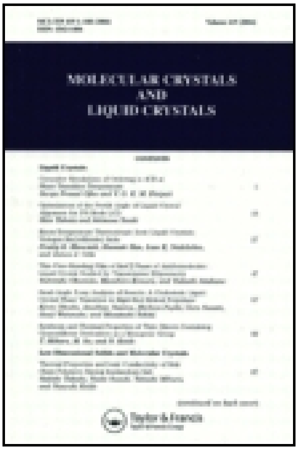

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Magnetic and Electrical Properties of Qn $(TCNQ)_2$

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Magnetic and Electrical Properties of $Qn(TCNQ)_2$

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High precision magnetic susceptibility, low frequency ESR, dc and ac conductivity measurements are presented with particular attention to separate intrinsic and spurious e.g. chain end effects.

A model, where both electron–electron and polaronic interactions and disorder effects are of importance is proposed to account for the experimental results.

In this paper we present evidence which show that in the donor-acceptor salt[1] $Qn(TCNQ)_2$ both structural peculiarities: the 1d arrangement of the donors and acceptors, and the random donor arrangement are of importance. The central features of a model we propose include: (i) A band gap in the single particle excitations arising from long range electron–electron interaction together with polaronic effects, and an associated singlet ground state, (ii) Band tailing into the correlation gap arising from disorder effects with subsequent localization leading to a mobility gap, to the existence of both localized and extended electronic states and a smeared out collective excitation spectrum.

The dc and microwave conductivity are shown in Figure 1, the insert shows the low temperature data of Buravov *et al.*[1] The good reproducibility from sample to sample shows, that both the dc and ac conductivity is an inherent property. δ is larger by about a factor of 10 than that corresponding to the maximum phonon assisted hopping conductivity $\sigma \approx 3\text{–}5\ \Omega^{-1}\ \text{cm}^{-1}$ and therefore the low temperature activation energy $\Delta E = 0.03$ eV reflects a gap in the extended electron states.[2] The overall behaviour of $\sigma_{dc}(T)$ is well described by an extended Hubbard model where nearest neighbour Coulomb interactions are responsible for the band gap in quater filled band appropriate for the complex (1 : 2) salts.[3] The ac conductivity indicates at the same time a contribution coming from hopping between localized states in the band gap, in a similar way than that observed in amorphous semiconductors.

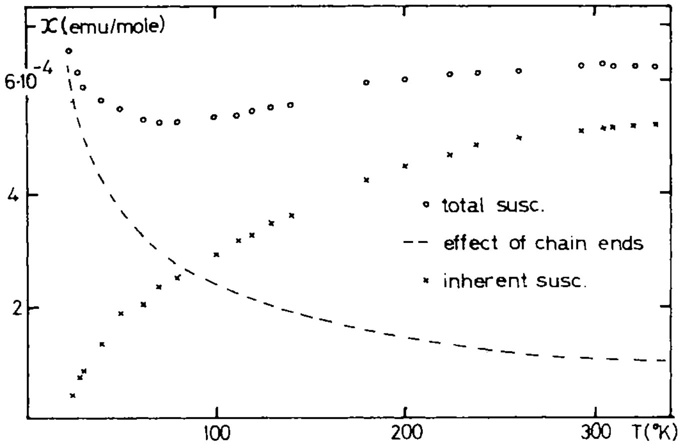

FIGURE 1

The effects of chain ends on the susceptibility has been demonstrated before,[4] Figure 2 shows the measured total susceptibility and the contribution of chain ends together with the inherent susceptibility characteristic to infinite chains. The diamagnetic contribution was evaluated by comparing the static susceptibility with that measured by the Schumaker–Slichter method. The nonmagnetic (i.e. singlet) ground state is the consequence of

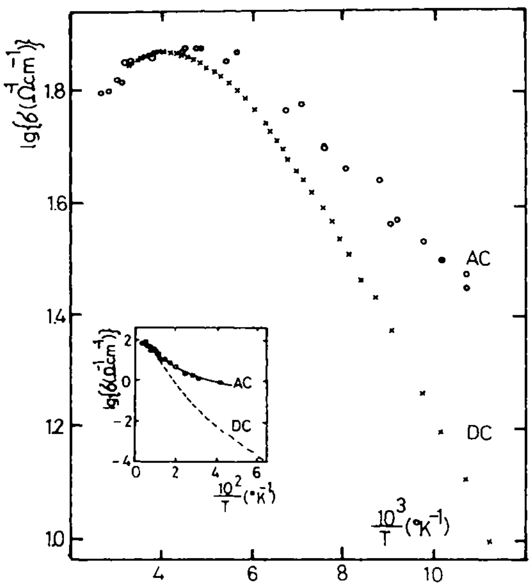

FIGURE 2

the electron–electron and polaron interactions (which at the same time open up a gap in the single particle excitations). The susceptibility however is not simple singlet-triplet excitation, but can be well fitted with a smeared out excitation spectrum assuming J varies between 0.01 and 0.1 eV. We believe, this smearing is due to disorder, and is related to the disorder effect evidenced by the difference between the dc and ac conductivity.

We do not find clear indication for a smeared out phase transition, but note that the disappearance of $\sigma_{ac} - \sigma_{dc}$ and the behaviour $\rho \sim T$ above the conductivity maximum[2] indicates, that the effect of band gap is strongly reduced at temperatures $kT > \Delta E$.

The existence of a single particle gap and the singlet ground state is a general feature of the 1 : 2 salts of TCNQ. For large band gaps (characteristic to the less conducting salts) the role of disorder is weak and all excitations are relatively sharp as evidence by the vanishing dispersion of the conductivity, small dielectric constant and by the well defined singlet-triplet excitations. For small band gaps (observed in the good conductors) the effect of disorder is enhanced and smears out both the collective and single particle excitation spectrum as demonstrated here on the $Qn(TCNQ)_2$. Salts with intermediate band gaps, like $NMeQn(TCNQ)_2$,[5] the magnetic and electric properties are between that found in well conducting and less conducting compounds.

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