HEAT CAPACITY FOR SOME CHOLESTEROL DERIVATIVES

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abstract: The heat capacity was established from DSC data by O'Neill method on characteristic temperature ranges of each compound regarding their behaviour under dynamic step of temperature. Dependences C_P=C_P (T) for cholesteryl- p-thiophenoxy- phenyl-carbamate, cholesteryl- p-(p'-chlor)-thiophenoxy- phenyl-carbamate and cholesteryl- p-(p'-brom)-thiophenoxy- phenyl-carbamate was correlated with phase transitions. Radical influences at C-3 upon thermodynamic measurements calculated were established.

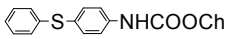
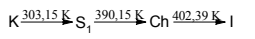
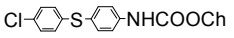
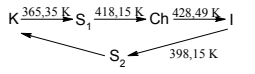
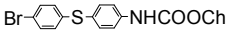
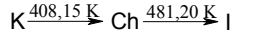
Introduction

Study of liquid crystals raises an important focus today in science and research with applicability in various fields like biology, medicine and engineering.

Liquid crystals represent an intermediary order degree between regular crystals and isotropic crystals. As the liquid crystals have the same positional order degree like the solids, their show a large variety of fault and discontinuity in their macroscopic structure. Faults in liquid crystals could be produced with translation or rotation destruction symmetry. These modifications have effect on thermal behaviour of the compounds with liquid crystals properties.

Sterols themselves have not liquid crystals properties but sterolic derivates substituted with different groups at C-3 lied to derivates, which have such kind of properties.

Table 1. The structure and polymorphism of the studied cholesteryl derivates

No	Compound	Structure	Polymorphism
1	Cholesteryl- p-thiophenoxy-phenyl-carbamate		
2	Cholesteryl- p-(p'-chlor)-thiophenoxy- phenyl-carbamate		
3	Cholesteryl- p-(p'-brom)-thiophenoxy- phenyl-carbamate		

This paper continues a thermodynamic study of same cholesteryl carbonates by heat capacity study of these compounds [1÷4].

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The structure and mesophases of the compounds aim in our study are shown in Table 1.

The heat capacity was established from DSC data by O'Neill method [5] on characteristic temperature ranges of each compound regarding their behaviour under dynamic step of temperature.

Results and Discussions

Dependences $C_P=C_P(T)$ for analysed compounds are shown in Fig. 1.

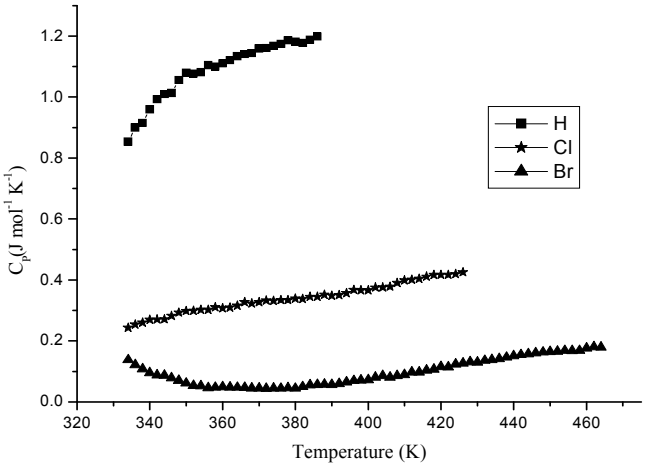

Fig. 1 *Dependences $C_P=C_P(T)$*

Equations, which describe these dependences, are shown in Table 2.

Table 2. Equation for dependences $C_P=C_P(T)$

Compound	Temperature range (K)	$C_P=C_P(T)$ (J mol^{-1} K^{-1})	r^2
1	334÷350	–3.63233+0.01347·T	0.988
	352÷386	–0.37812+0.00414·T	0.992
2	334÷426	–0.33289+0.00177·T	0.991
3	380÷464	–0.60671+0.00171·T	0.995

By monitoring the curves shown in Fig. 1 and mathematic equation of dependences $C_P=C_P(T)$ could establish some important conclusion.

CHOLESTERYL- P-THIOPHENOXY- PHENYL-CARBAMATE

On (334÷350) K temperature range it was established a linear type which correspond to stability domain for smectic mesophase which is characterized by a orientational order of the molecular long axes an d a disposing of the molecular centres in equidistant planes [6].

On (352÷386) K temperature ranges the relation $C_P=C_P(T)$ is linear too but with a different slope and corresponds to transition Smectic ⟶ Cholesteric ⟶ Isotrop liquid. On transition Smectic ⟶ Cholesteric the molecules pass from a parallel orientation after a

preferred direction named diretrix to a structure that have orientational order of the molecular long axes but with a type of disorder of centres of gravity as in a fluid liquid [7].

CHOLESTERYL- P-(P'-CHLOR)-THIOPHENOXY- PHENYL-CARBAMATE

For this compound molar heat capacity rises linear with temperature on (346÷426) K range. In this domain of temperature occur transitions Crystal $\longrightarrow$ Smectic $\longrightarrow$ Cholesteric $\longrightarrow$ Isotrop liquid that have structure characteristic presented at ansubstituted compound.

CHOLESTERYL- P-(P'-BROM)-THIOPHENOXY- PHENYL-CARBAMATE

At this compound, which have a similar structure with substituted chlor compound, heat molar capacity rises linear with temperature on (370÷470) K, corresponding transitions Crystal $\longrightarrow$ Smectic $\longrightarrow$ Cholesteric $\longrightarrow$ Isotrop liquid.

Conclusions

At substituted compounds with chlor and brom, the straight lines of dependences $C_P=C_P(T)$ are, in good approximation, parallels. The chlor and brom have compatible atomic volume. These substitutes are bound to a carbon atom of aromatic ring and exercise towards molecule an electromer effect repulsive electron. In the same time, these atoms exercise an inductive electromer attractive electron. The prevalence of the inductive electromer for studied compounds confirms the Gray rule for terminal groups effect on *p*-substituted phenyl ring [8].

Also, at the same given temperature (identically for three compounds), for example 380 K, molar heat capacity value decrease from ansubstituted compound to p'-chlor substituted respectively p'-brom substituted.

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