

and two projections are presented in *Figure 10*. The model consists of two skew monomer layers. The molecule has five three-membered rings; the n.m.r. spectra suggest a minimum of four three-membered rings. The predicted spectrum of the model, however, agrees with the actual spectrum, since one of the protons at the tip of a three-membered ring is shifted down-field by van der Waals interaction with a nearby carbon.

The top monomer skeleton has four double bonds, which are cross-conjugated, and three cyclopropane rings. Two of the three carbons not part of double bonds or the three-membered rings are highly strained. Thus, only one carbon in the top layer of the molecule is not part of a pi system of some type. This layer is believed to be the chromophore responsible for the low-energy $\pi-\pi^*$ absorption.

The other monomer skeleton contains the naphthalene chromophore and two three-membered rings. This naphthalene chromophore is fully conjugated to only one of the three-membered rings. There are 11 new bonds in this model of dimer A. (These appear striped in the figures.) Five of these are part of cyclopropane rings. There are six crosslinking bonds between layers. Since there is one more double bond in dimer B, only ten new sigma bonds are formed. Four of these are involved in three-membered rings and six connect the monomer layers. This model discussed above represents the characteristics displayed by the n.m.r. spectra of dimer A, as well as the u.v. and visible spectra. It is intended as a possible structure for a member of a new class of compounds formed under high pressure. Other models have been constructed; however, the one presented here fits the observed data best. These other models are similar and may also represent molecules actually present in the mixture. Models have also been constructed representing dimer B. Both products are similar.

The same type of analysis gave structures for the pyrene tetramers. In *Figure 11* we show a stereoscopic representation for pyrene tetramer A.

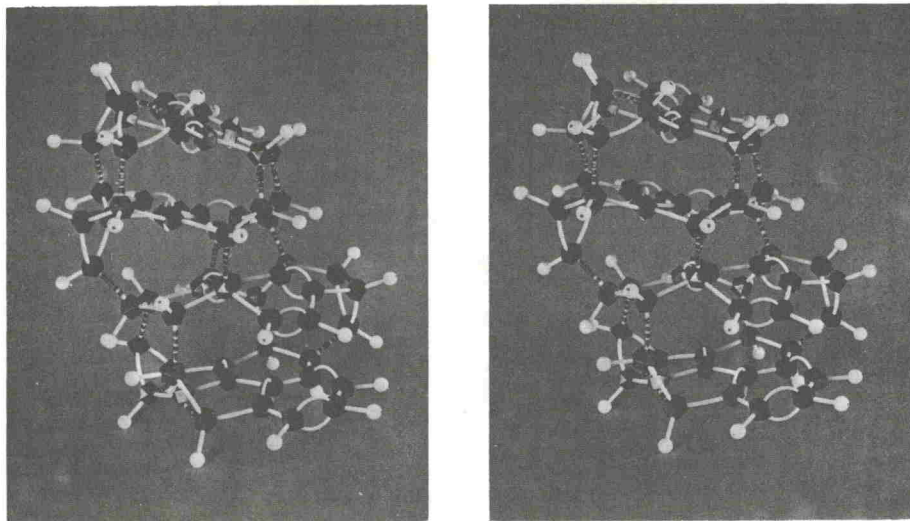


Figure 11. Stereoscopic view of pyrene tetramer A

The assignments are given in Table 1. It consists of four monomer-like layers turned as much as 90° out of alignment. A number of slightly different models were constructed, but this one best fits the data.

These products appear to be a new class of hydrocarbons. It is possible that one could construct electron donor-acceptor complexes with appropriate geometry and electronic structure so as to create a series of new products and to develop an organic chemistry of the solid state at high pressure.

BIANTHRONES

After optical excitation an electron may lose its energy in a number of ways. It may return to the ground state emitting fluorescent radiation or by a number of radiationless paths. It may undergo intersystem crossing to a triplet state and return to the ground state via phosphorescence or by radiationless processes. In a number of classes of molecules it may decay by one mechanism or another to a metastable state where it may remain for seconds or hours. This state will, in general, have a different (lower) excitation energy, so the material changes colour. This phenomenon is known as photochromism¹⁵. In organic materials the transformation to the meta-

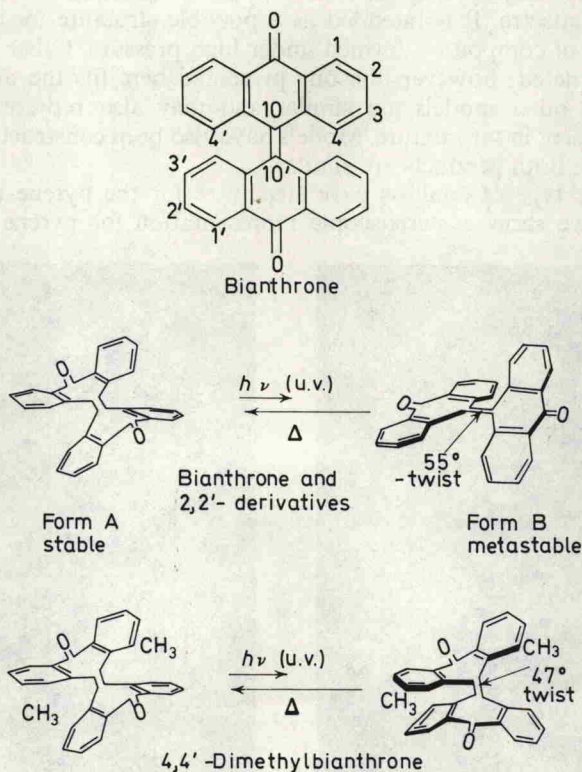


Figure 12. Structure and photochromic reactions of bianthrones