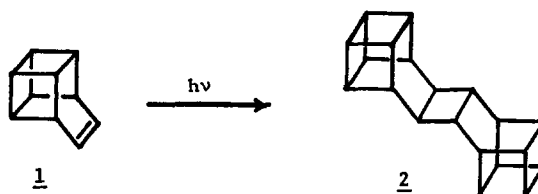


SYNTHESIS AND STRUCTURE OF BASKETENE PHOTODIMER, $C_{20}H_{20}$

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In a photochemical reaction not unlike that of other strained ring unconjugated olefins basketene, 1, undergoes cycloaddition to itself forming a dimer, $C_{20}H_{20}$. While the chemical and physical properties are consistent with a $2\pi + 2\pi$ photodimerization forming a highly strained system such as 2 together they were sufficiently ambiguous so as not to exclude other dimers.



To establish the structure an x-ray crystallographic study was undertaken.

The crystals of $C_{20}H_{20}$ were triclinic, space group P1, with: $a = 10.089$ (4), $b = 6.529$ (3), $c = 5.450$ (3) Å; $\alpha = 115.20$ (5), $\beta = 103.11$ (5), $\gamma = 76.35$ (5)°; $d_{\text{obsd}} = 1.36$, $d_{\text{calcd}} = 1.38$ g cm^{-3} ; $z = 1$. A total of 644 independent reflections was measured on a General Electric XRD-5 diffractometer with $\text{Cu K}\alpha$ radiation ($2\theta \leq 100^\circ$). The structure was solved by a combination of symbolic addition and Patterson methods. Hydrogens were located from a difference Fourier calculation. The final R is 8.6%. The average carbon-carbon bond length is 1.55 Å; and the average carbon-hydrogen length is 1.07 Å, exactly the values found for cubane². Furthermore, the bond lengths and angles of 2 agree well with those reported for basketene-9-ol p-bromobenzoate³ and basketene-9,10-dicarboxylic acid⁴. C-C-H angles in 2 are within the range of 105° to 127° ($\sigma = 5^\circ$) with two exceptions. These are angle C(7)-C(6)-H(6) and angle C(6)-C(7)-H(7) both of which are 135°. Many of the other bond lengths and angles which involve C(6) and C(7) are also anomalous reflecting a change of hybridization from the normal sp^3 .

