Neutral - Ionic Phase Transition in TTF-CA under Pressures

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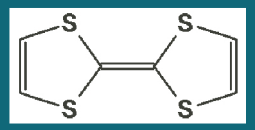
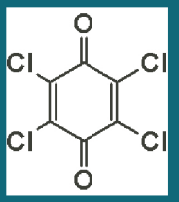
Contents

Introduction

TTF-CA : Quasi 1D System





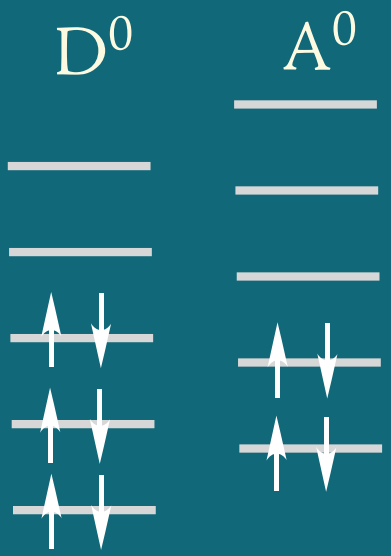
TTF (Donor Molecule) CA (Accepter Molecule)

Neutral (N) phase

$D^0A^0D^0A^0D^0A^0D^0A^0D^0A^0$

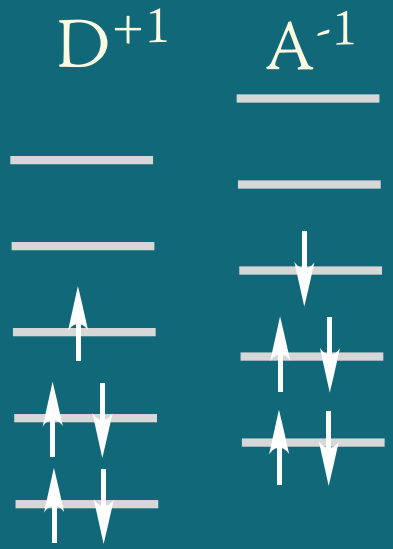
Ionic (I) phase

$D^{+1}A^{-1}D^{+1}A^{-1}D^{+1}A^{-1}D^{+1}A^{-1}D^{+1}A^{-1}$



Pressure,
lowering temperature

Costs electronic energy
Gets Mardelung energy



Band Insulator

Valence 0

Mott Insulator

Valence 1

Introduction

P-T Phase Diagram of TTF-CA

Ionic Phase

$D^+A^- D^+A^- D^+A^- D^+A^-$

Mott Insulator

non-mag

(Spin Peielrs,

lattice dimerization)

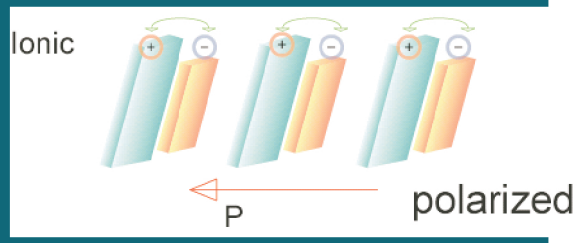
Pressure,
lowering temperature

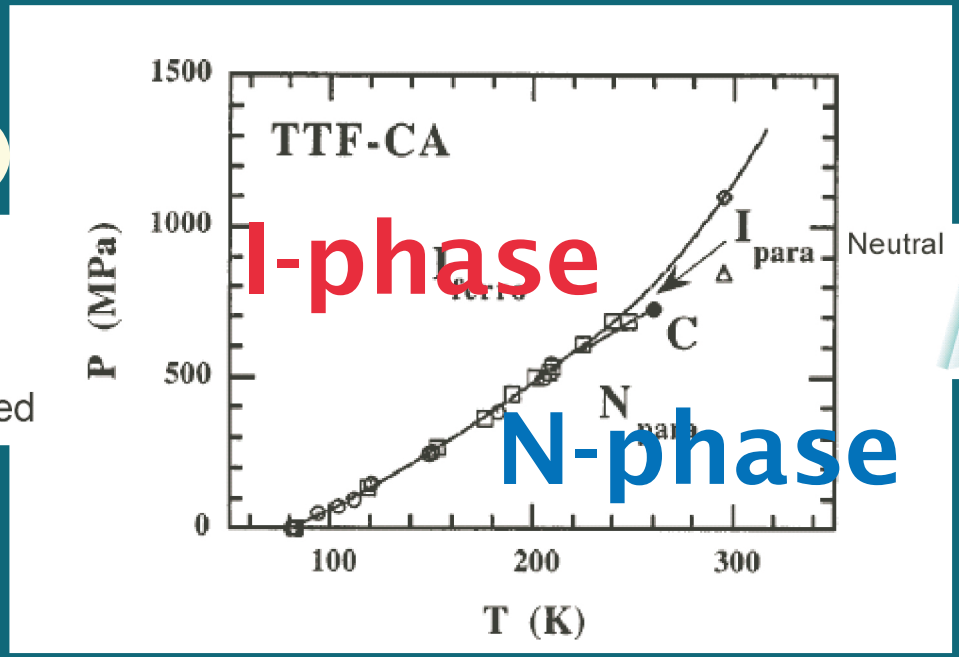
Neutral Phase

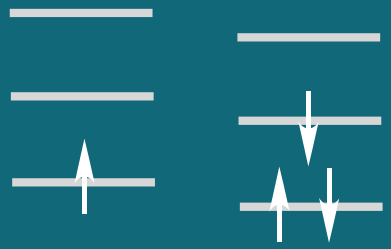
$D^0A^0D^0A^0D^0A^0D^0A^0$

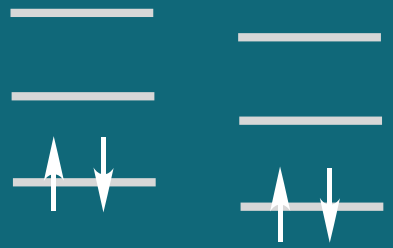
Band Insulator

non-mag



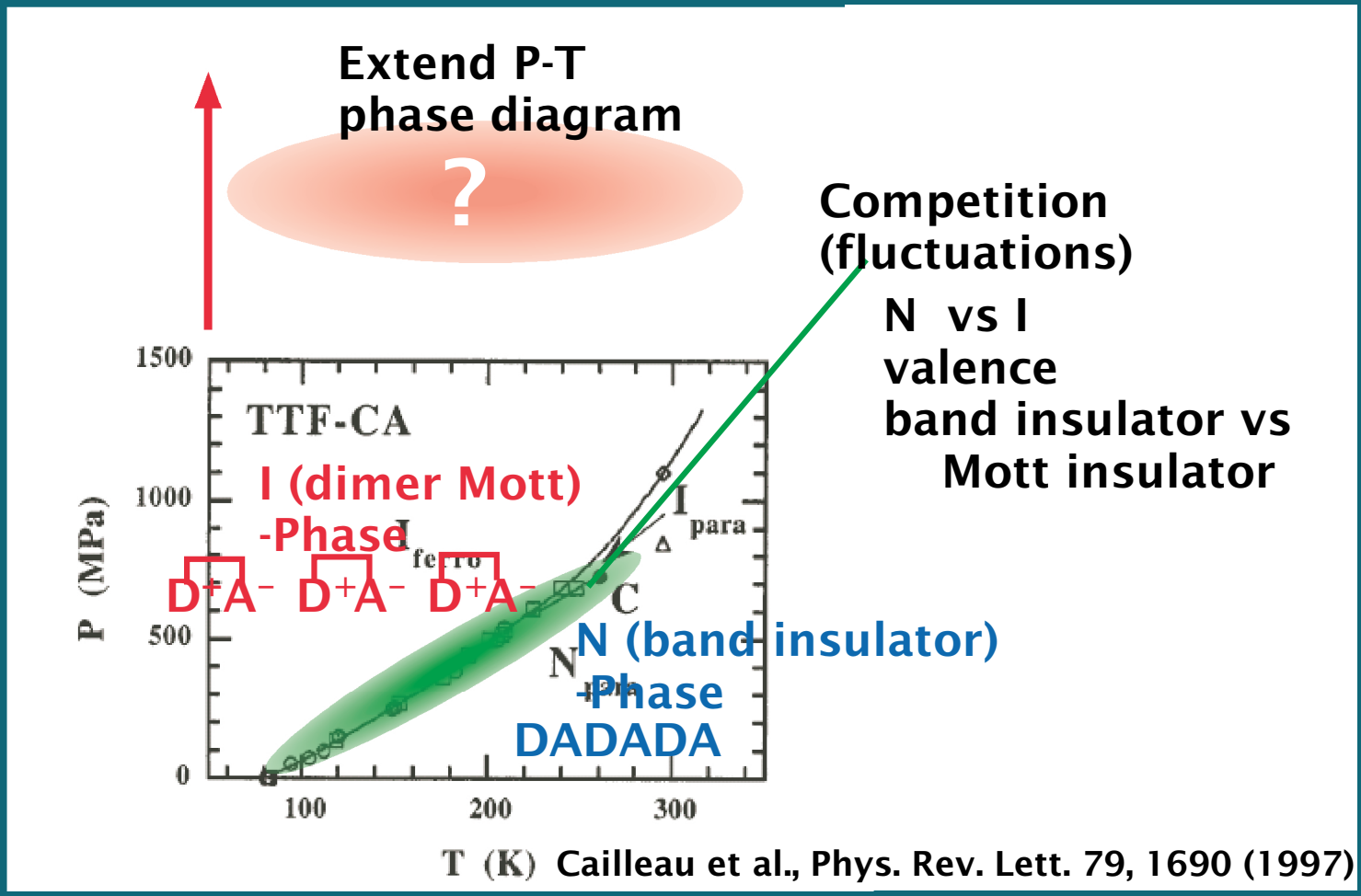






Cailleau et al., Phys. Rev. Lett. 79, 1690 (1997)

Motivation



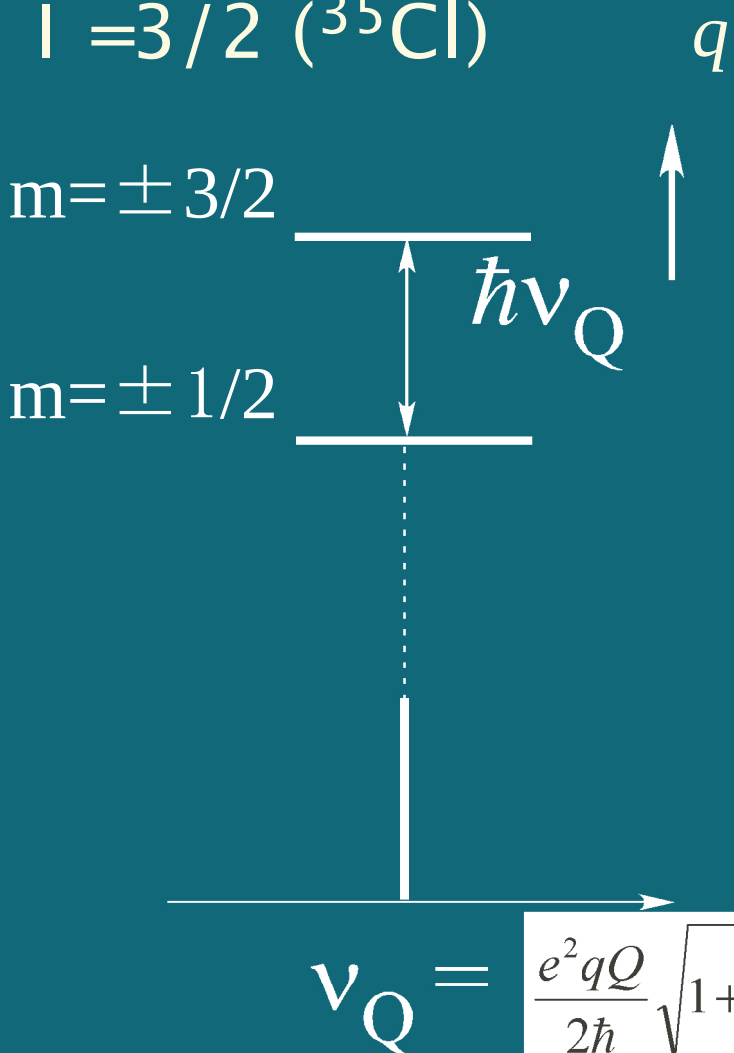
Cailleau et al., Phys. Rev. Lett. 79, 1690 (1997)

Experimental

^{35}Cl NQR and ^{1}H NMR

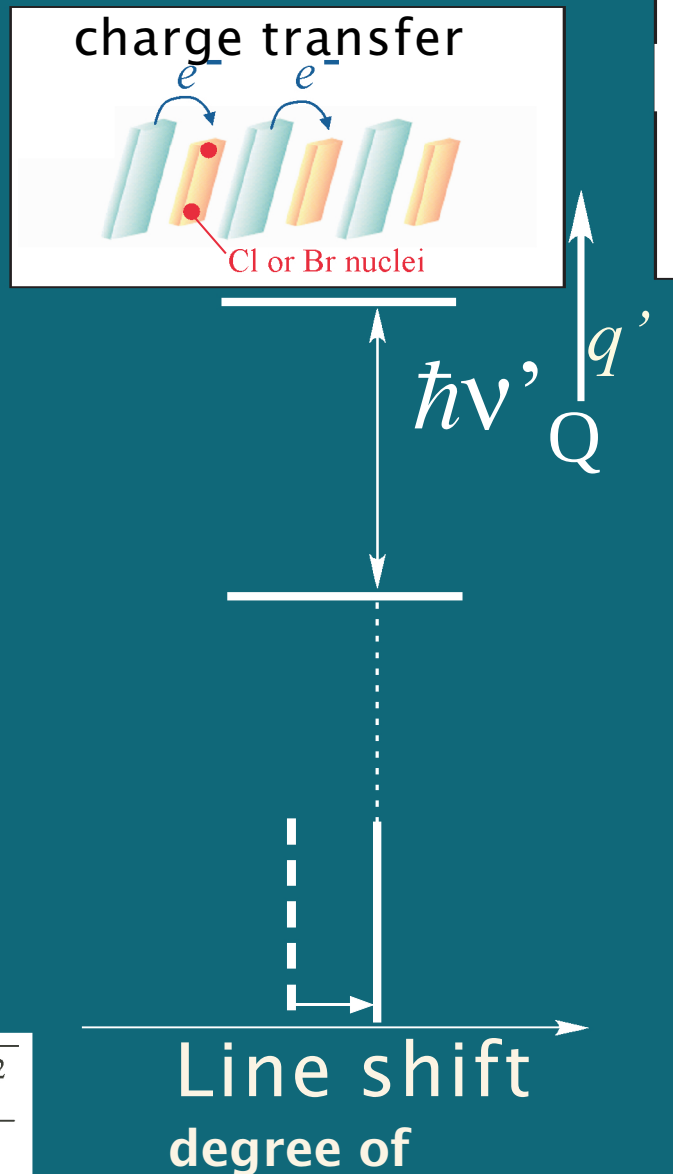
NQR I > 1, Quadrupole Moment couples to EFG.

I =3/2 (^{35}Cl)



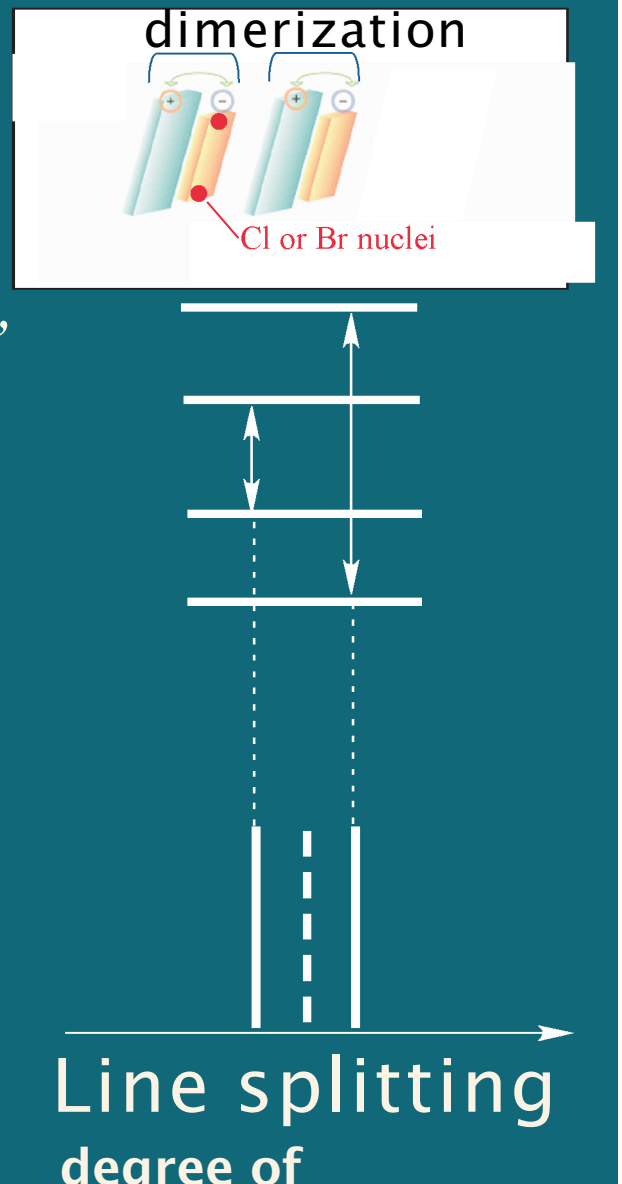
$$\nu_Q = \frac{e^2 qQ}{2\hbar}\sqrt{1+\frac{\eta^2}{3}}$$

q (Electric Field Gradient)



Line shift

degree of charge transfer,ρ



Line splitting

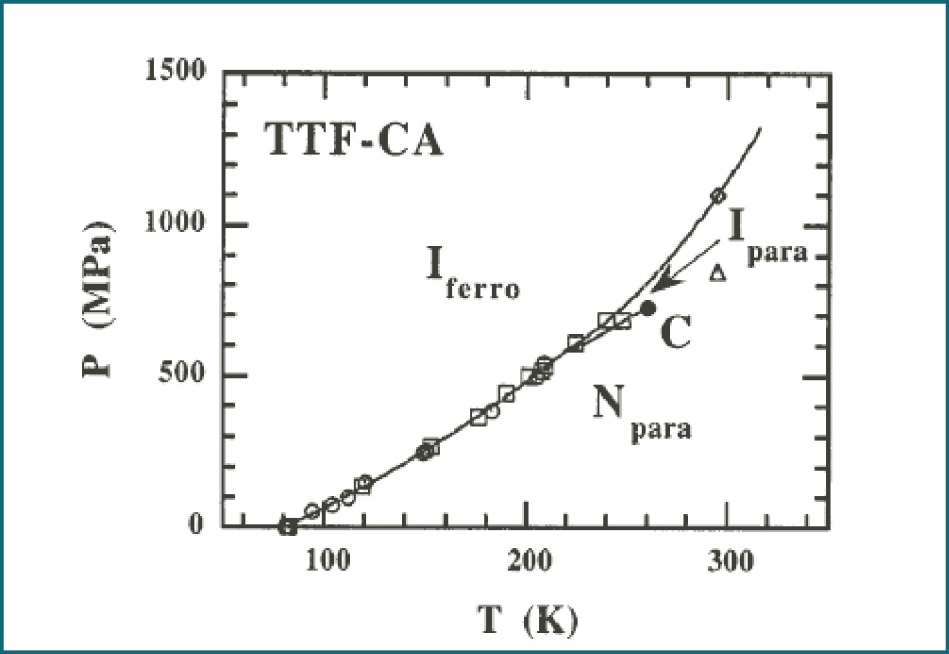
degree of lattice dimerization

Experimental

Cl NQR → charge

Cl NQR → lattice

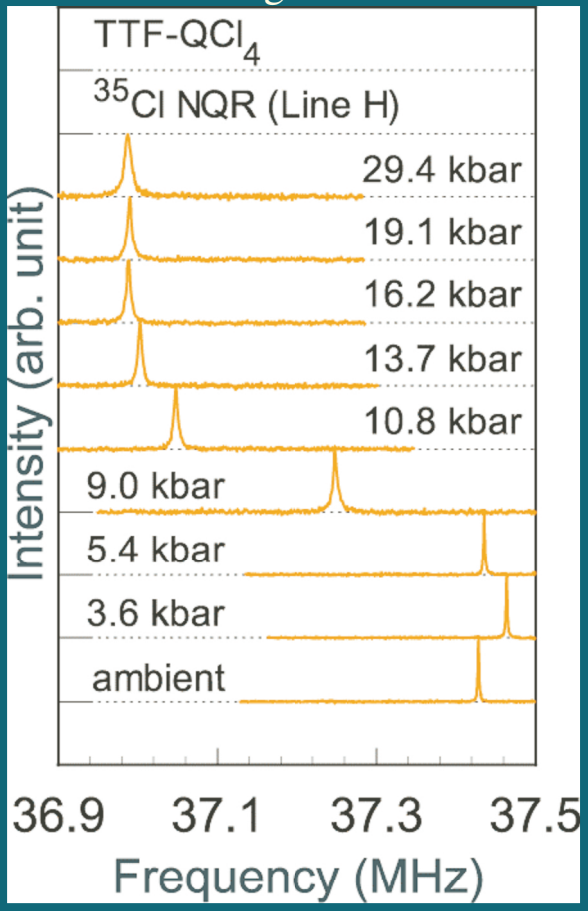
H NMR → spin

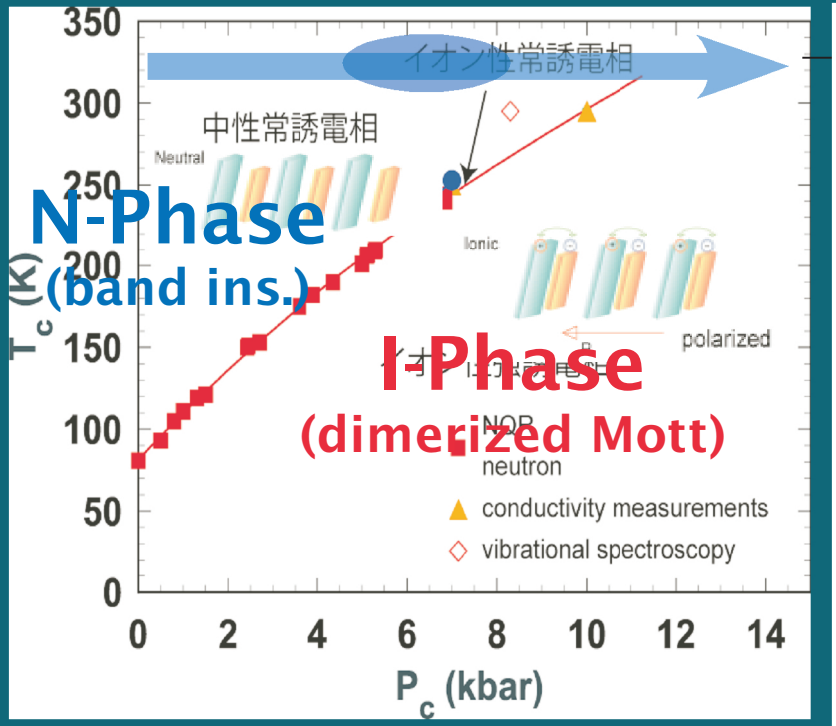


Results & Discussion

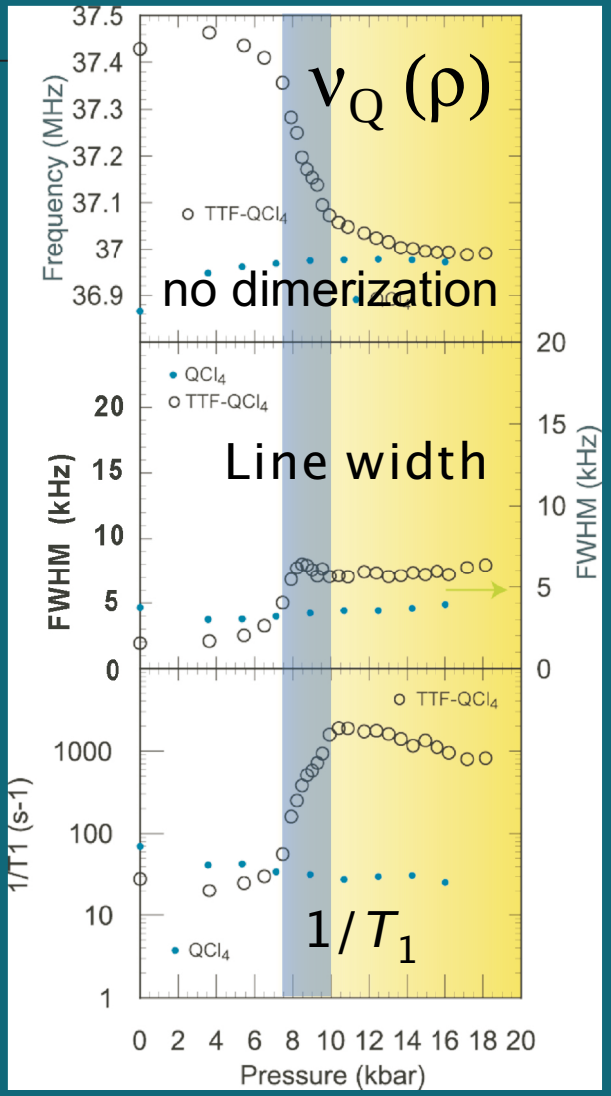
Pressure dependence of Cl NQR spectra at room temperature

Line Shift (without splitting)
Charge transfer





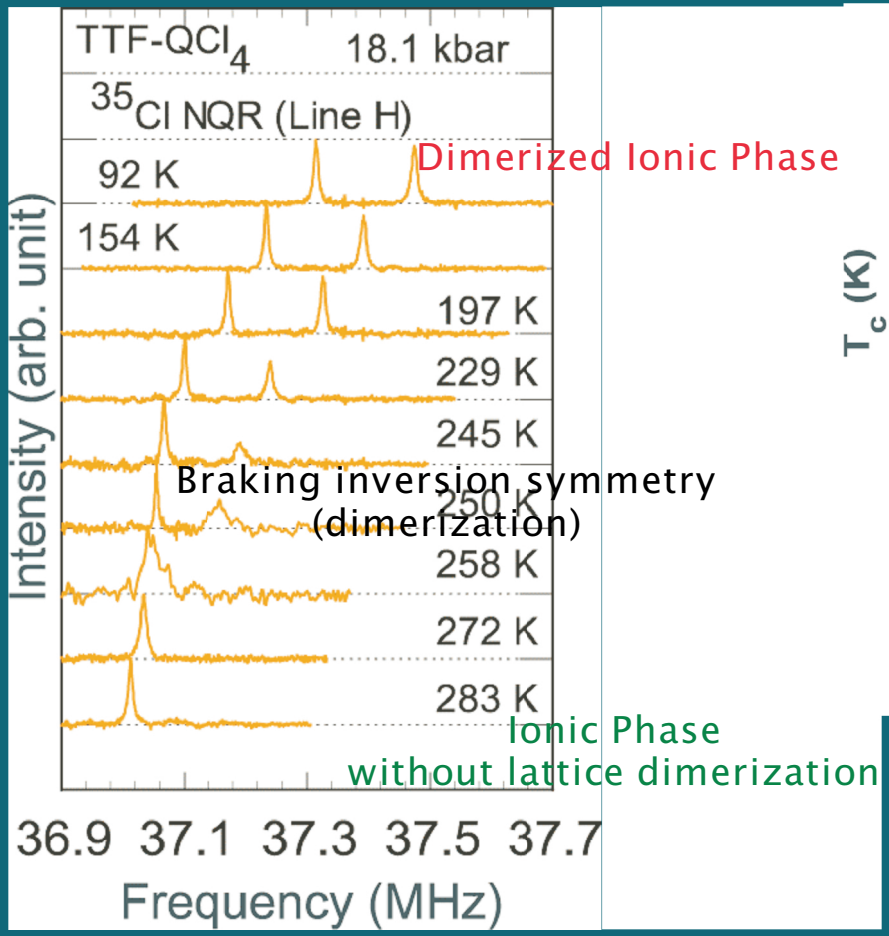
Cl NQR
N
I
(no dimerization)

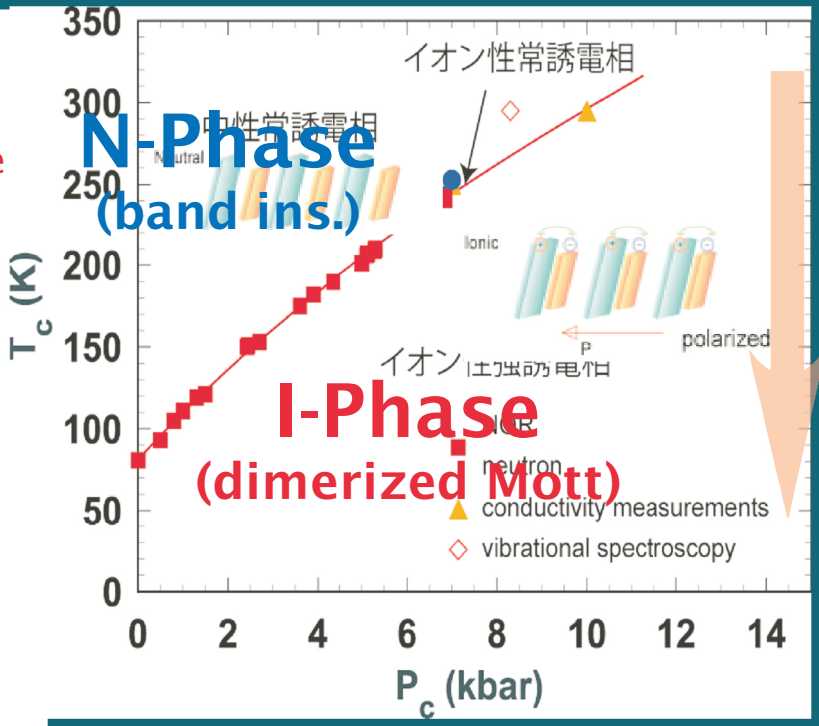


Results & Discussion

Temperature dependence under high pressure

Cl NQR



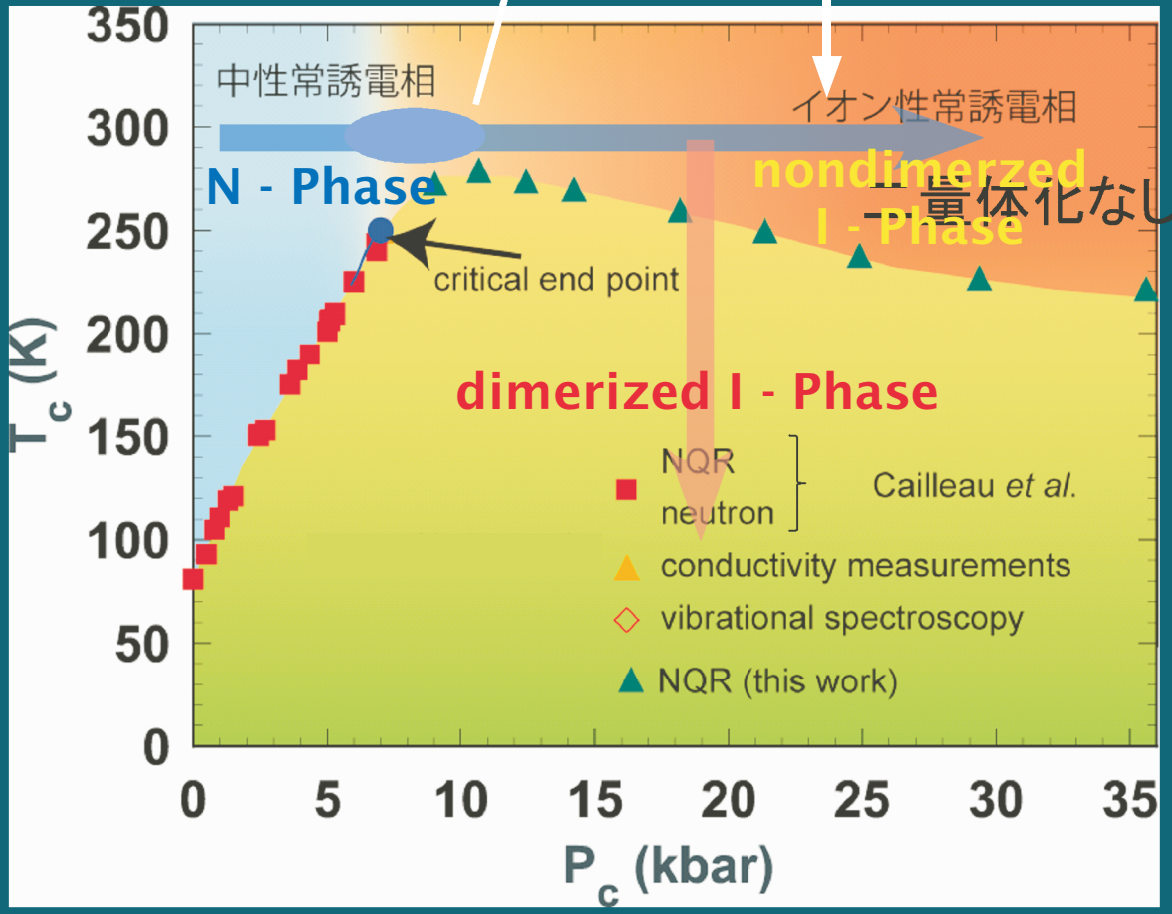


Results & Discussion

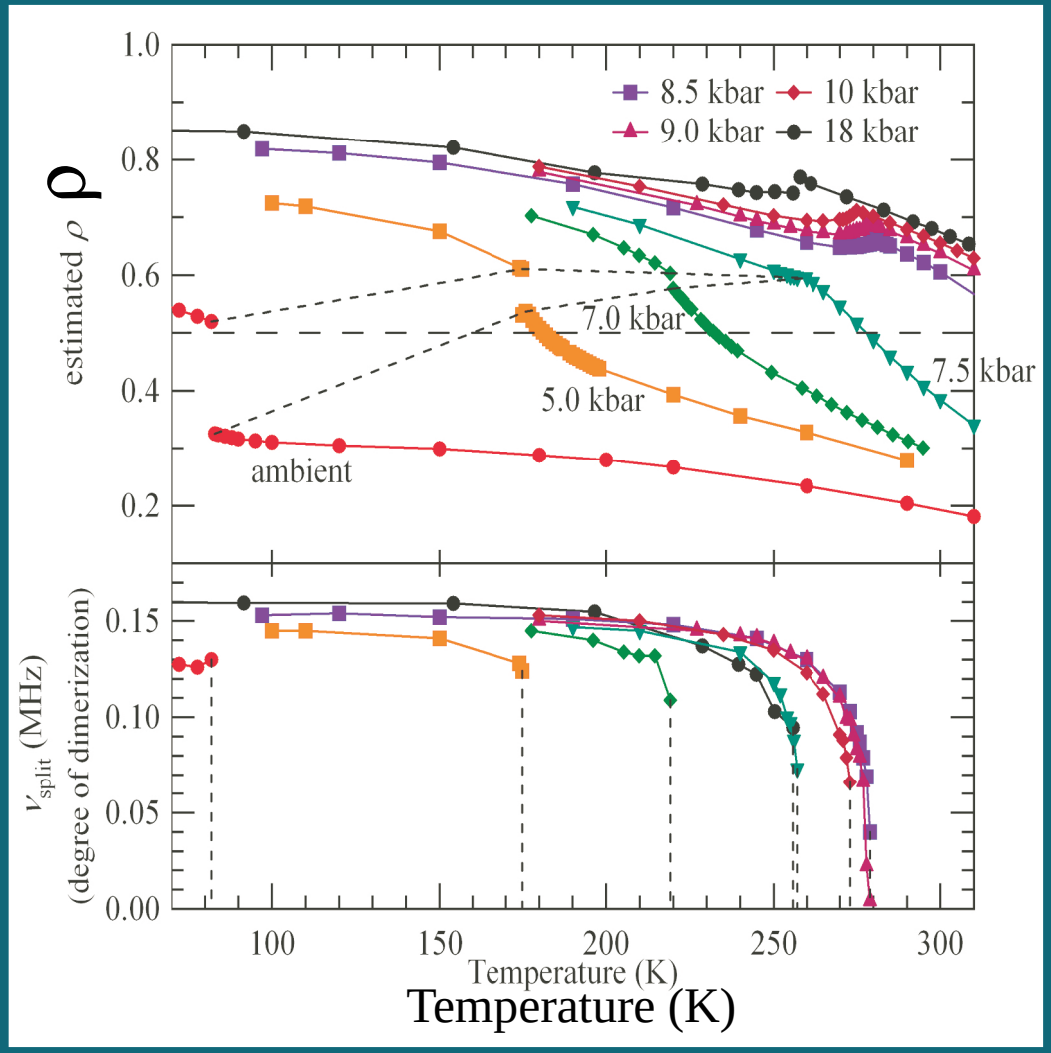
Extend P–T phase diagram up to 35 kbar

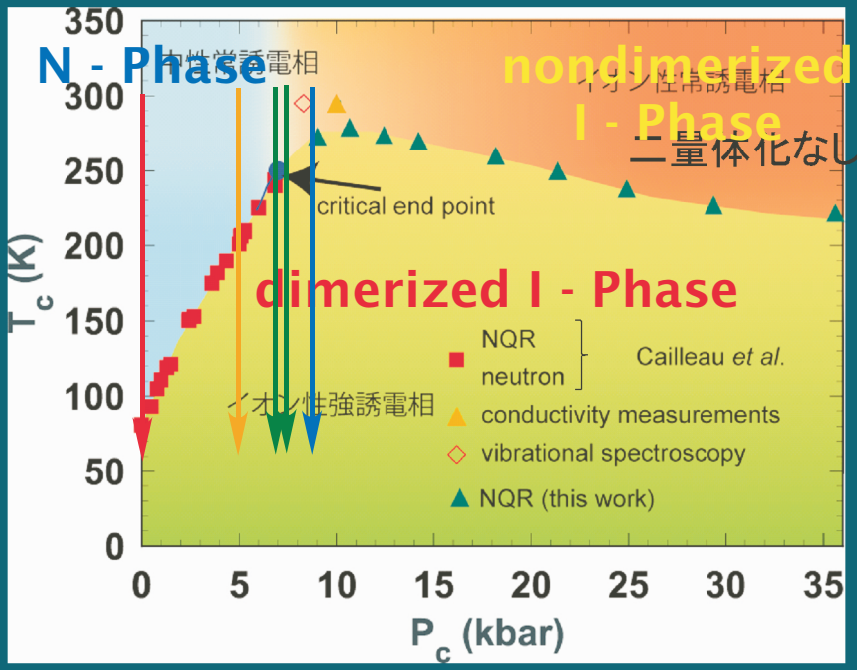
Non dimerized ionic phase

Crossover between N (band ins.) and I (Mott Ins,)

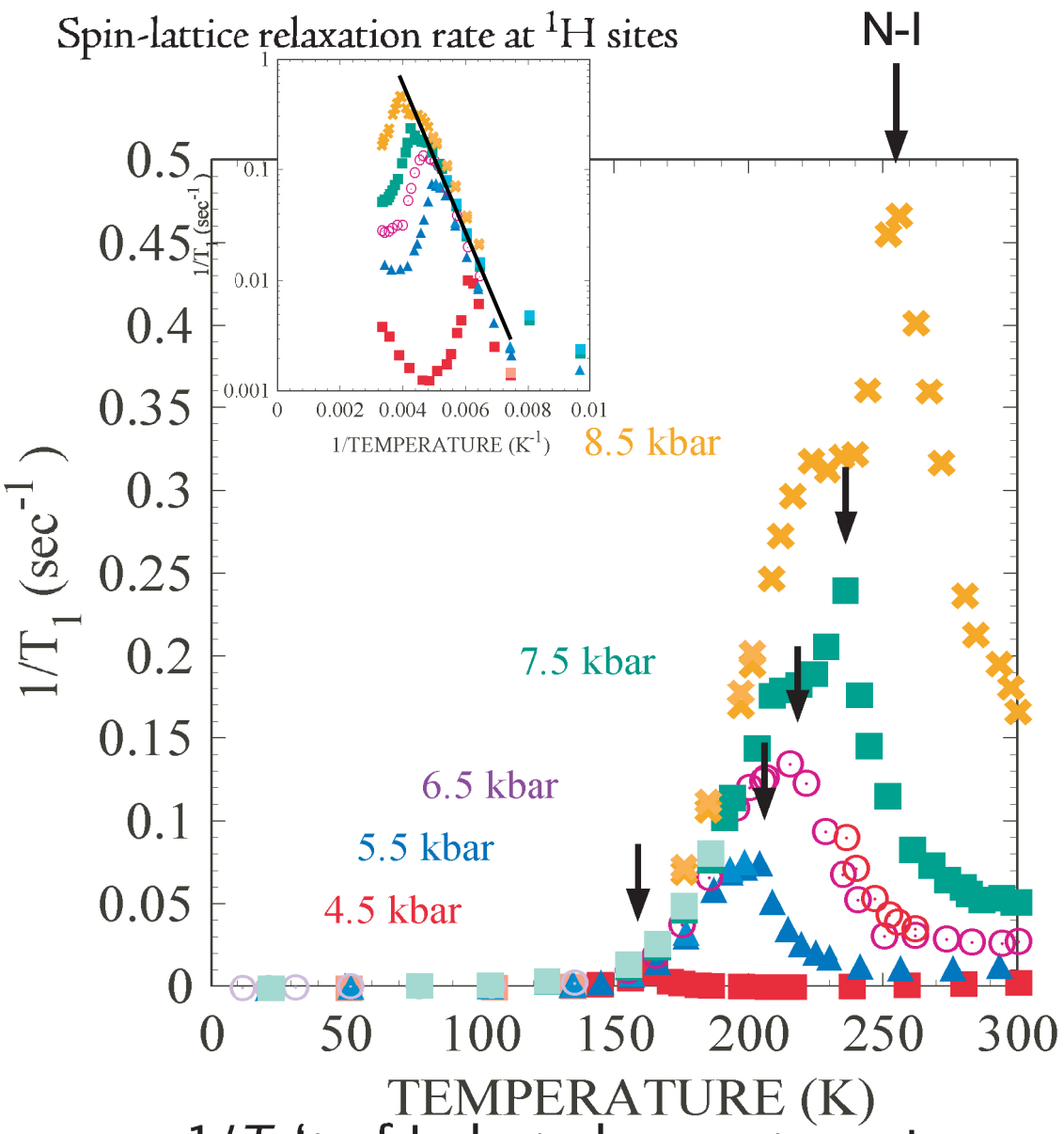


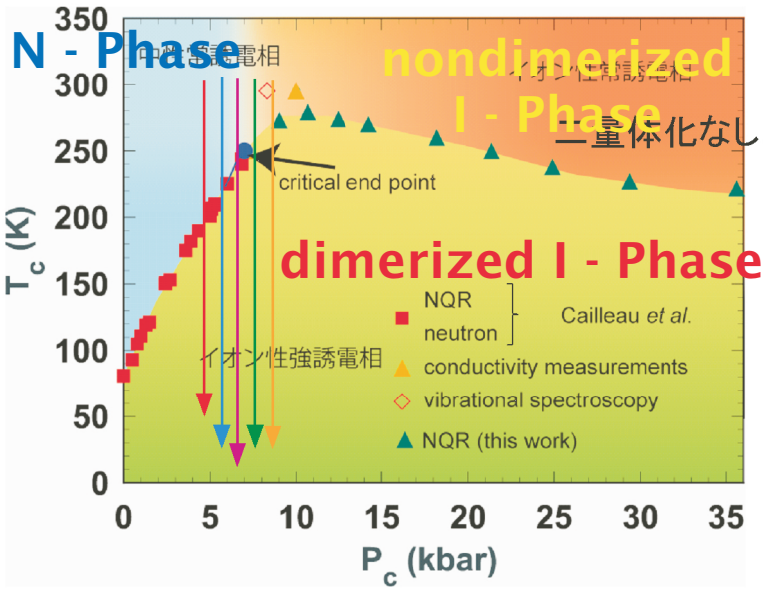
Results & Discussion





Results & Discussion





Large enhancement of $1/T_1$:
appearance of spin even in N-phase

Low pressure region :
N-I transition is accompanied with lattice dimerization.

Higher pressure region :
N-I transition temperature is higher than dimerization temperature.

$1/T_1$'s of I-phase have a same temperature dependence with $\Delta \sim 0.13$ eV.

Excitation of Spin soliton

DA DA DA D AD AD AD

Summary

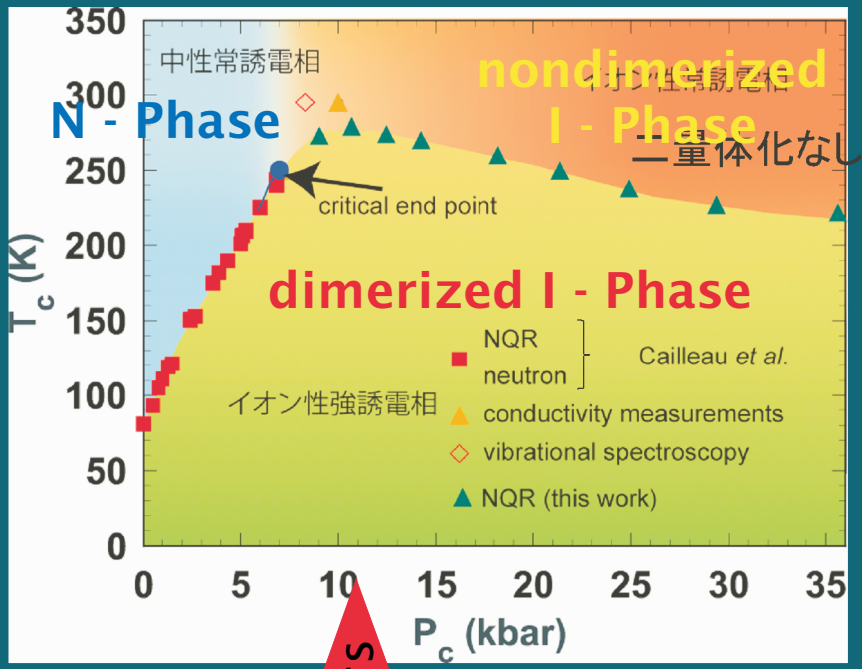
Resistivity, Cl NQR and 1H NMR studies have been performed in N-I phase transition of TTF-CA.

We extend the pressure region in P-T phase diagram.

We found
Non dimerized ferroelectric phase
large charge and spin fluctuations
at around the N-I crossover region

The spin appears even in N-phase.

The ferroelectric N-I transition is separated into N-I crossover (charge transfer) and ferroelectric transition (dimerization).



5 years