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# Molecular Crystals and Liquid Crystals

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# Infrared Modes of Charged Solitons

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#### INFRARED MODES OF CHARGED SOLITONS

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ABSTRACT Doping level and temperature dependence (4,2K-300K) of infrared absorption spectra of I<sub>2</sub> and MoCl<sub>5</sub> doped polyacetylene and deuterated polyacetylene are reported within spectral range 400-2000cm<sup>-1</sup> They exhibit two absorption ranges. The 1370 cm<sup>-1</sup> CH<sub>x</sub> mode (1160 cm<sup>-1</sup> for CD<sub>x</sub>) is a charged soliton mode. The low frequency part (400-1000 cm<sup>-1</sup> for CH<sub>x</sub>, 400-900 for CD<sub>x</sub>) can be analysed into resonant mode and doping species optical modes superimposed to a pinning mode.

## EXPERIMENTAL

Cis thin films (tickness about 1  $\mu$ m) synthesized by the usual Shirakawa's method were grown on KBr pellets, then thermally isomerized at 150°C during 20 minutes. MoCl<sub>5</sub> doping was performed in toluene and carbone disulphide solutions, iodine doping in gazeous phase.

### RESULTS

MoCl<sub>5</sub> doping results are mainly reported below. Most of iodine doping results will be published elswhere.

Two striking features appear in the absorption spectra. Strong narrow absorption at  $1370 \text{cm}^{-1}$  (1160 for CD<sub>x</sub>) and a broader absorption near  $870 \text{cm}^{-1}$  with a complex structure superimposed.

#### DOPING LEVEL AND TEMPERATURE DEPENDENCE

Main results are shown rather than a detailed discussion.

.The intensity of the  $1370 \mathrm{cm}^{-1}$  mode associated with the number of charged centers increases with doping

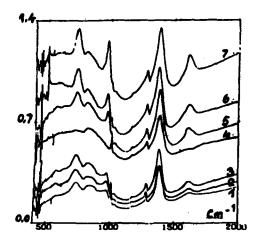


Figure 1 Absorption spectra of MoCl<sub>5</sub>doped CH<sub>x</sub>.1,2,3,5,6,7 in toluene solution.

4 in carbon disulphide solution (point that the bands at 730, 970, 1600 due to toluene solvated ion are mussing.

The intensity of this mode increases with decreasing temperature Fig 2.

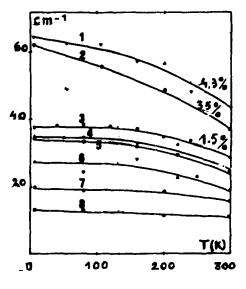


FIGURE 2 Strengh variation of the 1370cm $^{-1}$ mode with temperature for different doping level. 1,2,3 I doped CH  $_{\rm X}$  4,5,6,7,8 Mo Cl  $_{\rm 5}$  doped CH  $_{\rm X}$ 

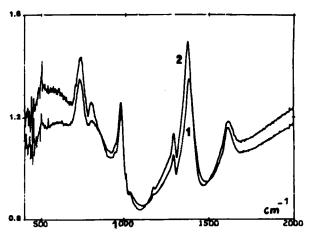


FIGURE 3 Absorption spectra of MqCl  $_5$  doped CH in toluène solution : 1 (300K). 2 (4,2K)

- . The broad band (bandwidth  $\sim 200 \text{cm}^{-1}$ ) strongly dependent of dopant concentration (Fig 1) and temperature (Fig 3.4) is the pinning mode of charged solitons.
- . Frequencies are shifted towards low energies.

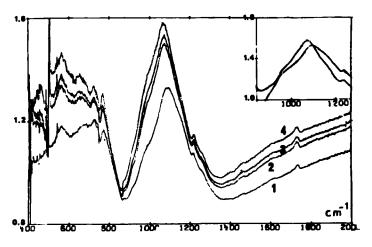


FIGURE 4 Evolution of 1370cm<sup>-1</sup>, and low frequency modes of MoCl<sub>5</sub> doped CD in carbone disulphide solution 1 (300K); 2 (220K), 3 (160K) 4 (4.2K)

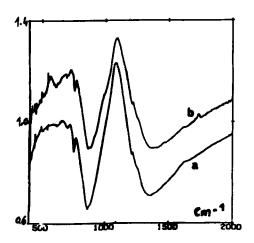


FIGURE 5 Absorption spectra of doped CD a:with Iodine b:with  $\operatorname{MoCl}_5$  in toluene solution

The superimposed structure can be analysed into:localised or resonant modes of the chain (730-820cm<sup>-1</sup>)

. Internal modes
of dopant species
(906-570cm<sup>-1</sup>) or
solvated ion
(977cm<sup>-1</sup>) Fig 5.
Similar results were obtained with iodine doping(Fig 6)

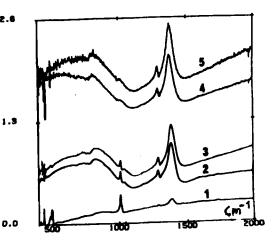


FIGURE 6 Absorption spectra of Iodine doped  $CH_{\chi}(2,3,4,5)$  1 undoped trans sample.