

are with the *D* ring. There are no intermolecular contacts between the bromophenol molecules and the *C* rings of steroid molecules.

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Lattice parameters and space groups of two stilbene substituents. By B. JOVANOVIĆ, *Department of Solid State Physics, Institute of Nuclear Sciences 'Boris Kidrič', Vinča, Beograd, P. O. Box 522, Yugoslavia* and I. GEORGESCU, *Polytechnical Institute, Bucarest, Roumania.*

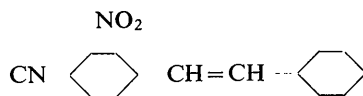
(Received 3 March 1969)

Crystals of 2-nitro-4-cyanostilbene, $C_{15}H_{10}N_2O_2$, are orthorhombic, space group either *Pnam* or *Pna2₁*, with 8 molecules in a unit cell of dimensions $a=13.84$, $b=7.20$, $c=24.88$ Å. 2-Nitro-4-cyano-4'-methoxystilbene, $C_{16}H_{12}N_2O_3$, has been crystallized in two forms, one yellow-green and the other orange. The orange crystals are triclinic, with 2 molecules in a unit cell of dimensions $a=8.38$, $b=13.06$, $c=7.25$ Å, $\alpha=97^\circ 30'$, $\beta=108^\circ$, $\gamma=71^\circ$.

The compounds 2-nitro-4-cyanostilbene and 2-nitro-4-cyano-4'-methoxystilbene are interesting organic scintillating and conducting materials (Georgescu & Giusca, 1966). The two stilbene substituents were synthesized by condensation of 3-nitro-4-methylbenzotrile with benzaldehyde and 3-nitro-4-methoxybenzaldehyde in the presence of piperidine as a catalyst, at a temperature of about 140°C (Ullmann & Gschwind, 1908). A few good crystals were obtained by repeated crystallization in absolute ethanol.

X-ray single-crystal and powder diffraction techniques were used, with Ni-filtered Cu radiation, to determine the cell parameters.

(1) 2-Nitro-4-cyanostilbene, structural formula



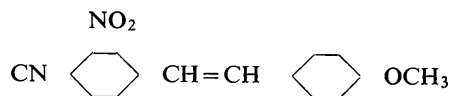
The crystals are thin tablets (001) of a yellow-green colour, and twinning along the *c* axis is frequently observed. A few monocrystals were selected for single-crystal measurements. From rotation and Weissenberg photographs, the crystals were found to be orthorhombic with the unit-cell parameters:

$$\begin{aligned} a &= 13.841 \pm 8, & b &= 7.199 \pm 6, \\ c &= 24.882 \pm 30 \text{ (three standard deviations) } \text{ \AA}, \\ V &= 2480 \pm 6 \text{ \AA}^3, \\ Z &= 8, & D_m &= 1.26 \pm 0.02 \text{ g.cm}^{-3} \end{aligned}$$

and $D_x = 1.34 \text{ g.cm}^{-3}$.

The systematic extinctions: reflexions $0kl$ present for $k+1=2n$; reflexions $h0l$ present for $h=2n$, lead to space group *Pna2₁* or *Pnam*.

(2) 2-Nitro-4-cyano-4'-methoxy stilbene, structural formula



This compound shows two kinds of crystals having yellow-green and orange colour respectively. The powder diffraction data clearly confirm the existence of two structural isomers. The single-crystal study was carried out only on the orange type of crystals. The unit cell is triclinic with:

$$\begin{aligned} a &= 8.377 \pm 13, \\ b &= 13.065 \pm 30 \text{ (two standard deviations)}, \\ c &= 7.246 \pm 10 \text{ \AA}, \\ \gamma &= 71^\circ 14' \pm 30', \\ \alpha &= 97^\circ 30' \pm 2^\circ, \\ \beta &= 108^\circ \pm 30', \\ V &= 702 \pm 4 \text{ \AA}^3; \\ Z &= 2 \end{aligned}$$

and $D_x = 1.28 \text{ g.cm}^{-3}$.

Possible space groups are *P1* or *P1̄*. The value of the β angle is consistent with that obtained by measurement on the optical goniometer.

No further work on these compounds is contemplated at present.

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