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Efficient Synthesis of 1,1-Diaryl 1,2-Dienes via Pd(0)-Catalyzed Coupling of Aryl Halides with Allenic/Propargylic Zinc Reagents

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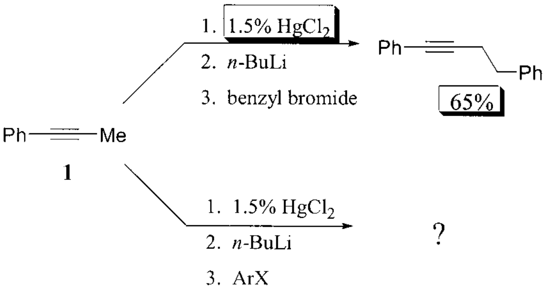
Introduction

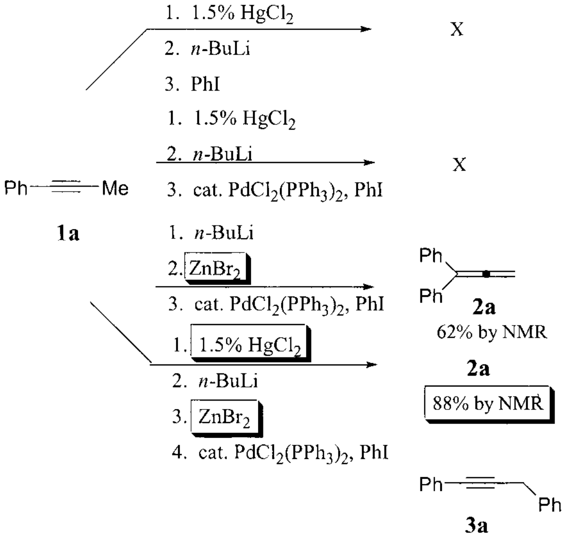
The synthesis and chemistry of allenes are of current interest due to their high and unique reactivities.[1−5] The reactivities of the two C═C bonds in allenes can be differentiated via delicate tuning of the steric and electronic factors.[1,4,5] Allenes are usually prepared by one of the following methodologies: (1) elimination of substituted alkenyl triflates/halides or allylic halides;[6] (2) reductive elimination of two vicinal halogen atoms from 2,3-dibromoalkenes;[7] (3) addition of organometallic reagents or metal hydrides to propargylic halides and analogues;[8] (4) rearrangement of acetylenic systems;[9] (5) reaction of 1,1-dihalocyclopropanes with MeLi;[10,13] (6) addition of organolithiums to vinylacetylenes;[11] and (7) coupling reaction of allenic metallic reagents with organohalides.[12] Some of the methodologies listed here require lengthy procedures to prepare the starting materials and thus lack efficiency. Moreover, the methods for the synthesis 1,1-diaryl-1,2-allenes seem limited probably due to the steric hindrance and instability.[13]

Recently, we developed a $HgCl_2$-catalyzed monolithiation reaction of 1-aryl-1-propynes.[14] The organolithium intermediates formed could be trapped by benzylic halides,[14] allylic halides,[15] and primary alkyl halides[15] to provide synthetically useful substituted 1-aryl-1-alkynes as the major product. In this paper, we would like to disclose our new results on the reaction of the organolithium intermediates with aryl halides (Scheme 1).

Scheme 1



Scheme 2



Results and Discussion

The treatment of 1-phenyl-1-propyne with *n*-BuLi in the presence of 1.5 mol % of $HgCl_2$ in THF at −78 °C followed by the addition of PhI did not afford any coupling product(s); the Pd-catalyzed coupling reaction of the corresponding organolithiums with iodobenzene did not work either. However, in the presence of 1.5 mol % $HgCl_2$, together with the addition of 1.5 molar equiv of $ZnBr_2$ after the lithiation, the organic zinc reagent thus formed by transmetalation reacted smoothly with PhI under the catalysis of $PdCl_2(PPh_3)_2$ to afford 1,1-diphenylallene in 88% NMR yield (Scheme 2). No reaction was observed with phenyl bromide (entry 2, Table 1). The interesting point here is that even if the monolithiation reaction was performed in the absence of $HgCl_2$, with the addition of $ZnBr_2$, 1,1-diphenylallene was formed in 62% NMR yield (see also entries 10 and 13, Table 1). All these facts indicate the following: (1) $ZnBr_2$, similar to $HgCl_2$, effects the equilibrium between monolithiation and bislithiation of 1-phenyl-1-alkynes;[14,16] (2) $HgCl_2$ has a dramatic effect on the monolithiaton of 1-phenyl-1-

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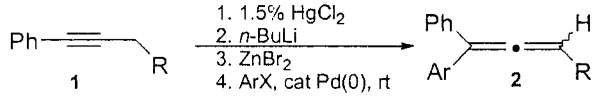
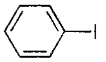
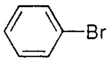
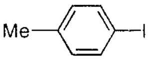
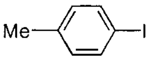
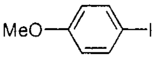
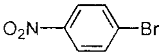
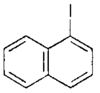
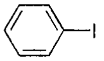
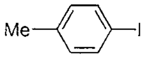
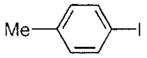
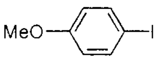
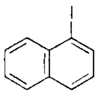
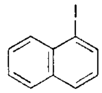
10.1021/jo981315o CCC: $15.00

Table 1. Synthesis of 1,1-Diaryl 1,2-Dienes via the Pd(0)-Catalyzed Coupling Reaction



entry	R	catalyst[a]	ArX	time (h)	product	yield (%)[b]
1	H(**1a**)	B		5	**2a**	83
2	**1a**	B		3.5	**2a**	0
3	**1a**	B		3	**2b**	79
4	**1a**	A		2.5	**2b**	49
5	**1a**	B		8	**2c**	69
6	**1a**	A		7	**2d**	55
7	**1a**	B		3.5	**2e**	55
8[c]	n-C_3H_7 (**1b**)	B		2	**2f**	75
9[c]	**1b**	B		1.5	**2g**	68
10[c,d]	**1b**	B		1.5	**2g**	36
11[c]	**1b**	B		8	**2h**	45
12[c]	**1b**	B		1.5	**2i**	54
13[c,d]	**1b**	B		1.5	**2i**	45

[a] A = $PdCl_2(PPh_3)_2$, B = $Pd(PPh_3)_4$; [b] Isolated yield; [c] The monolithiation reaction was performed at rt for 100 min before the addition of $ZnBr_2$. [d] No $HgCl_2$ was added.

alkynes (Scheme 2, also compare entries 9 /10, 12/13, Table 1).

The ^1H NMR spectrum of the crude product mixture revealed that allene **2a** was the only product formed, while the formation of its regioisomer, 1,3-diphenyl-1-propyne **3a**, was <2%, if any (Scheme 2). Some representative examples are summarized in Table 1. The following points should be noted: (1) the coupling reaction is generally smooth, and the reactivity of $Pd(PPh_3)_4$ is, in most cases, higher than that of $PdCl_2(PPh_3)_2$ (compare entries 3 and 4, Table 1); (2) the $HgCl_2$-catalyzed monolithiation also works for 1-aryl-1-alkynes other than 1-aryl-1-propynes,[14,16] but higher temperature (rt) is required for the lithiation reaction (entries 8–13, Table 1);[15] (3) under the same conditions, alkenyl iodide, i.e., 1-iodo-(1*E*)-hexene, did not afford the corresponding cross-coupling product in decent yield.

A plausible mechanism for this reaction is the oxidative addition reaction of an organic halide with Pd(0) to form an organopalladium intermediate ArPdI, which would be trapped by the allenic zinc reagent **4** and the propargylic zinc reagent **5**[17] formed by the transmetalation reaction of the organolithiums with $ZnBr_2$ to afford the allenic aryl palladium intermediate **6**[18] and the proparglic aryl palladium intermediate **7**, respectively. Rearrangement of **7** to **6**[19] followed by a reductive elimination reaction produced 1,1-diaryl-1,2-diene **2** as the sole product and regenerated the zerovalent Pd catalyst (Scheme 3).

In summary, we have developed an efficient methodology for the mild synthesis of the sterically hindered 1,1-diaryl-1,2-dienes. The scope of this reaction and the regiochemistry to provide the opposite regioisomers, i.e., alkynes **3**, are being investigated in our laboratory.

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[17] Quenching of the reaction mixture of 1-phenyl-1-propyne, *n*-BuLi, $HgCl_2$ (1.5 mol %), and $ZnBr_2$ in THF with water afforded the mixture of 1-phenylpropadiene (44% by NMR) and 1-phenyl-1-propyne (38% by NMR); see the Experimental Section for details.

[18] For a seminal paper, see: Negishi, E.; King, A. O.; Okukado, N. *J. Org. Chem.* **1977**, *42*, 1821. For a most recent review, see: Negishi, E.; Liu, F. In *Metal-Catalyzed Cross-Coupling Reactions*; Stang, P., Diederich, F., Eds.; VCH: Weinheim, 1998; pp 1–47.

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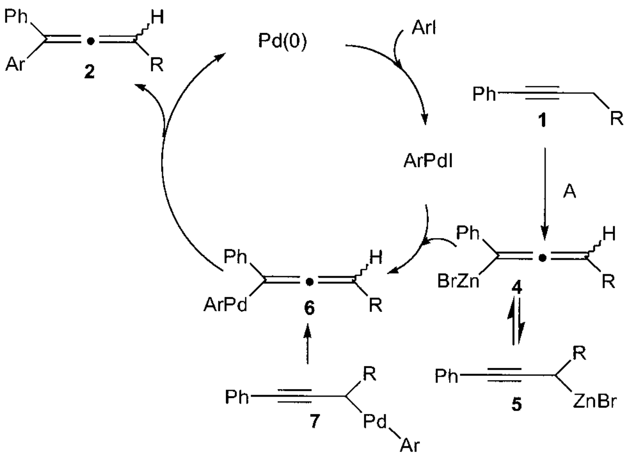
Scheme 3



A = a) 1.5% $HgCl_2$; b) *n*-BuLi; c) $ZnBr_2$

Experimental Section

Materials. *n*-BuLi (from Fluka, 1.6 M in hexanes), bromobenzene, iodobenzene, 1-iodonaphthalene, *p*-methylphenyl iodide, *p*-nitrophenyl bromide, and *p*-methoxyphenyl iodide are commercially available and used as is. ^1H NMR spectra were measured using $CDCl_3$ as the solvent and Me_4Si as the internal standard. The NMR yields were measured using CH_2Br_2 as the internal standard.

Reaction of 1-Phenyl-1-propyne, *n*-BuLi, and Iodobenzene. To a solution of $HgCl_2$ (4 mg, 0.015 mmol, 1.5 mol %) and 1-phenyl-1-propyne (116 mg, 1 mmol) in THF (2 mL) in a dry Schlenk tube was added *n*-BuLi (0.7 mL, 1.6 M in hexanes, 1.1 mmol) at −78 °C under N_2. After 100 min at −78 °C, iodobenzene (224 mg, 1.1 mmol) in THF was added. No reaction was observed after 4 h at room temperature, as monitored by TLC (eluent: petroleum ether (60−90 °C)).

$PdCl_2(PPh_3)_2$-Catalyzed Reaction of Iodobenzene with the Organolithiums Formed by the Reaction of 1-Phenyl-1-propyne and *n*-BuLi in the Presence of 1.5 mol % $HgCl_2$. To a solution of $HgCl_2$ (4 mg, 0.015 mmol, 1.5 mol %) and 1-phenyl-1-propyne (116 mg, 1 mmol) in THF (2 mL) in a dry Schlenk tube was added *n*-BuLi (0.7 mL, 1.6 M in hexanes, 1.1 mmol) at −78 °C under N_2. After 100 min at −78 °C, $PdCl_2(PPh_3)_2$ (36 mg, 0.05 mmol, 5 mol %) and phenyl iodide (224 mg, 1.1 mmol) were added. No reaction was observed after 7 h at room temperature, as monitored by TLC.

$PdCl_2(PPh_3)_2$-Catalyzed Coupling Reaction of Aryl Iodides with Organozincs Formed by the Reaction of 1-Phenyl-1-propyne, *n*-BuLi, and $ZnBr_2$ in the Absence of $HgCl_2$. To a solution of 1-phenyl-1-propyne (116 mg, 1 mmol) in THF (2 mL) in a dry Schlenk tube was added *n*-BuLi (0.7 mL, 1.6 M in hexanes, 1.1 mmol) at −78 °C under N_2. After 100 min at −78 °C, dry $ZnBr_2$ (338 mg, 1.5 mmol) in THF (5 mL) was added. After 10 min at this temperature the reaction mixture was warmed to room temperature for 20 min, $PdCl_2(PPh_3)_2$ (36 mg, 0.05 mmol, 5 mol %) and phenyl iodide (224 mg, 1.1 mmol) were added at room temperature, and the resulting mixture was stirred. After the reaction was complete, as monitored by TLC (eluent: petroleum ether (60−90 °C)), it was quenched with water and extracted with petroleum ether (60−90 °C). Drying over $MgSO_4$ and rotary evaporation afforded 1,1-diphenylpropadiene (**2a**)[13] in 62% NMR yield: liquid; ^1H NMR (300 MHz) δ 5.30 (s, 2H), 7.20−7.50 (m, 10H); MS (*m*/*e*) 192 (M^+, 100); IR (neat) 1938 cm^{-1}.

Pd(0)-Catalyzed Coupling Reaction of Aryl Iodides with Organozincs Formed in the Presence of $HgCl_2$. Synthesis of 1-Pheny-1-(4′-methylphenyl)propadiene (2b). Typical Procedure. To a solution of $HgCl_2$ (4 mg, 0.015 mmol, 1.5 mol %) and 1-phenyl-1-propyne (116 mg, 1 mmol) in THF (2 mL) in a dry Schlenk tube was added *n*-BuLi (0.7 mL, 1.6 M in hexanes, 1.1 mmol) at −78 °C under N_2. After 100 min at −78 °C, dry $ZnBr_2$ (338 mg, 1.5 mmol) in THF (5 mL) was added. After 10 min at this temperature, the reaction mixture was warmed to room temperature for 20 min, and $Pd(PPh_3)_4$ (58 mg, 0.05 mmol, 5 mol %) and *p*-methylphenyl iodide (262 mg, 1.2 mmol) were added. After the reaction was complete, as monitored by TLC (eluent: petroleum ether (60−90 °C)), it was quenched with water and extracted with petroleum ether (60−90 °C). Drying over $MgSO_4$, rotary evaporation, and chromatography on silica gel (eluent: petroleum ether (60−90 °C)) afforded 163 mg (79%) of 1-phenyl-1-(4′-methyl-phenyl)propadiene (**2b**): liquid; ^1H NMR(300 MHz) δ 2.39 (s, 3H), 5.26 (s, 2H), 7.10−7.45 (m, 9H); MS (*m*/*e*) 206 (M^+, 100); IR (neat) 1940 cm^{-1} ; HRMS calcd for $C_{16}H_{14}$ 206.1092, found 206.1092.

The following compounds were prepared similarly; the catalyst used and reaction time were listed in Table 1.

1,1-Diphenylpropadiene (**2a**) was isolated in 83% yield.

1-Phenyl-1-(4′-methoxylphenyl)propadiene (2c): yield 69%; liquid; ^1H NMR(300 MHz) δ 3.80 (s, 3H), 5.32 (s, 2H), 6.90-(d, *J* = 6.82 Hz, 2H), 7.20−7.40 (m, 7H); ^{13}C NMR δ 209.74, 159.01, 136.63, 129.61, 128.48, 128.42, 127.25, 127.19, 114.07,108.76, 77.89, 55.18; MS (*m*/*e*) 222 (M^+, 100); IR (neat) 1939 cm^{-1}; HRMS calcd for $C_{16}H_{14}O$ 222.1041, found 222.1048.

1-Phenyl-1-(4′-nitrophenyl)propadiene (2d): yield 55%; liquid; ^1H NMR (300 MHz) δ 5.38 (s, 2H), 7.25−7.45 (m, 5H), 7.50 (d, *J* = 8.71 Hz, 2H), 8.18 (d, *J* = 8.72 Hz, 2H); MS (*m*/*e*) 237 (M^+, 100); IR (neat) 1920 cm^{-1}; HRMS calcd for $C_{15}H_{11}NO_2$ 237.0787, found 237.0787.

1-Phenyl-1-(1′-naphthyl)propadiene (2e): yield 55%; liquid; ^1H NMR (300 MHz) δ 5.23 (s, 2H), 7.10−7.60 (m, 9H), 7.80−7.95 (m, 3H); MS (*m*/*e*) 242 (M^+, 70.64), 241 (100); IR (neat) 1930 cm^{-1}; HRMS calcd for $C_{19}H_{14}$ 242.1092, found 242.1115.

For the synthesis of compounds **2f**−**i**, the monolithiation was carried out at room temperature.

1,1-Diphenyl-1,2-hexadiene (2f): yield 75%; liquid; ^1H NMR (300 MHz) δ 1.04 (t, *J* = 7.35 Hz, 3H), 1.50−1.80 (m, 2H), 2.45−2.65 (m, 2H), 6.55 (t, *J* = 3.05 Hz,1H), 7.10−7.60 (m, 10H); MS (*m*/*e*) 234 (M^+, 16.42), 205 (100); IR (neat) 1928 cm^{-1}; HRMS calcd for $C_{18}H_{18}$ 234.1404, found 234.1413.

1-Phenyl-1-(4′-methylphenyl)-1,2-hexadiene (2g): yield 68%; liquid; ^1H NMR (300 MHz) δ 1.02 (t, *J* = 7.35 Hz, 3H), 1.55−1.75 (m, 2H), 2.35 (s, 3H), 2.45−2.65 (m, 2H), 6.53 (t, *J* = 3.05, 1H), 7.05−7.45(m, 9H); MS(*m*/*e*) 248 (M^+, 50.88), 205 (100); IR (neat) 1926 cm^{-1}; HRMS calcd for $C_{19}H_{20}$ 248.1560, found 248.1570.

1-Phenyl-1-(4′-methoxylphenyl)-1,2-hexadiene (2h): yield 45%; liquid; ^1H NMR (300 MHz) δ 1.02 (t, *J* = 7.35 Hz, 3H), 1.50−1.75 (m, 2H), 2.40−2.65 (m, 2H), 3.82 (s, 3H), 6.53 (t, *J* = 3.05 Hz, 1H), 6.87 (d, *J* = 6.82 Hz, 2H), 7.15−7.45 (m, 7H); MS (*m*/*e*) 264 (M^+, 100); IR (neat) 1935 cm^{-1}; HRMS calcd for $C_{19}H_{20}O$ 264.1059, found 264.1515.

1-Phenyl-1-(1′-naphthyl)-1,2-hexadiene (2i): yield 54%; liquid; ^1H NMR (300 MHz) δ 1.03 (t, *J* = 7.31 Hz, 3H), 1.55−1.80 (m, 2H), 2.45−2.86 (m, 2H), 6.35 (t, *J* = 2.95 Hz, 1H), 7.18−7.65 (m, 9H), 7.70−7.95 (m, 2H), 8.20−8.30 (m, 1H); MS (*m*/*e*) 284 (M^+, 41.92), 241 (100); IR (neat) 1939 cm^{-1}; HRMS calcd for $C_{22}H_{20}$ 284.1560, found 284.1565.

Quenching of the Reaction Mixture of Allenylzinc Bromide and Propargylzinc Bromide with H_2O. To a solution of $HgCl_2$ (4 mg, 0.015 mmol, 1.5 mol %) and 1-phenyl-1-propyne (116 mg, 1 mmol) in THF (2 mL) in a dry Schlenk tube was added *n*-BuLi (0.7 mL, 1.6 M in hexanes, 1.1 mmol) at −78 °C under N_2. After 100 min at −78 °C, dry $ZnBr_2$ (338 mg, 1.5 mmol) in THF (5 mL) was added. After 10 min at this temperature, the reaction mixture was warmed to room temperature for 20 min, quenched with water, extracted with diethyl ether, and dried over $MgSO_4$. Rotary evaporation afforded the crude products, which were analyzed by ^1H NMR spectroscopy using CH_2Br_2 as the internal standard. 1-Phenylpropadiene:[20] yield 44% by NMR; ^1H NMR (300 MHz) δ 5.10 (d, *J* = 6.75 Hz, 2H), 6.10 (t, *J* = 6.75 Hz, 1H), 7.05−7.30 (m, 5H). 1-Phenyl-1-propyne: yield 38% by NMR.

Acknowledgment. We thank the NNSF of China, Laboratory of Organometallic Chemistry, Chinese Academy of Sciences, and Shanghai Institute of Organic Chemistry for financial support.

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(20) Skattebol, L. *Acta Chem. Scand.* **1963**, *17*, 1683.

Supporting Information Available: The ^{1}H NMR spectra of the compounds **2b**−**i** (9 pages). This material is contained in libraries on microfiche, immediately follows this article in the microfilm version of the journal, and can be ordered from the ACS; see any current masthead page for ordering information.

JO981315O

Additions and Corrections

Vol. 63, 1998

Franklin, A. Davis,* Ping Zhou, Christopher K. Murphy, Gajendran Sundarababu, Hongyan Qi, Wei Han, Robert M. Przeslawski, Bang-Chi Chen, and Patrick J. Carroll . Asymmetric Fluorination of Enolates with Nonracemic *N*-Fluoro-2,10-Camphorsultams.

Page 2275. A number of the compound signs in Table 1 were incorrect. A corrected table follows.

Table 1. Fluorination of Camphorsultams 5 to *N*-Fluorocamphorsultams 3 at −40 °C for 1.5 h

entry	sultam	conditions concentration/solvent	products (% yield)	δ(^{19}F) ppm of **3** (*J*, Hz)
1	(−)-**5a** (X = H)	(0.1 M)/1:1 CHCl$_3$:CFCl$_3$	(−)-**3a** (67) [75%]	−65.5 (br, s)
2	(−)-**5b** (X = Cl)	(0.1 M)/1:1 CHCl$_3$:CFCl$_3$	(−)-**3b** (67), **6b** (13), (−)-**7** (5)	−53.9 (48.4)
3		(0.2 M)/1:1 CHCl$_3$:CFCl$_3$	(−)-**3b** (56), **6b** (9), (−)-**7** (11)	
4	(+)-**5b** (X = Cl)	(0.2 M)/1:1 CHCl$_3$:CFCl$_3$	(+)-**3b** (56), **6b** (12), (−)-**7** (10)	
5		(0.4 M)/1:1 CHCl$_3$:CFCl$_3$	(+)-**3b** (58), **6b** (11), (−)-**7** (12)	
6		(0.2 M)/CHCl$_3$	(+)-**3b** (67), **6b** (7), (−)-**7** (11)	
7		(0.2 M)/4:5:1 CHCl$_3$:CFCl$_3$:EtOH	(+)-**3b** (35), **6b** (0), (−)-**7** (0)	
8	(−)-**5c** (X = OMe)	(0.2M)/1:1 CHCl$_3$:CFCl$_3$	(−)-**3c** (25), **6c** (35)	−55.6 d (44.0)
9	(+)-**5c** (X = OMe)	(0.2M)/1:1 CHCl$_3$:CFCl$_3$	(+)-**3c** (31), **6c** (40)	
10	(+)-**5c** (X = OME)	(0.2M) CHCl$_3$	(+)-**3c** (42), **6c** (21)	
11	(+)-**5c** (X = OME)	(0.6M) CHCl$_3$	(+)-**3c** (34), **6c** (33)	

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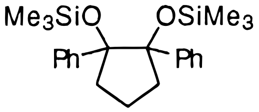
Toshikazu Hirao,* Motoki Asahara, Yasuaki Muguruma, and Akiya Ogawa. Highly Diastereoselective Pinacol Coupling of Secondary Aliphatic Aldehydes Induced by a Catalytic System Consisting of Vanadium Complex, Chlorosilane, and ZincMetal.

Page 2813, eq 2. The diastereoselectivity of structure **4** should be drawn as follows:



4

(*dl*/*meso* = 9/91)

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Tushar A. Kshirsagar* and Laurence H. Hurley. A Facile Synthesis of 5-Mesyl-3-benzylbenz[*e*]indole: Implications for the Involvement of a *p*-Quinone Methide Intermediate.

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