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N.M.R. PROTON LINESHAPE IN SINGLE CRYSTALS (TMTSF)2 X AND ANTIFERROMAGNETIC SATELLITES.

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Abstract Beetwen 1.2K and 4.2K in the metallic state of relaxed (TMTSF)2 CLO4, the tunneling of methyl groups gives a central line and four symmetrical satellites in proton N.M.R.. In quenched (TMTSF)2CLO4 and (TMTSF)2PF6 new satellites give the orientation and amplitude of the local fields (15 G in CLO4 and 27 G in PF6) corresponding to an S.D.W. amplitude of 13% and 25% respectively. The S.D.W. seems incommensurate to the lattice.

INTRODUCTION

We have measured the N.M.R. line shape using a home made Robinson box (1) in a magnetic field 0.43 T perpendicular to the a axis. In the normal state the structure comes from dipolar interaction averaged by tunneling of protons in methyl group and in the S.D.W. phase additionnal satellites appear, associated to the field created by the antiferromagnetic sublattices.

N.M.R. LINE SHAPE OF METHYL GROUPS IN THE NORMAL STATE

In the metallic relaxed state of (TMTSF)2 ClO4 (one hour and half from 50K to 4,2K) we observe a central line and four symmetrical lines as function of field H angle with respect to the molecular axis in complete agreement with the theory of Clough (2): In the case of a fast quantum tunneling with respect to dipolar interaction, each methyl has a central line and two

symmetrical lines at distance $3/4\ \hbar\gamma_p/R^3\ (1-3\cos^2\Theta)$ (γ_p is the proton gyromagnetic ratio, R = 1.75A is the distance between protons and Θ is the angle between field and the normal to the methyl plane). When the field is parallel to the molecule's plane , the four methyls (3) are divided into two types characterized by two angles Θ_1 and Θ_2 with respect to fields with $\Theta_1-\Theta_2=70°$.

STUDY OF ANTIFERROMAGNETIC SATELLITES

In the quenched state of (TMTSF)2 ClO4 (by quenching from 70 K to 4.2K in 13 seconds), the S.D.W. gives additionnal satellites as shown in Fig 2 at a distance of 15 G. Fig 3 presents the satellites observed in (TMTSF)2 PF6, for some angles they are resolved in two satellites and a broad central line in the same range of intensity. On the contrary in quenched (TMTSF)2 ClO4 the intensity of satellites is much weaker than that of the central line which remains approximatively similar to the one in the metallic relaxed state at all angles excepted for a strong broadening of methyl structure . This difference can be explained by a model where in the quenched state there are antiferromagnetic domains (around 20 to 40 % of volume) and metallic domains. The change of lineshape as a function of the magnetic field's angle with b' axis in the plane perpendicular to a axis, can be explained by the change of the local field projections Hi on the applied field H. In PF6 we observe a local field of 26 G at angle -15° and one of 18 G at angle 10° from the axis b. In ClO4 we observe two much weaker satellites superposed to the methyl lines, of approximate amplitude 15 G at angle 35° with respect to the

molecular axis.

We have calculated the local fields created by a S.D.W with a nesting vector $[\pi/a, \pi/b, \pi/c]^*$ and a spin $\underline{S}$ oriented along the anisotopy axis b' (as observed by A.F. resonance (4)) using the spin densities calculated by Metzger (5) (the density on carbon atoms contributes around 25% to the local fields): we expect two large local fields of 127 and 94 G at angle 11° and -26° respectively from molecular axis, and two smaller fields. the amplitude of these local fields agree with experiments if the amplitude of S.D.W. is taken as 25% in PF6 and 13% in C104 of the one for $1/2/_b$ per molecule.

CONCLUSIONS

Our N.M.R. lineshape agrees fairly well with that calculated from Clough theory (2). The c.w. N.M.R can be useful for orientation of crystals because of the high sensitivity of lineshape to angle variations, in particular we have identified macled crystals.

The interpretation of the magnetic states of (TMTSF)2 C104 and (TMTSF)2 PF6 seems more complex than expected: uncertainties remain for the nesting vector's components of the quasi onedimensional Fermi surface of the S.D.W., the number of superposed equivalent components, and their relative phases. A more detailed comparison of N.M.R. lineshapes with the theoretical local fields corresponding to the different types of possible S.D.W. can determine the structure of the S.D.W.. The anomalous broadening of all the N.M.R.lines seems explained by the incommensurability of the nesting vector with the molecular lattice.

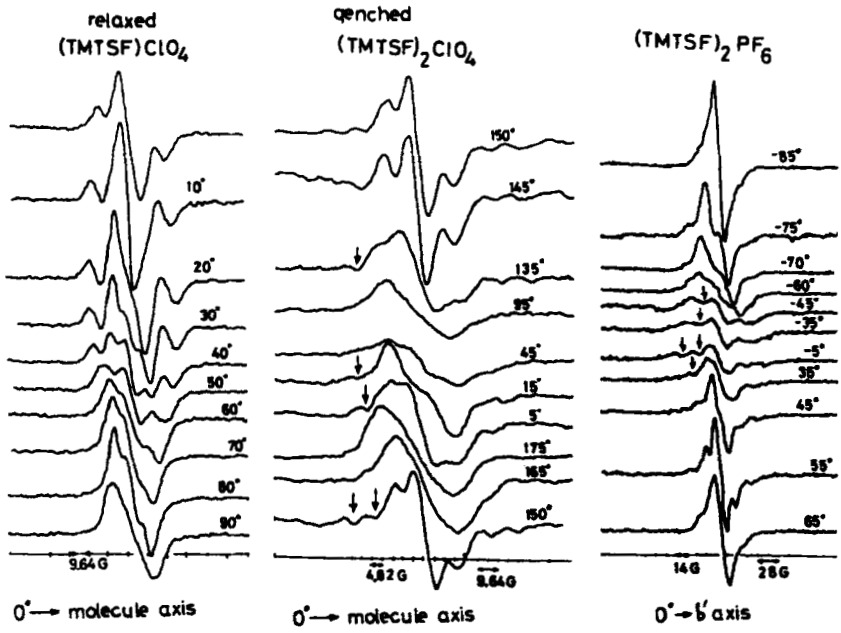

FIGURE 1 FIGURE 2 FIGURE 3
C.W. N.M.R. derivatives as function of magnetic field's angle (to a axis). For PF6, the field scale is three times smaller. The arrows indicate the A.F. satellites.

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