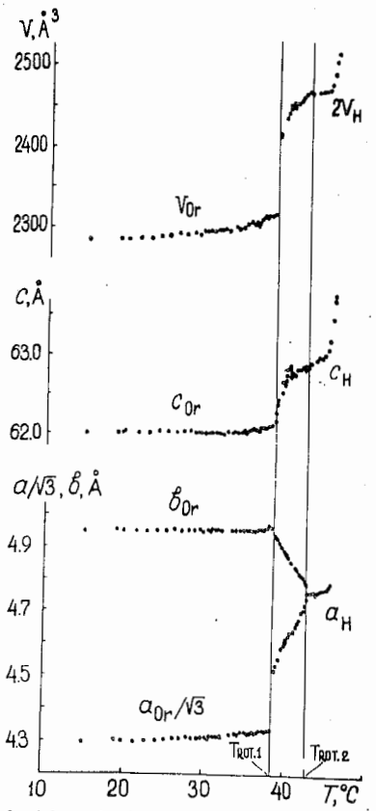


Fig.1

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

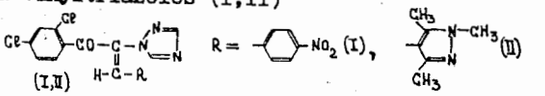
Molecules (aliphatic chains) are packed in the paraffin structure by the principle "a bulge into a hollow", they are located in each other's potential field and perform torsional vibrations around their axes relatively to the fixed equilibrium positions. At heating to $T_{rot.1}$ energy is achieved, 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, γ=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, α=85,91(1), β=82,50(1), γ=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 MoKα 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, β=106.85(1)°, V=0.8307nm³, Z=4, Dc=1.492g.cm⁻³, Mr=186.66, μ=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, μ=84.325cm⁻¹, the final R=0.047, Rw=0.047. The max. $\Delta\rho$ are 0.258e/Å³ and 0.530e/Å³ respectively.

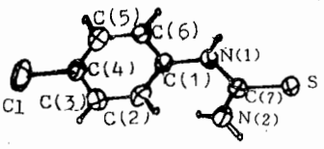


Fig. 1. The perspective view of (I)

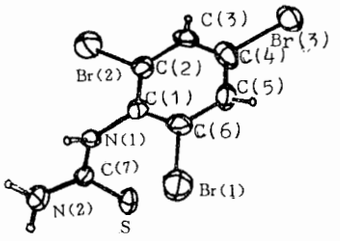


Fig. 2. The perspective View of (I)

The calculations indicate, both in (I) and (II), the thiourea moiety is coplanar. But the dihedral angles between it and the benzene rings are 70.1° and 30.5°, respectively. Due to the steric effect of the Brs a hydrogen bond formed by S and N(2)' of a nearest neighbor, the dihedral angle for (II) (30.5)° is much smaller than that of (I) (70.1)°. The lack of conjugation between the thiourea plane and benzene plane is also illustrated by the bond length C(1)-N(1) (0.1434 and 0.1464nm, normal N-C single bond). In (I), the bond lengths of C(7)-N(1),C(7)-N(1),C(7)-N(2), and C(7), the bond angles of S-C(7)-N(1),S-C(7)-N(2), and N(1)-C(7)-N(2) are close to the corresponding bond lengths and angles of thiourea (Truter, M. R., Acta Crystallogr., 22, 556 (1967)). In (II), N(1) together with the strong electron-attracting tribromo-phenyl group, contributes to larger π-electron density than the others of thiourea. Therefore the bond lengnth of C(7)-N(1) (0.1267nm) is observed to be shorter than the corresponding one in thiourea (0.133nm).

PS-06.05.03 CRYSTAL STRUCTURE AND CONFORMATION OF N-(3-AMINO- PROPYL)CARBAZOLE By D.Kumaran*, S.Eswaramoorthy and M.N.Ponnuswamy, Department of Crystallography and Biophysics, University of Madras, Guindy Campus, Madras-600 025, India.

In view of the proved carcinogenicity of many compounds derived from carbazole, it is worthwhile to study the crystal and molecular structure of N-(3-aminopropyl) carbazole. The compound crystallizes in the monoclinic space group $P2_1/c$ with cell constants a = 16.242(1), b = 5.521(3), c = 13.054(1)Å, β= 92.90(1)° and V = 1169.08Å^3. The other relevant details are as follows: $C_{15}H_{12}N_2$, M_r = 220.28, Z = 4 and D_x = 1.250 Mgm^{-3}. The structure is solved by direct methods and refined by full-matrix least-squares to an R-value of 0.071 for 1907 observed reflections. The carbazole ring is planar with maximum deviation of 0.28(4)Å. The aminopropyl group is also planar and subtends an angle of 73.5(1)° to the carbazole moiety. The structure is stabilised by Vander Waal's forces.

PS-06.05.04 CRYSTAL STRUCTURE OF 2,2'-DIFORMYL 4,4'-DIMETHYL-6,6'-[PIPERAZINE-1,4-DIYL BIS-(METHYLENE)] BIS PHENOL. by S.Shanmuga Sundara Raj, K.Gunasekaran*, D.Velmurugan and K.K.Chacko, Department of Crystallography and Biophysics, University of Madras, Guindy campus, Madras-600 025,INDIA

The development of the chemistry of binuclear complexes has been stimulated by a desire to synthesize model systems that may "mimic" the active sites of metello biomolecules. The X-ray study of the title compound was carried out to yield information about the conformational features and the effect of the size of the piperazine substituent on the molecular conformation. The compound crystallizes in the orthorombic system, space group $P2_12_12_1$ with a=8.687(1),b=13.228(2),c=17.029(3)A, V=1956.7(2)A^3, Dcal=1.30Mgm^{-3} and Z=4. The structure was solved by direct methods and refined by full-matrix least-squares methods to a final R-index of 0.046, for 1995 observed reflections. The phenyl rings are planar and both the phenyl rings are coplanar. The piperazing ring adopts chair conformation and orients 98.9(1)° and 104.0(1)° with respect to the two phenyl rings. The molecules are held together by van der Waals forces.

PS-06.05.05 CRYSTAL STRUCTURE OF 2,6-BIS-(N-METHYLENE MORPHOLINO)-4-CHLORPHENOL. by S.Shanmuga Sundara Raj, D.Velmurugan* and E.Subramanian, Department of Crystallography and Biophysics, University of Madras, Guindy campus, Madras-600 025, INDIA

The study of polymetallic in which coupling between metals is propagated via a bridging molecule has direct application to the design of novel magnetic and electronic solid state materials and for an understanding of the role of polymetallic sites in biological processes. The nature and the magnitude of the interactions depend on the bridge, metal-metal separation, the bond angles at the bridging atoms, the dihedral angle between the planes containing the metal ions and the stereochemistry around the metal ions. Here we report the structure analysis of a bridging ligand molecule by X-ray methods. The title compound, $C_{16}H_{23}N_2O_3Cl$, crystallizes in the monoclinic system, space group $P2_1/c$ with a=10.798(2), b=10.771(3), c=14.235(4)A β=94.65(2) V=1650.1(7)A^3, Dx=1.32mgm^{-3} and Z=4. The structure was solved by direct methods and refined by full-matrix least-squares methods to a final R-index of 0.052, for 2803 observed reflections. Both the morpholino rings adopt chair conformation and orient 49.4(1)° with respect to each other. The molecules are held together by van der Waals forces.

PS-06.05.06 CRYSTAL AND MOLECULAR STRUCTURES OF SOME ACRIDINE DIONES by J.Sivaraman[1], K.Subramanian*[1],. D.Velmurugan[2], E.Subramanian[2], and V.T.Ramakrishnan[3], [1]Department of Physics, Anna University, Madras-25, INDIA; [2]Department of Crystallography and Biophysics, University of Madras, Madras-25, INDIA; [3]Department of Organic Chemistry, University of Madras, Madras-25, INDIA

Amino acridinyl derivatives have been used as anti tumour and antibacterial agents. X-ray studies on three different derivatives have been carried out. Compound I: 10-[4-methylphenyl]-9-methyl-3,4,6,7,9,10-hexahydro 1,8 [2H,5H]acridinedione ($C_{21}H_{23}NO_2$) P21/c, with a=9.108(1), b=11.405(2), c=17.482(2)A, β=102.8(1)°. The structure was solved by Direct methods and refined to a final R=0.066. The central part of acridine ring adopts a twist conformation while the outer 6-membered rings adopt either a sofa or "half-chair" conformation and the planar phenyl ring is axial to the central ring. The acridine system is considerably folded along the bonds at the ring junctions. Compound II : 10-[Methylphenyl] -9[2-chlrophenyl] 3,4,6,7,9,10-hexahydro-1,8(2H,5H)- acridinedione ($C_{26}H_{24}NO_2Cl$): Crystal data Pi, with a=10.715, b=11.183, c=9.267A, α=90.3°, β=105.6° and γ=88.6°, Z=2. Trial structure refined to R=0.093. Compound III : 3,3,5,5,-tetramethyl 10-(4-