and then chromatographed on silica (40 × 3.8 cm; $CHCl_3$–MeOH, 19:1). The benzyl derivative emerged as the major product and crystallized in colorless needles (1.39 g; mp 151–151.5 °C) after addition of petroleum ether (bp 40–60 °C) to a solution in $CHCl_3$–EtOH. Rechromatography of early contaminated fractions gave a further quantity (80 mg; total yield 71%) of crystalline product, mp 151–152 °C. Anal. Calcd for $C_{17}H_{20}N_2O_5$: C, 61.43; H, 6.07; N, 8.43. Found: C, 61.37; H, 6.12; N, 8.05.

**Comparison by TLC of 5′-*O*-Tosylthymidine and $O^2$,5′-Cyclothymidine as Precursors of Thymidine 5′-Phosphonates.** Experiments were carried out on a 0.03–0.10 mmol scale.

**A. Reaction with Bis(dihydroxyphosphinomethyl)-phosphinic Acid (10).** (i) Acid **10** (24 mg, 0.09 mmol), tri-*n*-octylamine (95 mg, 0.27 mmol), and 5′-*O*-tosylthymidine (12 mg, 0.03 mmol) were heated in DMF (0.3 mL) in a closed tube at 120 °C. No substantial darkening occurred. Samples were taken at 2.5 and 4 h. (ii) The procedure was the same as in (i), but with $O^2$,5′-cyclothymidine[17] (13; 7 mg, 0.03 mmol) in place of **4**. The solution darkened within a few minutes of the start of heating.

Reaction mixtures (i) and (ii) gave similar patterns on TLC (*n*-PrOH–2 N aqueous $NH_3$, 7:3), compound **5** being a major product in both cases. There was no significant difference between the 2.5- and 4-h samples.

**B. Reaction with Methylenediphosphonic Acid.** Conditions were similar to those described in A, but with tri-*n*-butylamine as base (2 or 4 mol/mol of diphosphonic acid) and a heating time of 2.5 h. Compound **7** was formed in each case as a major product; the proportion of base was not critical. TLC (as in A) showed that the cyclothymidine reaction produced an additional, though minor, UV-absorbing product moving just ahead of **7**; in other respects the TLC patterns were closely similar.

**Acknowledgment.** This investigation was supported by Cancer Research Campaign Grant No. 410/B/973/73. I am greatly indebted to Dr. Philip Loftus (Imperial Chemical Industries Corporate Laboratory, Runcorn, Cheshire) for running and interpreting the $^{31}P$ NMR spectra, to Mrs. Elizabeth Summers (Department of Chemistry, King's College, London, WC2R 2LS) for those NMR spectra run on the Bruker 90-MHz instrument, to Dr. Michael Jarman, of this Institute, for the mass spectra, and to Dr. Andrzej Okruszek (see ref 3) for kindly providing a sample of his thymidine triphosphonate (**5**) before he had completed its purification. Microanalyses were carried out by Butterworth Laboratories Ltd., Teddington, Middlesex, England.

**Registry No.** **4**, 7253-19-2; **5** tetrasodium salt, 71370-59-7; **7** trisodium salt, 71370-60-0; (*R*)-**8**, 71393-23-2; (*S*)-**8**, 71425-91-7; **9**, 365-07-1; **10**, 22401-27-0; **11** ammonium salt, 71370-61-1; **11** sodium salt, 38379-51-0; **12** diammonium salt, 71370-62-2; **12** disodium salt, 71370-63-3; **13**, 15425-09-9; methylenediphosphonic acid, 1984-15-2; tetraethyl methylenediphosphate, 1660-94-2; phosphoric acid, 7664-38-2; 3′-*o*-benzylthymidine, 63593-01-1; benzyl chloride, 100-44-7; 5′-*o*-tritylthymidine, 7791-71-1.

(17) A. M. Michelson and A. R. Todd, *J. Chem. Soc.*, 816 (1955).

## Synthesis and Thermal Reactions of 5,5-Diphenylcyclopentadiene[1]

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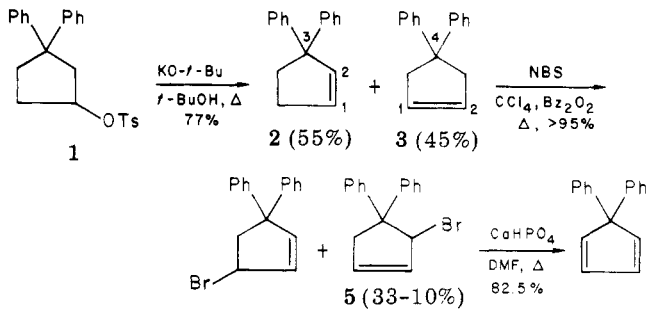
The *gem*-diphenyl function is not easily introduced into molecules. Probably, introduction of this function via diphenyldiazomethane or diphenylketene is most commonly employed. Because other work required *gem*-diphenyl functionality in bi- and tricyclic structures, we considered the possibility that 5,5-diphenylcyclopentadiene could serve usefully in the synthesis of such compounds. 5,5-Disubstituted cyclopentadienes of various types are indeed known. The alkyl examples, for instance, have a number of syntheses, proceeding from a cyclopentanone,[2] bicyclopentanes,[3] or cyclopentenones.[4] The 5,5-diphenyl analogue appears to be unreported previously, although the 1,4,[5] the 1,2,[6] and the 2,3[7] isomers, have been described. We report here the synthesis, characterization, thermal rearrangement, and Diels-Alder reactivity of this interesting diene.

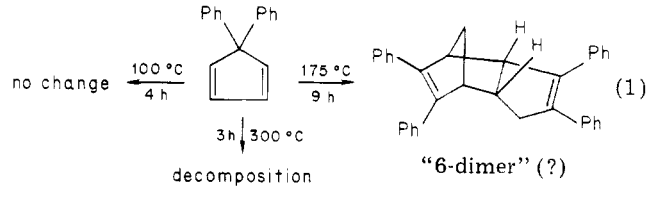
Scheme I




### Results and Discussion

5,5-Diphenylcyclopentadiene (**6**) was prepared in a straightforward sequence from 3,3-diphenylcyclopentyl tosylate (**1**). These reactions are summarized in Scheme I.

Diene **6** showed no change in its NMR, IR, or UV spectra upon being heated neat under nitrogen at 100 °C for 4 h. A solution of **6** in hexadecane, when heated under nitrogen in a sealed tube at 300 °C for 3 h, underwent extensive degradation. Better control of the process was achieved by heating **6** in benzene-$d_6$ under nitrogen in a sealed NMR tube at 175 °C for 9 h, with NMR analysis being conducted each hour. No further change was observed after 3–4 h, however. Evaporation of the solvent left a solid, mp 136–138 °C dec, which exhibited *no vinyl proton* resonance in its NMR spectrum. Attempts to purify this crude solid by crystallization were unsuccessful, and the structure "**6**-dimer" for this material must be considered tentative (eq 1).[8]




(1) Taken from the M.S. Thesis of S.Z.A., 1978.

(2) C. F. Wilcox, Jr., and M. Mesirov, *J. Org. Chem.*, **25**, 1841 (1960).

(3) P. Eilbracht, P. Dahler, and W. Totzauer, *Tetrahedron Lett.*, 2225 (1976).

(4) R. Holder, J. Dahler, W. Baker, and R. Gilbert, Abstracts of Papers, 175th National Meeting of the American Chemical Society, Anaheim, Calif., March, 1978, paper ORGN 80.

(5) N. Drake and J. Adams, Jr., *J. Am. Chem. Soc.*, **61**, 1326 (1939). This is presumably the same diene as that prepared by W. Borsche and W. Menz, *Chem. Ber.*, **41**, 209 (1908), and believed by them to be the 1,3 isomer. Another preparation is due to M. Gonikberg and A. Gavrilova, *Zh. Obshch. Khim.*, **22**, 1384 (1952); *Chem. Abstr.*, **47**, 5901 (1953).

(6) G. Rio and M. Chariffi, *C. R. Hebd. Seances Acad. Sci., Ser C*, **268**, 1960 (1969).

(7) C. F. H. Allen, J. E. Jones, and J. A. Vanallan, *J. Org. Chem.*, **11**, 268 (1946). These authors name the diene "3,4-diphenylcyclopentadiene", but it is the 2,3 isomer.

(8) This dimer (mp 171–172 °C) was reported by Rio and Chariffi[6] to form along with others from 1,2-diphenylcyclopentadiene. Its structure was supported by (unreported) spectra. Compound "**6**-dimer" was not obtained in pure enough condition to make a comparison.

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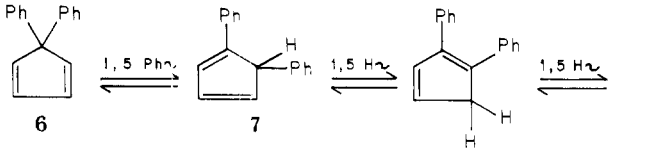
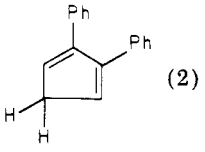
The change in NMR spectrum as **6** was heated suggested that sigmatropic rearrangement of **6** to other isomers was occurring.[9] This process can be summarized as shown in eq 2.

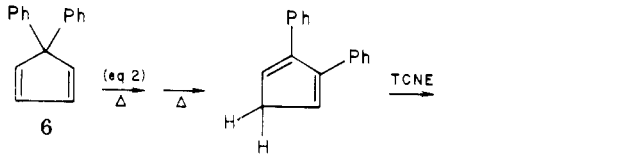



6 7 8



9 (2)

If other isomers were in fact formed, then perhaps a better dienophile could trap them more efficiently. To this end, a solution of **6** and tetracyanoethylene in xylene was refluxed (~140 °C) for 4 h. Although other adduct(s) were apparently present as well, the principal adduct, mp 230–231 °C, was isolated in >65% yield (yield of all adducts was 87%). Its $^1H$ and $^{13}C$ NMR spectra (see Experimental Section) strongly support structure **10** shown in eq 3, the product expected for capture of **9**. Interestingly, no reaction of **6** itself with TCNE occurred upon attempted reaction of the two compounds in refluxing carbon tetrachloride for 18 h.



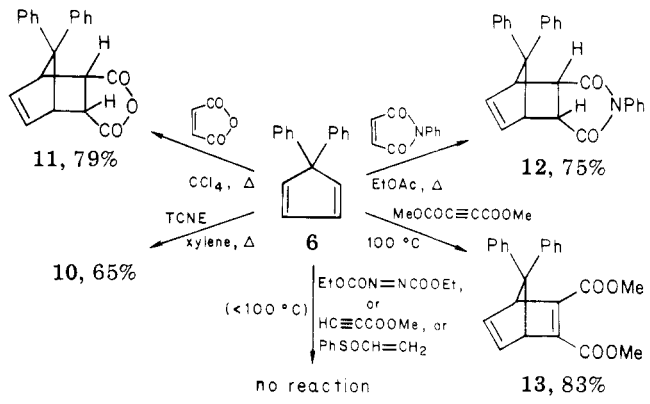

6 10 (3)

**Diels–Alder Reactions.** Diene **6** underwent cycloaddition to form well-characterized adducts with maleic anhydride, *N*-phenylmaleimide, and dimethyl acetylenedicarboxylate at temperatures of 76–100 °C and with tetracyanoethylene at 140 °C. As mentioned above, this last cycloaddition gave rearranged product, unlike the others. Phenylazomaleianil gave an adduct, but attempts to characterize the material were only partially successful. Diethyl azodicarboxylate, methyl propiolate, and phenyl vinyl sulfoxide[10] did not react with diene **6** under the conditions employed (<100 °C).

These reactions are grouped in Scheme II.

The additions in Scheme II establish that diene **6** is a well-behaved conjugated diene, giving the expected adducts with *reactive*, *disubstituted* dienophiles. It is, therefore, a useful reagent for the introduction of *gem*-diphenyl groups, as was hoped for at the outset of this work. Less reactive dienophiles are ineffectual, although higher temperatures would probably afford products from the isomeric **9** formed by thermal rearrangement of **6**. Diene **6** is clearly affected by steric problems, and no adduct with both exo substituents and the bridge *gem*-diphenyl function has been made. Apparently this steric problem causes TCNE to await the formation of **9** and thus to form **10** instead.

Scheme II




## Experimental Section

**General.** Melting points were taken on a calibrated Fisher-Johns block and are uncorrected, as are the boiling points. Infrared spectra ($\nu$) were determined on a Perkin-Elmer Model 700 instrument. Only structurally significant or intense absorptions are listed. Ultraviolet spectra ($\lambda_{max}$) were recorded on a Cary Model 14 or a Perkin-Elmer Model 575 spectrometer. Nuclear magnetic resonance spectra ($\delta$) were obtained on Varian EM-360 ($^1H$) and Varian FT-80 ($^{13}C$) spectrometers using tetramethylsilane as an internal reference. Mass spectra ($m/e$) were taken on a Varian EM-600 instrument. Microanalyses were performed by Micro-Tech Laboratories, Skokie, Ill.

**3,3- and 4,4-Diphenylcyclopentenes (2, 3). 3,3-Diphenylcyclopentanone** was prepared from 3,3-diphenyladipic acid[11] as reported[12] (60%, mp 85–87 °C (lit.[12] mp 87–88 °C)). Use of pure, recrystallized acid is important for a respectable yield. The ketone was reduced with lithium aluminum hydride in the usual manner to **3,3-diphenylcyclopentanol** (93%, mp 54–56 °C (lit.[13] mp 55–57 °C)). To a solution of this alcohol (4.0 g, 16.8 mmol) in dry ether (80 mL) was added a solution of *n*-butyllithium in hexane (Alfa, 2.2 M, 10 mL). After the solution was stirred briefly, a solution of *p*-toluenesulfonyl chloride (6.43 g, 33.7 mmol) in dry ether (30 mL) was added dropwise with stirring. After the material had been stirred overnight, water was added, and the layers were separated. The aqueous layer was extracted with some ether, and the extract was combined with the original ether phase. This material was washed with hydrochloric acid (10%), sodium bicarbonate solution, and brine and finally dried over magnesium sulfate. The solvent was removed under vacuum, and the product was recrystallized from ether in the freezer overnight to afford **3,3-diphenylcyclopentyl tosylate** (1): 4.3 g; 65%; mp 78–79 °C (lit.[13] mp 80–81.5 °C).

Potassium *tert*-butoxide (Aldrich, 2.0 g, 17.8 mmol) was dissolved in freshly distilled *tert*-butyl alcohol (75 mL). To the stirred solution was slowly added tosylate **1** (3.5 g, 8.9 mmol), and the mixture was then heated under reflux overnight. Water (200 mL) was added, and the solution was extracted three times with ether. The combined ether extracts were washed with water, hydrochloric acid (10%), sodium bicarbonate solution, and brine and finally dried over anhydrous magnesium sulfate. The ether was removed, and the residual oil was distilled in a Kugelrohr apparatus at 120 °C (0.5 mm) to afford the olefin mixture **2** and **3**: 1.51 g; 77%; $\nu$ (neat) 1665 cm$^{-1}$ (C=C); $\delta$ ($CCl_4$) for **2**, 7.29 (PhH, 10 H, s), 6.2 (H-2, 1 H, d, $J \sim 5$ Hz), 5.94 (H-1, 1 H, d), 2.51 ($CH_2$'s,

(9) Cf. M. F. Semmelhack, H. N. Weller, and J. Clardy, *J. Org. Chem.* **43**, 3791 (1978).

(10) We thank Professor L. A. Paquette (The Ohio State University) for details on the preparation of this sulfoxide, which has been used in Diels–Alder processes quite successfully as an acetylene equivalent. Cf. L. A. Paquette, R. E. Moerck, B. Harirchian, and P. D. Magnus, *J. Am. Chem. Soc.*, **100**, 1597 (1978). We also are indebted to Mr. A. Patel for preparing the sulfoxide and attempting its reaction with diene **6**.

(11) W. Herz and G. Caple, *J. Org. Chem.*, **29**, 1696 (1964).

(12) A. Warshawsky and B. Fuchs, *Tetrahedron*, **25**, 2633 (1969).

(13) J. W. Wilt, R. A. Dabek, and K. C. Wetzel. *J. Org. Chem.*, **37**, 425 (1972).

4 H, s, isochronous); δ for **3**, 7.29 (PhH, 10 H, s), 5.89 (vinyl H's, 2 H, s), 3.1 ($CH_2$, 4 H, s). NMR analysis indicated a composition of **2**:**3** of 55:45.[14]

Anal. Calcd for $C_{17}H_{16}$: C, 92.68; H, 7.32. Found: C, 92.64; H, 7.41.

**5-Bromo-3,3-diphenyl- and 3-Bromo-4,4-diphenylcyclopentene (4, 5).** To a mixture of olefins **2** and **3** prepared as described above (1.1 g, 5 mmol) in carbon tetrachloride (100 mL) was added *N*-bromosuccinimide (NBS, Aldrich, 0.9 g, 5 mmol) and benzoyl peroxide (10 mg). The solution was then refluxed for 1.5 h, at which time the solution which originally was yellow and contained the *N*-bromosuccinimide as an insoluble solid on the bottom became clear with succinimide as a white solid on the top. After filtration of the succinimide and removal of the solvent, a clear oil remained (ca. 1.5 g, ~100% yield). This oil was used quickly in the following step because it colored on standing and appeared somewhat labile. Cursory NMR analysis indicated that **4** predominated in the product [δ ($CDCl_3$) 5.17 (>CHBr, 1 H, t, $J \sim 6$ Hz)] with varying amounts of **5** (10–33%) [δ ($CDCl_3$) 5.67 (>CHBr, 1 H, m)].

Use of 1,2-dibromotetrachloroethane[15] instead of NBS was unsatisfactory.

**5,5-Diphenylcyclopentadiene (6).** The allylic bromide mixture of **4** and **5** (ca. 1.5 g, 5 mmol) was dissolved in freshly distilled *N*,*N*-dimethylformamide (50 mL) containing suspended finely powdered calcium hydrogen phosphate (3.44 g, 20 mmol of the monohydrate which had been dried at 120 °C for 12 days) and stirred at 80 °C for 12 h.[16] The cooled mixture was poured into water (200 mL), the supernatant material was decanted from the solid present, and both were then extracted thoroughly with ether (each 3 × 50 mL). The combined extracts were washed three times with water and then with brine and finally dried over magnesium sulfate. Removal of the ether left an oil which was distilled in a Kugelrohr apparatus at 100 °C (0.3 mm) to afford diene **6** as a colorless oil (0.9 g, 82.5%) which eventually solidified (quickly when seeded) to a colorless, crystalline mass, mp 45–46 °C. Further data for **6** are: *m/e* 218 ($M^+$); ν (neat) 1590 (conjugated C=C), 1481, 1440, 730, and 690 $cm^{-1}$ (Ph); $\lambda_{max}$ (isooctane) 235 (ε 7280), 260–270 complex (ε ≃ 3300) nm.[17] The $^1H$ NMR spectrum ($CCl_4$, $Me_4Si$) showed the aromatic protons at δ 7.23 (10 H, s) and the vinyl protons as two complex doublet resonances ($J \sim 6$ Hz) at δ 6.79 (2 H, H-1, 4, m) and δ 6.36 (2 H, H-2, 3, m). The seven-line $^{13}C$ NMR spectrum ($CDCl_3$, $Me_4Si$) was taken in a solution containing 12 mol% $Cr(acac)_3$, a $T_1$ suppressor: δ 144.96 (C-1,4), 141.88 (C-2,3), 31.89 (C-5). The phenyl carbons were observed at δ 129.55 (ipso), 128.30 (ortho), 127.67 (meta), and 126.65 (para).

Anal. Calcd for $C_{17}H_{14}$: C, 93.54; H, 6.46. Found: C, 93.21; H, 6.60.

Use of 1,5-diazabicyclo[5.4.0]undec-5-ene ("DBU") to effect dehydrobromination led to resinous material.

**Thermal Reactions of Diene 6.** Heating 200 mg of diene **6** (no solvent) at 100 °C under nitrogen for 4 h led to no change in its $^1H$ NMR spectrum. A solution of **6** (79 mg) in hexadecane (0.75 mL) sealed under nitrogen in a small tube was heated in a tube oven at 300 °C for 3 h. The material turned brownish-black and had obviously undergone extensive decomposition. In a third reaction, diene **6** (218 mg, 1 mmol) was dissolved in benzene-$d_6$ (Norel, 1 mL) and sealed under nitrogen in an NMR tube. The material was heated in a tube furnace at 175 °C for a total of 9 h, with interuptions each hour to observe by NMR the transfer of the vinyl protons to the aliphatic region (δ 1–4), with eventual development of a triplet at δ 3.0 ($J \sim 7$ Hz) clearly evident in a complex group of multiplets (δ 1.90–3.90). No vinyl proton resonance (δ 4.5–7.0) was evident. The transformation appeared to be complete in ca. 3–4 h, with no significant change thereafter. Evaporation of the solvent left an orange-yellow solid (ca. 200 mg), mp 136–138 °C dec. Attempts to recrystallize this solid or to sublime it were unsuccessful. A final study identical with the above was conducted at 130 °C, leading to NMR changes that were completed in ca. 9 h.

**Diels–Alder Reactions. Diene 6 and Maleic Anhydride.** Diene **6** (218 mg, 1 mmol) and recrystallized maleic anhydride (107 mg, 1.1 mmol) in carbon tetrachloride (5 mL) were heated under reflux for 12 h. The solvent was removed, and the residue was recrystallized from chloroform–acetone to afford **7,7-diphenyl-5-norbornene-*endo*-2,3-dicarboxylic acid anhydride (11)**: 250 mg; 79%; mp 266–267 °C; ν (KBr) 1850, 1770 $cm^{-1}$ (–COOCO–); δ (acetone-$d_6$) 7.34 (PhH, 10 H, br m), 6.31 (vinyl H's, 2 H, t), 4.57 (H-1, 4, 2 H, m), 3.72 (H-2, 3, 2 H, m).

Anal. Calcd for $C_{21}H_{16}O_3$: C, 79.73; H, 5.10. Found: C, 79.62; H, 5.09.

**Diene 6 and *N*-Phenylmaleimide.** Diene (218 mg, 1 mmol) and *N*-phenylmaleimide (Aldrich, 190 mg, 1.1 mmol) were refluxed in ethyl acetate (5 mL) for 3 h. Processing the reaction as above led to ***N*,7,7-Triphenyl-5-norbornene-*endo*-2,3-dicarboximide (12)**: 290 mg; 75%; mp 221–222 °C from chloroform and petroleum ether; ν (KBr) 1775, 1700 $cm^{-1}$ (–CON(CO–)–); δ ($CDCl_3$) 7.47 (PhN<, 5 H, br s), 7.28 (7,7-PhH's, 10 H, br s), 6.30 (vinyl H's, 2 H, br s), 4.39 (H-1, 4, 2 H, br s), 3.57 (H-2, 3, 2 H, br s).

Anal. Calcd for $C_{27}H_{21}O_2N$: C, 82.84; H, 5.41. Found: C, 82.73; H, 5.36.

**Diene 6 and Dimethyl Acetylenedicarboxylate.** Diene **6** (218 mg, 1 mol) and the diester (Aldrich, 142 mg, 1 mmol) were heated at 100 °C without solvent for 2 h. Upon cooling the solution, a crystalline solid formed which was recrystallized from ethanol to produce **dimethyl 7,7-diphenylnorbornadiene-2,3-dicarboxylate (13)**: 300 mg; 83%; mp 120–121 °C; ν (KBr) 1723, 1633 $cm^{-1}$ (C=CCOOR); δ ($CDCl_3$) 7.29 (PhH, 10 H, m), 6.87 (vinyl H's, 2 H, m), 4.86 (H-1, 4, 2 H, m), 3.77 ($OCH_3$, 6 H, s).

Anal. Calcd for $C_{23}H_{20}O_4$: C, 76.65; H, 5.59. Found: C, 76.40; H, 5.63.

**Diene 6 and Tetracyanoethylene ("TCNE").** An attempted reaction of diene **6** with TCNE as above ($CCl_4$, reflux, 18 h) led to no reaction. Instead, diene **6** (218 mg, 1 mmol) and TCNE (Aldrich, 128 mg, 1 mmol) were heated under reflux in xylene (10 mL) for 4 h. The solution was cooled, and the solid that precipitated was collected: 300 mg; 87%; mp 227–232 °C. NMR analysis indicated that more than one adduct was present, but recrystallization several times from chloroform gave the principal component (>65%), **2,3-diphenyl-5,5,6,6-tetracyanonorbornene (10)**, a rearranged adduct: mp 230–231 °C; ν (KBr) 2320 $cm^{-1}$ (CN); δ (acetone-$d_6$) 7.49 (PhH, 10 H, br m), 4.83 (H-1, 4, 2 H, sharp m), 2.82, 2.35 ($CH_2$, 2 H, AB *q*, $J \sim 11$ Hz); $^{13}C$ δ ($CDCl_3$, 5 mol% $Cr(acac)_3$ present) 45.45 (C-1, 4), 46.13 (C-7), 60.43 (C-5, 6), 109.58 (endo CN), 110.87 (exo CN), 131.19 (C-2, 3). The aromatic carbons exhibited δ 130.40 (ipso), 127.85 (ortho), 127.13 (meta), and 126.94 (para).

Anal. Calcd for $C_{23}H_{14}N_4$: C, 79.95; H, 4.07. Found: C, 79.67; H, 3.97.

**Other Attempted Diels–Alder Reactions.** An adduct was produced from diene **6** and *N*-phenylazomaleianil (Aldrich), treated as described for the adduct **12**. The orange product, mp 221–223 °C from chloroform, exhibited proper spectra but repeatedly incorrect microanalyses. "Purification" seemingly made the compound even worse. The following are summaries of other additions (1 mmol scale) attempted with diene **6** and mentioned dienophiles: diethyl azodicarboxylate ($CCl_4$, reflux, 7 days), no reaction; methyl propiolate (neat mixture, 100 °C, 3 h), no reaction; phenyl vinyl sulfoxide (neat mixture, 100 °C, 3 h), no reaction.

**Acknowledgment.** Acknowledgment is made to the donors of the Petroleum Research Fund, administered by The American Chemical Society, for support of this research.

**Registry No.** 1, 32812-61-6; **2**, 22351-60-6; **3**, 36666-03-2; **4**, 71516-76-2; **5**, 71516-77-3; **6**, 71516-78-4; **10**, 71516-79-5; **11**, 71516-80-8; **12**, 71516-81-9; **13**, 71516-82-0; 3,3-diphenylcyclopentanone, 16020-97-6; 3,3-diphenylcyclopentanol, 24771-20-8; maleic anhydride, 108-31-6; *N*-phenylmaleimide, 941-69-5; dimethyl acetylenedicarboxylate, 762-42-5; TCNE, 670-54-2.

(14) This rough equivalence of **2** and **3** was observed in all of the half-dozen or so preparations performed.

(15) E. S. Huyser and D. N. DeMott, *Chem. Ind. (London)*, 1954 (1963).

(16) Cf. J. S. Swenton and G. L. Smyser, *J. Org. Chem.*, **43**, 165 (1978).

(17) There appears to be no particular electronic influence between the chromophores. Compare cyclopentadiene, $\lambda_{max}$ (isooctane) 239 nm (ε 3400), and diphenylmethane, $\lambda_{max}$ (iso-octane) 262 nm (ε 5000).