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

\[
\text{Cl} - \text{C}=\text{N} - \text{S} - \text{O}_2 - \text{H}
\]

Crystal (I) is monoclinic: \(a=0.974(1), b=20.341(2), c=6.567(1), \beta=91.10(1), p-a\),

g = 0.028(35) mm. Crystal (II) is triclinic: \(a=7.634(1), b=10.578(1), c=11.078(2), \alpha=65.31(1), \beta=72.13(1), \gamma=72.13(1), \gamma=0.029(1648) \text{mm.}

It was determined that the substitution of the 4-nitrophenyl cycle in (I) for the bulky pyrazole 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 C1 - H - intermolecular contact occurs in (II) equal to 3.46Å, stabilizing the trisole cycle position. At the same time, the Z-configuration is well preserved in (I) and (II).

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, the rot.1 energy is achieved, at which molecules escape the potential barrier and take a different conformation. After that, molecules continue torsional vibrations, but relatively to positions changing in time and space. 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

**REFERENCES:**

- \(06.05.01\) THE X-RAY ANALYSIS OF TWO NEW N-VINYLTIAZOLES, By Matsuoka S.T., Kimer K.H., Stenghach B.R., Rechter M.A., Gavrin V.R.
  Institute of Chemistry, Academy of Sciences of Moldova. Chișinău, 277028, Moldova.

Among N-vinyltriazole derivatives some compounds with antifungal activity are known. In order to understand the dependence between the activity of these molecules and their structures we have carried out X-ray investigations.

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**Fig. 1.** The perspective view of (I)
PS-06.05.03 CRYSTAL STRUCTURE AND CONFORMATION OF N-(3-AMINO-PHENYL)CARBAZOLE BY D.Kumaraswamy, S.Eswaramoorthy and M.N.Ponnusamy, 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-aminophenyl) carbazole. The compound crystallizes in the monoclinic space group P2₁/c with cell constants a = 16.242(1) Å, b = 5.251(3) Å, c = 15.854(1), β = 92.981° and V = 1169.886 Å³. The other relevant data are as follows: C₂₀H₁₈N₂, M₀ = 228.39, Z = 4. The structure is solved by direct methods and refined by full-matrix least-squares to an R-value of 0.051 for 1983 observed reflections. The carbazole ring is planar with maximum deviation of 0.20(4) Å. The aminoaryl group is planar and subtends an angle of 75.5(1)° to the carbazole moiety. The structure is stabilised by Vander Waal’s forces.

PS-06.05.05 CRYSTAL STRUCTURE OF 2,2'-DIFORMYL 4,4'-DIMETHYL-6,6'-PIPERAZINE-1,4-DYI BIS-(3-METHYL-YLENE) BIS PHENOL BY S.Shamugam Sandara 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 bisnuclear complexes has been stimulated by a desire to synthesise model systems that may mimic the active sites of metallo 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 orthorhombic system, space group P2₁₂₁ with a = 6.687(1), b = 13.228(2), c = 17.092(3), β = 90°, 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 piperazine ring adopts chair conformation and orient 98.8(1)° and 104.0(1)° with respect to the two phenyl rings. The molecules are held together by van der Waals forces.

PS-06.05.06 CRYSTAL STRUCTURE OF 2,4-BIS-(N-METHYL-MORPHOLINO)-4-CHLOROPHENOL BY S.Shamugam Sudharra Raj, D.Velmurugan* and E.Subramanian, Department of Crystallography and Biophysics, University of Madras, Guindy campus, Madras-600 025, INDIA.

The study of polynuclear 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 polynuclear 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, C₁₇H₁₇N₂O₂Cl, crystallizes in the monoclinic space group P2₁/c with a = 16.103(2), b = 10.774(3), c = 14.237(4), β = 94.854(2), V = 1650.17(8), Z = 2. 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 morpholinol rings adopt chair conformation and orient 49.4(1)° with respect to each other. The molecules are held together by van der Waals forces.

Amino acridinyl derivatives have been used as anti tumour and antihistamine agents. X-ray studies on three different derivatives have been carried out. Compound I: 10-(4'-methylphenyl)-9-(N-methyl)-3,4,6,7,9,10-hexahydro-1,8,2H-acridinedione (C₁₉H₁₄NO₂) P2₁/c, with a = 9.108(1), b = 11.405(2), c = 17.482(2), β = 102.81(1). The structure was solved by Direct methods and refined to a final R = 0.066. The central part of the 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: 20-(Methylphenyl)-8-(2-chlorophenyl)-3,4,6,7,9,10-hexahydro-1,8,2H-acridinedione (C₁₉H₁₄NO₂Cl): Crystal data P2₁, with a = 10.715, b = 11.483, c = 9.976A, 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-