

PRESSURE ON THE ELECTRONIC STATES OF ORGANIC SOLIDS

Table 1. Structural features of products from pyrene and perylene complexes with iodine

	Pyrene tetramers		Perylene dimers	
	A	B	A	B
Number of protons	40	40	24	24
Total paraffinic protons	31	30	19	17
(a) normal ring protons	14	13	7	7
(b) three-membered ring protons at $\delta = 1.1$	5	4	4	4
(c) protons shifted downfield	12	13	8	6
Total olefinic protons	3	5	2	4
(a) at normal position	0	1	1	1
(b) shifted up field by benzene ring	3	4	1	3
No. of aromatic protons	6	5	3	3
Three-membered rings	6	5	5	4
Total aromatic rings	2	2	2	2
aromatic rings with protons	2	2	1	1
Naphthalene chromophore	0	0	1	1
Total olefin bonds	8	9	4	5
olefin bonds with protons	2	3	2	3
New bonds	18	17	11	10

field protons in dimer A are at 1.1 p.p.m. For a system with no methyl groups one would anticipate that these would be on three-membered rings. It should be noted that, in the absence of proton rearrangement, all paraffinic protons must be tertiary. Some of the protons on a three-membered ring were on carbons also involved in five-membered rings formed by the rearrangement of the original six-membered rings. These appear at 1.5 p.p.m. For dimer A, there were a minimum of four three-membered rings. Those protons appearing between 1.6 and 3.0 p.p.m. were shifted downfield by double bonds or by aromatic rings.

For details concerning the electronic and molecular spectra and the

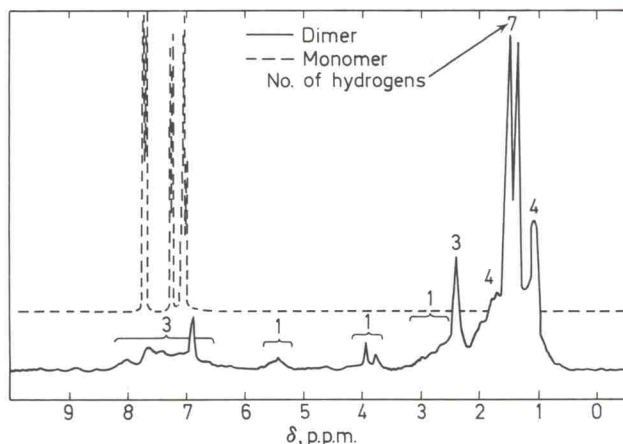


Figure 8 N.m.r. spectrum of perylene and of perylene dimer A

mass spectrum as well as a discussion of how they contribute to the structural determination the reader is referred to the original paper¹⁴.

A model of dimer A has been developed which includes all of the characteristics listed in *Table 1*. It is shown in a stereoscopic representation in *Figure 9*

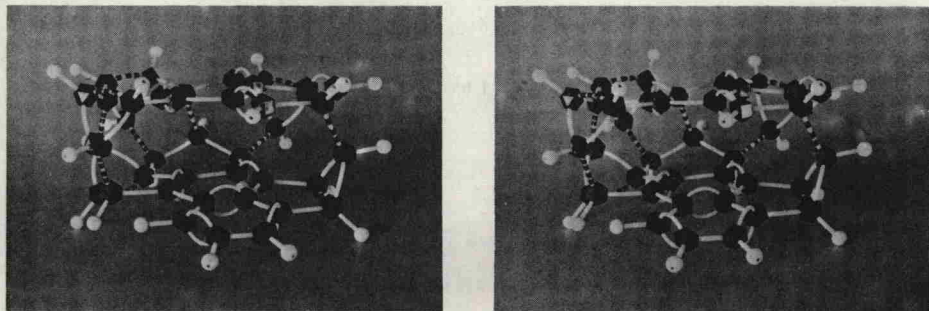


Figure 9. Stereoscopic view of perylene dimer A

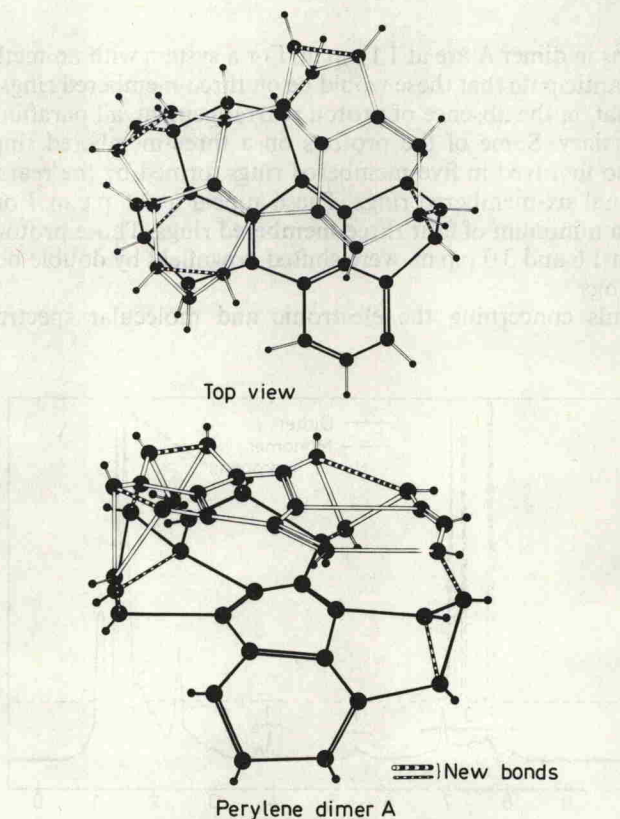


Figure 10. Front and top view of perylene dimer A