**NQR Study of Neutral-Ionic Transition on TTF-$QCl_4$**

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The quasi-one-dimensional mixed-stack charge transfer complex, tetrathiafulvalene-*p*-chloranil (TTF-$QCl_4$), is known to exhibit the temperature- and pressure-induced neutral-ionic phase transition. [1] In the ionic phase, tetrathiafulvalene (TTF) and *p*-chloranil ($QCl_4$) are dimerized and a ferroelectric behavior is observed. This transition is characterized by the degree of charge transfer $\rho$ between the electron donor molecule, TTF, and the electron acceptor molecule, $QCl_4$, and by their dimerization. Pressure-Temperature phase diagram, where the 1st order phase transition line divides the states with a critical end point around 0.7 GPa is suggested. [2]

We report the results of $^{35}Cl$ NQR studies on TTF-$QCl_4$ under pressures. Fig. 1 shows the temperature dependence of NQR frequency under various pressures. At ambient pressure (not shown here), the frequency of resonance line increases with decreasing temperature, and a line splitting, which indicates dimerization, occurs at the transition temperature. The averaged frequency of the split lines has a discontinuous drop at the transition temperature. This shows that a charge transfer suddenly occurs at the transition. Under 0.5 GPa, however, the resonance frequency starts to decrease with temperature before the line splitting occurs at $T_D$, where the dimerized phase appears. This indicates the continuous development of charge transfer above $T_D$. With increasing pressure, the line splitting at $T_D$ becomes moderate.

These results suggest that an ionic phase without dimerization, *i.e.* ionic paraelectric phase, is more developed at higher pressures.

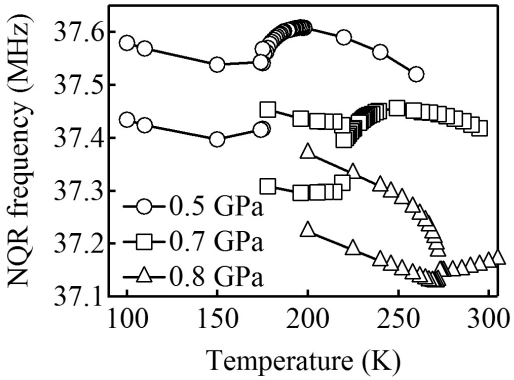


Fig. 1: Temperature dependence of the NQR frequency under various pressures.

[1] J. B. Torrance *et al.*, Phys. Rev. Lett. 46 (1981) 253.
[2] M. H. Lemée-Cailleau *et al.*, Phys. Rev. Lett. 79 (1997) 1690.