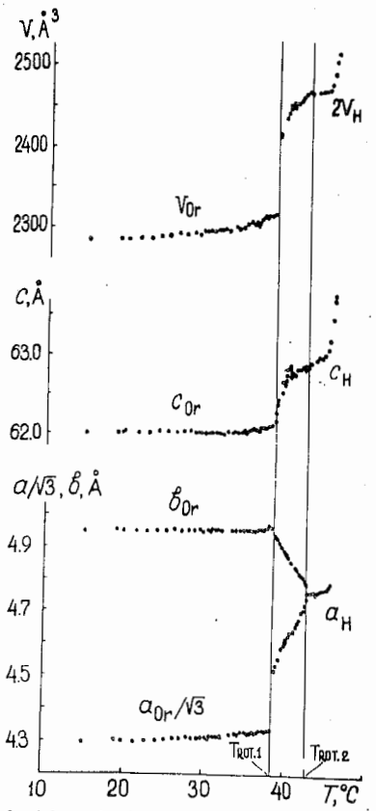



Fig.1

diagram of polymorphism of the paraffin $C_{23}H_{48}$.

$T_{rot.1}$ – temperature of new phase transformation

$T_{rot.1} - T_{rot.2}$ life period of the new polymorphic modification $Or_{rot.1}$

Crystalline $Or_{cryst.}$ and rotational-crystalline $Or_{rot.1}$. rhombic modifications differ in character of thermal motion of molecules.

H – hexagonal rotational-crystalline modification

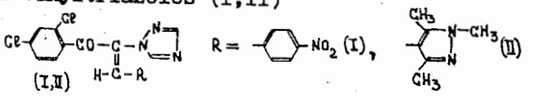
Molecules (aliphatic chains) are packed in the paraffin structure by the principle "a bulge into a hollow", they are located in each other's potential field and perform torsional vibrations around their axes relatively to the fixed equilibrium positions. At heating to $T_{rot.1}$ energy is achieved, at which molecules can escape the potential barrier and take a different orientation. After that molecules continue torsional vibrations, but relatively to positions changing in time and assemblage. The first-order phase transition discovered in paraffins may appear characteristic for other compounds performing transition to rotational-crystal state. The described transformations make paraffins close to liquid crystals.

## 06.05 – Conformation Analysis

**PS-06.05.01** **THE X-RAY ANALYSIS OF TWO NEW N-VINYLTRIAZOLES.** *By Malinovsky S.T., Krimer M.Z., Stynghach E.P., Rechter M.A., Zavodnik V.E.*
*Institute of Chemistry, Academy of Sciences of Moldova. Kishinev, 277028, Moldova.*

Among N-vinyltriazols derivatives some compounds with strong fungicide activity are known. In oder to understand the dependence between the activity of these molecules and their structure we have carried out X-ray investigations.

In this paper we give the results of X-ray analysis of two representatives of N-vinyltriazoles (I,II)




Crystal(I) is monoclinic: a=9,974(1), b=20,341(2), c=8,567(1)Å, $\gamma$=91,10(1)°, sp. gr. $P2_1/b$, R=0,028(835 ref.). Crystal(II) is triclinic: a=7,634(1), b=10,578(1), c=11,702(2)Å, $\alpha$=85,91(1), $\beta$=82,50(1), $\gamma$=72,13(1)°, sp.gr. P1, R=0,029(1648 ref.). It was determined that the substitution of the 4-nitrobenzene cycle in (I) for the bulky pyrazol cycle in (II), alters the molecular structure as a whole by rotation of the fragment containing the carbonyl group and the chlorobenzene ring by 164°. As a result a Cl-N intermolecular contact occurs in (II) equal to 3.46Å, stabilizing the triazol cycle position. At the same time the Z-configuration is well preserved in (I) and (II).

**PS-06.05.02** CRYSTAL AND MOLECULAR STRUCTURES OF P-CHLOROPHENYL-THIOUREA (I) AND 2, 4, 6-TRIBROMO-PHENYL-THIOUREA (II). By Mao Zhihua*, Zhou Zhonghua, Den Wengli and Hong Zhou, Department of Chemistry and Center of Analysis and Measurement, Sichuan University, Chengdu, Sichuan, China; Shan Shuxiang, Department of Biological Engineering, Sichuan University, Chengdu, Sichuan, China.

Thiourea and its derivatives have important significance in medicine and biology, from 1950s to now, scientists have been studying their anti tuberculosis activity and toxicity in rats and insects, and found that their biological activities depend upon N-substituted groups in thiourea. The biological activity of some of them are notable and have a widely useful future. Therefore we determined the crystal structures of the title compounds and studied their molecular structures. A colorless bright crystal for (I) and a pale yellow one for (II) both with suitable sizes were used for the measurements. Diffraction data were collected in $\omega/2\theta$ mode on a ENRAF NONIUS CAD4 diffractometer using MoK$\alpha$ radiation. A total of 1666 unique reflections for (I) and 2448 for (II) were collected in a range of $2° \leqslant \theta \leqslant 25°$. All calculations were performed on a PDP11/44 computer with SDP program package. The reflections for $I \geqslant \sigma(I)$ (1330 and 1207 respectively) were used in the measurements and refinements. Both the structures were solved by direct methods. The crystallographic data are as follows: crystal (I) is monoclinic, space group $P2_1/a$, a=1.0671(1), b=0.8912(1), c=0.9128(1)nm, $\beta$=106.85(1)°, V=0.8307nm³, Z=4, Dc=1.492g.cm⁻³, Mr=186.66, $\mu$=6.325cm⁻¹, the final R=0.029, Rw=0.031; Crystal (II) is orthorhombic, space group Pcab, a=0.9997(2), b=0.7876(4), c=2.7920(3)nm, V=2.1984nm³, Z=8, Dc=2.35g.cm⁻³, Mr=388.92, $\mu$=84.325cm⁻¹, the final R=0.047, Rw=0.047. The max. $\Delta\rho$ are 0.258e/Å³ and 0.530e/Å³ respectively.

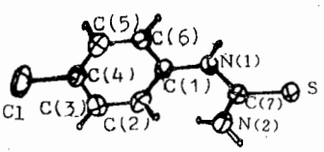



Fig. 1. The perspective view of (I)