Multiscale phenomena in molecular matter



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## Positron annihilation in smectic E phase of 4 - alkyl -4 -isothiocyanatobiphenyl (6TCB)

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Positron annihilation lifetime spectroscopy (PALS) has been employed for characterization of the local structure in molecular substances such as polymers or liquid crystals. When a positron enters an insulator solid it can form a bound state with an electron called positronium (Ps). Ps is located in low electron density regions like local free volume holes. Ps can be formed in two spin states: para-Ps (p-Ps) and ortho-Ps (o-Ps) due to possible positron and electron spin alignment, i.e., antiparallel and parallel, respectively. In vacuum, the selfannihilation lifetime of o-Ps is 142 ns and it decays into three quanta while the p-Ps lifetime is much shorter, i.e., 125 ps with decay into two quanta. The relative abundance of these two spin states is 1:3. In molecular solids, due its to relatively long lifetime, o-Ps interacts with the electrons of surrounding molecules. Its lifetime is determined mainly by the annihilations of the positron with one of these external electrons. This process is called *pick-off* annihilation. It causes shortening of the o-Ps lifetime to several nanoseconds. The lifetime of o-Ps annihilating in the pick-off process is connected to the free volume hole radius and it is a basis of broadly understood positron porosimetry.

In case of liquid crystals not only local microstructure but also molecular dynamics can influence the Ps lifetime as it was demonstrated in our studies of supercooled smectic E (SmE) phase of 4TCB [1,2]. The obtained value of *o*-Ps for 4TCB can be explained by formation of Ps bubbles due to a liquid-like state of the butyl chains molecules in the SmE phase and the lamellar structure with nano-segregation of alkyl chains and other parts of molecules proposed by Saito et al. [3].

The present studies were performed for the other member of the nTCB homologous series, i.e. 6TCB. The obtained temperature dependencies of the *o*-Ps lifetime and its intensity for the supercooled SmE phase indicate two processes taking place during heating of the sample. Softening of the glass phase and cold crystallization occurring simultaneously cannot be resolved in positron lifetime measurements as it was in the case of 4TCB thanks to difficult and lengthy crystallization of the latter. The proposed explanation of the obtained dependencies may shed light on the results of previous positron lifetime studies of supercooled liquid crystals reported in the literature.

## References

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