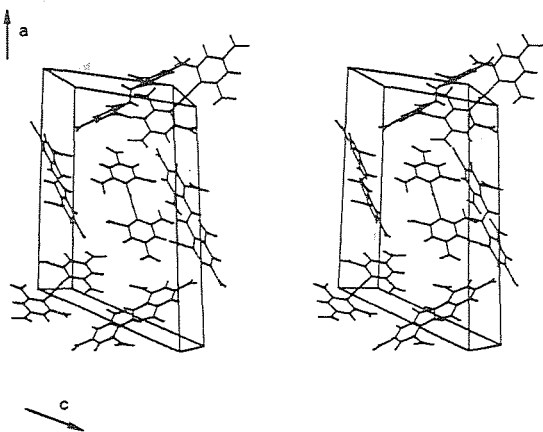


09.2-6 CRYSTAL STRUCTURE OF HNS,
2,2',4,4',6,6'-hexanitrostilbene.

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Monoclinic, $P2_1/c$, $a=22.326(7)\text{\AA}$, $b=5.5706(9)\text{\AA}$,
 $c=14.667(2)\text{\AA}$, $\beta=110.04(1)^\circ$, $V=1714(1)\text{\AA}^3$, $Z=4$,
 $D_m=1.74(1)$, $D_x=1.745(1)$, $\text{Cu K}\alpha_1 \lambda=1.54051\text{\AA}$,
 $\mu=13.30\text{ cm}^{-1}$, $F(000)=912$, room temperature,
 $R=0.060$ for 2345 independent reflections, $R_w=0.057$



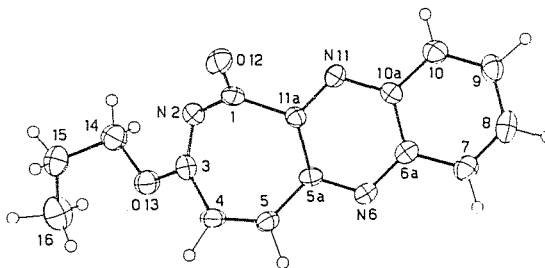
Two different molecules have a symmetry centre either in 2(d) or in 2(c). Their benzene planes are parallel and respectively 1.298Å and 1.428Å apart. NO₂ groups are twisted in the range 5.51° to 48.64° with respect to carbon rings. Molecules are tilted with regards to the axes and make an herringbone pattern. The most compact molecules stacking is along \vec{b} .

09.2-7 CRYSTAL AND MOLECULAR STRUCTURE OF 1-OXO-3-PROPOXYAZEPINO[7,6-b]QUINOXALINE. By Bruna Bovio, Dipartimento di Chimica Generale, Università di Pavia, Italy.

In the course of investigations of photochemical decomposition of 2-azido-1-(3,5-dimethylpyrazolyl)phenazine in n-propylalcohol solution, a compound C₁₅H₁₃N₃O was isolated from the several reaction products. Since the determination of structural formula by chemical means appears to be not smooth and IR, ¹H NMR, and mass spectra do not permit to attribute unambiguously the structure to the title compound, it was deemed necessary to carry out a single-crystal X-ray analysis.

Crystals are triclinic: space group $P\bar{1}$ with $a=7.289(2)$
 $b=14.414(5)$ $c=6.797(2)$ $\alpha=83.56(3)$ $\beta=68.73(3)$
 $\gamma=86.58(4)^\circ$ $Z=2$.

The structure was solved by direct methods and refined by full-matrix least-squares to a final R value of 0.047 ($R_w=0.024$) for 908 reflections having $I \geq 2\sigma(I)$.



The seven-membered ring exhibits a marked puckering: the puckering parameters, calculated according to Cremer and Pople (J. Am. Chem. Soc., 1975, 97, 1354) are

$$\begin{aligned} q_2 &= 0.604 & \phi_2 &= 358.8^\circ \\ q_3 &= 0.161 & \phi_3 &= 188.5^\circ \\ q_3 &= 0.626 & \theta &= 75.0^\circ \end{aligned}$$

These puckering parameters describe a distorted boat. The direction of the distortion is given by θ , which is smaller than 90°; therefore the ring is distorted from the pure boat in the direction of a chair. Indeed, the bow angle is 44.5°, whereas the stern angle is 24.9°. The double bonds are clearly localized at N(2)-C(3) = 1.277(5) and C(4)-C(5) = 1.326(6) Å, whereas the C(5a)-C(11a) bond = 1.418(5) which hinges the two condensed heterocycles, is longer than a double bond, because it takes part in the conjugation within the quinoxaline moiety. The shortening of the C(1)-N(2) bond, 1.382(5), suggests that there is some electron delocalization between the CO group and the adjacent N(2)-C(3) double bond; on the contrary the long C(1)-C(11a) bond, 1.519(5) Å, rules out any electron delocalization between the CO group and the quinoxaline moiety. All the bonds in the quinoxaline moiety have a partial double-bond character, thus reflecting the aromatic character of the quinoxaline: indeed the two condensed rings are nearly coplanar (dihedral angle 1.1°) in spite of their individual nonplanarity. With regard to the propoxy chain, it is worthwhile to remark the short C(3)-O(13) ether bond (1.335(5) Å) which suggests that there is some electron delocalization between O(13) and the adjacent N(2)-C(3) double bond.