The large and negative value of ϵ_1 found experimentally is accounted here by applying the phonon-drag theory. The positive value of ϵ_1 found for damaged samples is accounted by a broken-chain model.

Recent data by Tanner et al (1) raised again the question whether collective effects (2,3,4) or single particle theory (5,6,7) can account for transport phenomena in quasi-one-dimensional organic metals.

Tanner et al (1) obtained the ac conductivity $\sigma(\omega)$ and the dielectric constant ϵ_1 in the far infrared region (ω <400 cm⁻¹), for 25 K < T < 160 K . The main features of their results are: (i) Rapid decrease of the conductivity with increasing frequency at ω = 20 cm⁻¹ (ii) Large (in absolute value) and negative dielectric constant (ϵ_1 = -10⁴)

These experimental results are in sharp contradiction with previous results of Gunning et al (8) who found a positive dielectric constant $\epsilon_1{}^{=}$ +2500. This positive dielectric constant invoked the collective approach which yields a positive ϵ_1 . Another possible explanation for the positive dielectric constant was given by using a broken chain (9,10) model. This model applies to low-quality samples with damaged surfaces.

^{*} Bar Ilan University, Ramat-Gan, Israel.

In order to test which explanation is correct, one needs to measure ϵ_1 for very high quality samples. Indeed, the measurements by Jacobsen (11) and Tanner et al (1) for very high quality samples indicate a negative dielectric constant. Thus, the positive (8) ϵ_1 may be attributed to damaged areas near the surface which yield a large positive ϵ_1 .

While the negative sign of ε_1 is properly accounted for by the Boltzmann-Drude theory, the magnitude is not. $(\varepsilon_1)_{\rm Drude}^{\simeq}$ -200 at T= 100 K which is about two orders of magnitudesmaller than the experimental value.

We apply here the phonon-drag theory (12) and get

$$\sigma(\omega) = \sigma_{\rm dc} \left(1 + i\omega \tau_{\rm dc} + \frac{\tau_{\rm dc}}{\tau_{\rm el \rightarrow ph}} \right) \frac{i\omega \tau_{\rm ph \rightarrow el}}{1 + i\omega \tau_{\rm ph \rightarrow el}} - 1$$

$$\varepsilon_{1}(\omega) = -4\pi \sigma_{dc} \tau_{dc} \frac{1 + \tau_{ph \to el} / \tau_{el \to ph} + \omega \tau_{ph \to el}}{[1 - \omega^{2}_{dc} \tau_{ph \to el}] + \omega^{2}[\tau_{ph \to el} + \tau_{dc} (1 + X)]^{2}}$$

where $X = \tau_{ph \to el}/\tau_{el \to ph}$ and $\tau_{el \to ph}$, $\tau_{ph \to el}$ are the relaxation times for the electron (due to emission or absorption of a $2k_F$ phonon) and the $2k_F$ phonon (due to absorption or emission by an electron). At $\omega \to 0$ this yields $\epsilon_1 \simeq -10^4$ in good agreement with experiment. τ_{dc} is the relaxation time of the electron due to quadratic coupling (the 2-phonon mechanism) which dominates in TTF-TCNQ (7).

The sharp difference of ϵ_1 between different samples supports the idea of the existence of broken chains for which we get:

$$\sigma(\omega) = \frac{\sigma_{\text{bulk}}}{1 + (\omega/\omega_{\text{c}})^2} \left((\omega/\omega_{\text{c}})^2 + 1(\omega/\omega_{\text{c}}) \right)$$

where $\omega_{\rm c}=4\pi{\rm d}\sigma_{\rm bulk}/\varepsilon_{\rm o}$ and d is the width of the break, $\varepsilon_{\rm o}$ the effective dielectric constant of the broken section and ℓ is the length of the chain. Thus, the large positive $\varepsilon_{\rm l}$ is accounted for by this model.

Describing the bulk by the phonon-drag theory and the surface by a broken strand model with an effective medium calculation (taking into account also the transverse conductivity) we obtain good agreement with experimental results (Figs. 1, 2).

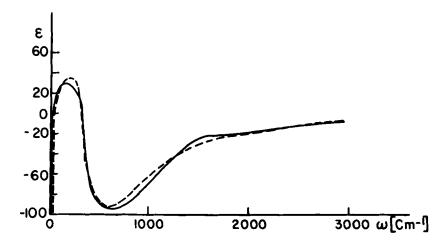


FIGURE 1 Dielectric constant $\epsilon_1(\omega)$ at T=100 K. Full line-experiment (ref. 11). Dashed line-present theory.

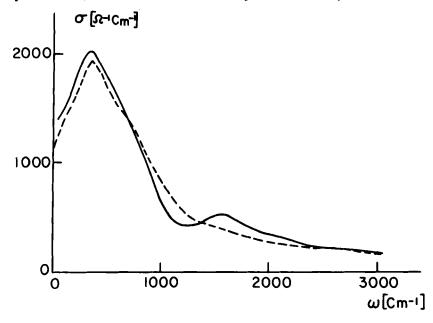


FIGURE 2 Conductivity $\sigma(\omega)$ at T=100 K. Full line - experiment (ref. 11). Dashed line - present theory.

REFERENCES

- D.B. Tanner, K. D. Cummings and C. S. Jacobsen, Phys. Rev. Lett. (in press).
- J. Bardeen, Solid State Commun. <u>13</u>, 357 (1973); D. Allender, J. W. Bray and J. Bardeen, Phys. Rev. <u>B9</u>, 119 (1974).
- D. B. Tanner, C. S. Jacobsen, A. F. Garito and A. J. Heeger, Phys. Rev. <u>B13</u>, 3381 (1976).
- A. J. Heeger, M. Weger and M. Kaveh, Proceedings of Dubrovnik Conference 1978; <u>Lecture Notes in Physics 95</u> p. 105 (Springer Verlag, New York, 1979).
- E. M. Conwell, Phys. Rev. <u>B22</u>, 1761 (1980); G. A. Thomas et al, Phys. Rev. B13, 5105 (1976).
- M. B. Salamon, J. W. Bray, G. de Pasqual, R. A. Craven
 G. Stucky and A. Schultz, Phys. Rev. <u>B11</u>, 619 (1975).
- 7. H. Gutfreund and M. Weger, Phys. Rev. <u>B16</u>, 1753 (1977).
- 8. W. J. Gunning, A. J. Heeger, T. F. Shchegolev and S. P. Zolotukhin, Solid State Commun. 25, 981 (1978).
- M. Weger and M. Kaveh, J. Phys. C: Solid State <u>12</u>, 2567 (1979).
- 10.S. Marianer, M. Kaveh and M. Weger, submitted to Phys. Rev.
- 11.C. S. Jacobsen, Proceedings of Dubrovnik, Conference 1978; <u>Lecture Notes in Physics 95</u> (Springer Verlag, New York, 1979) p. 223.
- 12. (a) M. Weger and H. Gutfreund, Comments on Solid State Physics, 8,135 (1978).
 - (b) M. Kaveh and M. Weger, Phys. Rev. <u>B20</u>, 2264 (1979).
 - (c) H. Gutfreund, M. Kaveh and M. Weger, Proc. Dubrovnik Conf. 1978; <u>Lecture Notes in Physics 95</u> (Springer Verlag New York, 1979) p. 105.
 - (d) M. Kaveh, H. Gutfreund and M. Weger, Phys. Rev. <u>B18</u>, 7171 (1978).