[2 + 4] Cycloadditions between germenes and .alpha.-ethylenic aldehydes and ketones: a route to germaoxacyclohexenes

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(*E*)-**2** (R = $CH_3(CH_2)_2$), 42067-72-1; (*E*)-**2** (R = $CH_3(CH_2)_4$), 31930-43-5; (*E*)-**2** (R = *n*-BuO), 138090-55-8; (*Z*)-**2** (R = *n*-BuO), 138090-56-9; (*E*)-**2** (R = $CH_3(CH_2)_6$), 90584-19-3; (*E*)-**2** (R = C_6H_5), 104014-92-8; (*E*)-**2** (R = *p*-$CH_3OC_6H_4$), 138090-59-2; **3** (R = $CH_3(CH_2)_2$), 13810-04-3; **3** (R = $CH_3(CH_2)_4$), 10175-53-8; **3** (R = $CH_3(CH_2)_6$), 18408-00-9; **3** (R = C_6H_5), 13183-69-2; **3** (R = *p*-$CH_3OC_6H_4$), 138090-52-5; **3** (R = *n*-BuO), 138090-53-6; **4**, 14355-62-5; **5**, 87555-71-3; **6**, 21209-32-5; **7**, 104014-91-7; **8**, 10399-74-3; $Rh_2(pfb)_4$, 73755-28-9; $Rh_2(oct)_4$, 73482-96-9; Et_3SiH, 617-86-7; $CH_3(CH_2)_2CH_2CH{=}CH_2$, 592-41-6; $CH_3(CH_2)_4CH_2CH{=}CH_2$, 111-66-0; $CH_3(CH_2)_6CH_2CH{=}CH_2$, 872-05-9; $C_6H_5CH_2CH{=}CH_2$, 300-57-2; *p*-$CH_3OC_6H_4CH_2CH{=}CH_2$, 140-67-0; *n*-$BuOCH_2CH{=}CH_2$, 3739-64-8; $PhCH{=}CH_2$, 100-42-5; $H_2C{=}CHCOOEt$, 140-88-5.

[2 + 4] Cycloadditions between Germenes and α-Ethylenic Aldehydes and Ketones: A Route to Germaoxacyclohexenes

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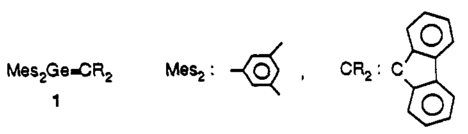
Dimesityl(fluorenylidene)germene (1) reacts with various α-ethylenic aldehydes and ketones to afford, by a [2 + 4] cycloaddition, the six-membered-ring heterocycles 2–7. Hydrolysis of these germaoxacyclohexenes leads to germylated aldehydes and ketones.

Introduction

Organometallic alkenes, such as silenes >Si=C<[1] and germenes >Ge=C<,[2] are now intensively studied. However, nothing is known about their reactivity toward α-ethylenic aldehydes and ketones, except the reaction between a silene and cyclopentadienones performed by Märkl.[3] Moreover, both [2 + 2] and [2 + 4] cycloadditions have been observed by Wiberg[4] in the reactions between transient silenes and germenes and benzophenone, which, in this case, behaves as a conjugated ketone.

We describe in this paper the reactivity of dimesityl(fluorenylidene)germene (1)[5] toward some α-ethylenic aldehydes (acrolein, methacrolein, and crotonaldehyde) and α-ethylenic ketones (methyl vinyl ketone, mesityl oxide, and tetraphenylcyclopentadienone).

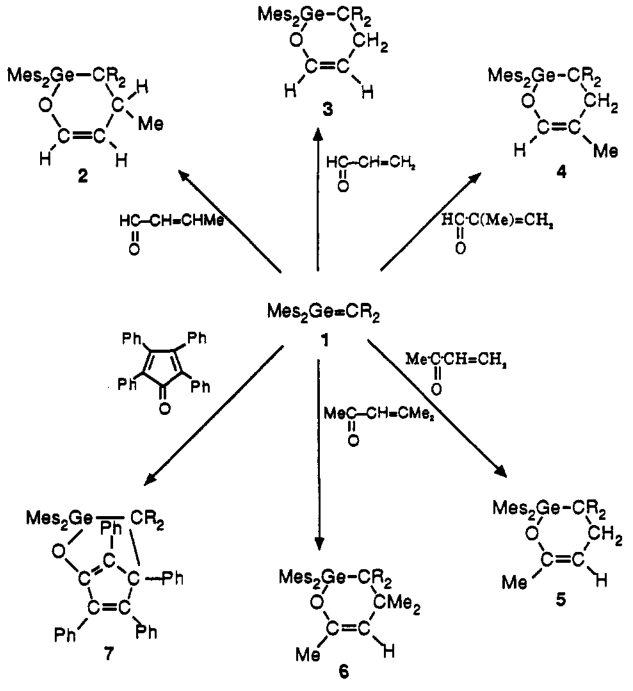


Results and Discussion

Two reactions could occur: [2 + 2] cycloaddition to the carbonyl group leading to germaoxetanes (I) or [2 + 4] cycloaddition with the formation of the corresponding six-membered rings (II).

Although these carbonyl derivatives have differing steric and electronic properties, particularly different electronic charges on carbons 2 and 4,[6] we have observed in all cases

Scheme I



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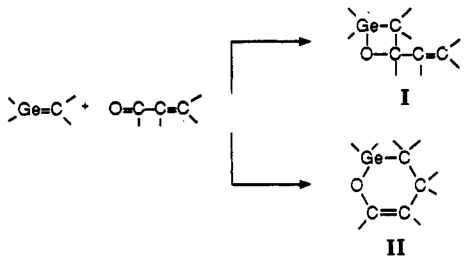


exclusive [2 + 4] cycloaddition leading to the corresponding six-membered germaoxacyclohexenes 2–7 (Scheme I).

All the reactions are facile and occur between −78 °C and room temperature, except in the case of tetraphenylcyclopentadienone, which requires 1 h heating in refluxing ether. The germaoxacyclohexenes 2–7 have been unambiguously characterized by NMR (see Tables I and II), IR (see Table IV), and mass spectroscopy (see Table III) and also by their chemical reactivity.

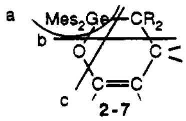
In the ^{13}C NMR spectra, the ethylenic carbon bonded to oxygen shows the expected characteristic low-field chemical shift (between 142 and 170 ppm). In germaoxetanes of type I, the carbon bonded to oxygen would be at higher field, around 80–90 ppm (for example 87.24 ppm in the case of the silaoxetane obtained by Märkl in the reaction between a silene and tetraphenylcyclopentadienone[3]). Moreover, only one signal is observed between 80 and 100 ppm for the ethylenic carbons, instead of the two expected in the region for four-membered rings I.

The large steric hindrance in these germaoxacyclohexenes is clearly demonstrated in their ^1H NMR spectra. At room temperature we observe for compounds 3–5 and 7 a slow rotation of the two mesityl groups, which appear as very broad signals about 1–1.20 ppm wide. In the case of 2, the rotation of one mesityl group is hindered (two singlets at 1.16 and 2.68 ppm for the inequivalent *o*-Me groups) whereas a very broad singlet is observed for the other mesityl groups. At −45 °C the NMR spectrum displays four singlets for the *o*-Me groups at 1.16, 1.72, 2.75, and 3.17 ppm.

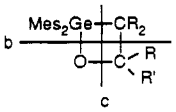
In the case of 6, which has the greatest steric hindrance, the rotation of both mesityl groups is hindered. We observe at room temperature nine signals between 0.33 and 3.17 ppm corresponding to the nine methyl groups. At 70 °C the signals at 3.17 and 1.95 ppm coalesce to a very broad singlet.

The two methyl groups on the carbon bonded to the fluorenyl group are very different (0.33 and 1.72 ppm). Because of the large steric hindrance, there must be folding of the ring, which results in very different positions of the methyl groups in relation to the fluorenyl group.

In mass spectroscopy, the most important fragment is always, except for 7, the germylene $[Mes_2Ge]^+$ (see Table III); the latter can arise from the germene $Mes_2Ge{=}CR_2$, observed in most cases (fragmentation b), but also, more



2-7



I

likely, from a [6] → [5 + 1] decomposition, since the $R_2CCC{=}CO$ moieties also are observed (fragmentation a). So it seems that the two types of fragmentation, a and b, occur in germaoxacyclohexenes 2–7; the cleavage according to c appears as a minor one, since $[Mes_2Ge{=}O]^+$ is only observed for 2 and 4. There is a great difference in the mass spectroscopy of four-membered heterocycles I (RR'

Table I. ^1H NMR Spectral Data (ppm) for Derivatives 2–7[a]

solvent	toluene-d_8	$CDCl_3$	$CDCl_3$	$CDCl_3$	C_6D_6	C_6D_6
compd	**2**	**3**	**4**	**5**	**6**	**7**
R_2CCMe	0.16 (d, $^3J_{HH}$ = 6.1 Hz)				0.33, 1.72	
o-Me	1.16, 2.68	1.73–2.46 (br s)	1.89 (br s)	1.23–2.55 (br s)	1.16, 1.96, 2.77, 3.17	1.19, 2.29 (br s), 2.92
C=CMe			1.56 (d, $^4J_{HH}$ = 1.3 Hz)	2.00 (d, $^4J_{HH}$ = 0.7 Hz)	2.15 (d, $^4J_{HH}$ = 0.8 Hz)	
p-Me	2.04, 2.26	2.27	2.24	2.23	2.01, 2.25	1.77, 1.92
R_2CCH_2 or R_2CCH	3.51–3.57 (m)	1.73–2.46 (m)	2.24–2.94 (m)	1.23–2.55 (m)		
OC=CH	4.42 (dd, $^3J_{HH}$ = 2.0 and 6.0 Hz)	4.85 (dt, $^3J_{HH}$ = 6.0 and 6.1 Hz)		4.65 (tq, $^3J_{HH}$ = 4.4, $^4J_{HH}$ = 0.7 Hz)	4.44 (q, $^4J_{HH}$ = 0.8 Hz)	
OCH=C	6.82 (dd, $^3J_{HH}$ = 6.0 Hz, $^4J_{HH}$ = 2.8 Hz)	6.91 (dt, $^3J_{HH}$ = 6.0, $^4J_{HH}$ = 1.5 Hz)	6.73 (m)			
H (arom Mes)	6.28, 6.52	6.77	6.73	6.72 (br s)	6.34, 6.59	6.39, 6.54
CR_2 Ph	6.62–7.97 (m)	7.11–7.96 (m)	7.10–7.92 (m)	7.06–7.90 (m)	6.87–7.83 (m)	6.00–7.95 (m)

[a] All signals without multiplicity are singlets.

Table II. ^{13}C NMR Spectral Data (ppm) (Solvent $CDCl_3$) for Derivatives 2–7

	2	3	4	5	6	7
p-Me	20.85, 21.16, 22.81	21.09	20.05 or 21.04	20.99	20.86, 21.18	20.75, 20.91
o-Me	22.96, 23.17	22.98	22.94	23.27	22.24, 22.90, 23.31, 24.13	23.63, 23.74
*Me*C=C			21.04 or 20.05	20.99	24.76	
MeCCR_2	15.34				26.35, 29.92	
CH_2		33.75	39.44	34.60		
R_2*C*Me	35.41				40.14	
CR_2 (*C*Ph)	52.76	47.96	47.62	48.10	56.51	62.74 (70.23)
OC=*C*	107.97	101.03	108.23	96.12	108.73	
O*C*=C	146.71	147.93	142.14	153.20	149.83	170.48

Table III. Mass Spectroscopy Data for 2–7 (EI, 70 eV, ^{74}Ge)

	m/e	Fragments	Rel. Int. %
2	546	M	10
	476	$Mes_2Ge{=}CR_2$	70
	329	$Mes_2Ge{=}O + H$	4
	327	Mes $Ge{=}CR_2$	2
	311	$Mes_2Ge - 1$	100
	235	$R_2CCH(Me)CHCHO + 1$	10
	220	R_2CCH CH CHO+1	10
	119	Mes	6
3	532	M	35
	313	Mes_2Ge • 1	100
	220	R_2CCH_2CH CHO	6
	203	R_2CCH_2C CH	5
	191	R_2CCH_2CH	30
	119	Mes	19
4	546	M	29
	476	$Mes_2Ge{=}CR_2$	11
	329	$Mes_2Ge{=}O + H$	8
	313	$Mes_2Ge + 1$	100
	235	$R_2CCH_2C(Me)CHO + 1$	8
	220	R_2CCH_2CCHO +1	12
	191	R_2CCH_2CH	37
5	546	M	5
	476	$Mes_2Ge{=}CR_2$	8
	313	$Mes_2Ge + 1$	100
	235	$R_2CCH_2CHC(Me)O + 1$	10
	220	$R_2CCH_2CHCO + 1$	15
6	574	M	4
	476	$Mes_2Ge{=}CR_2$	90
	311	$Mes_2Ge - 1$	100
	297	$Mes_2Ge{-}Me$	10
7	861	M +1	100
	741	M - Mes	10
	476	$Mes_2Ge{=}CR_2$	9
	385	$M - Mes_2Ge{=}CR_2$	25

Table IV. IR Data (cm^{-1}) for 2–7 ($CDCl_3$)

	6	2	3	5	4	7
ν(Ge—O)	1025.1	1023.0	1036.1	996.7	1030.4	1110.5
ν(C=C)	1670.1	1638.0	1634.7	1669.1	1665.5	1623.2

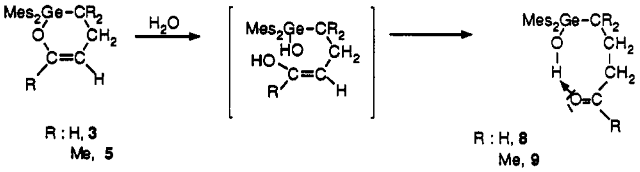
Table V. NMR (ppm) and IR (cm^{-1}) Data for 8 and 9

	8	9
	^1H NMR ($CDCl_3$)	
CH_3		1.10 (s)
*CH_2*CR_2	1.21–1.52 (m)	1.18–1.38 (m)
p-Me	2.22 (s)	2.02 (s)
o-Me	1.93 (s)	2.09 (s)
CH_2CO	3.00–3.19 (m)	3.31–3.49 (m)
H arom Mes	6.72 (s)	6.51 (s)
CR_2	7.52–7.96 (m)	7.00–7.84 (m)
CHO	9.28 (t, $^3J_{HH}$ = 1.5 Hz)	
	^{13}C NMR ($CDCl_3$)	
p-Me	20.97	20.94
o-Me	23.48	23.45
CH_2CR_2	28.19	29.53
Me		29.59
CH_2CO	38.13	37.28
CR_2	54.85	55.10
C_4, C_5	119.68	119.59
C_1, C_2, C_3, C_6, C_7, C_8	124.58, 126.96, 127.19	124.63, 126.70, 127.07
m-C Mes	129.36	129.28
p-C Mes, C_{10}, C_{11}	139.19, 141.93	139.07, 141.62
o-C Mes, C_{12}, C_{13}	142.96, 146.95	142.95, 147.16
C=O	202.05	208.61
	IR	
ν(OH)	3625.8 (free), 3416.1 (assoc)	3610.0 (free), 3447.6 (assoc)
ν(C=O)	1720.2	1708.0

= Ph_2, HPh),[7] where germanone $Mes_2Ge{=}O$ is the most important fragment.

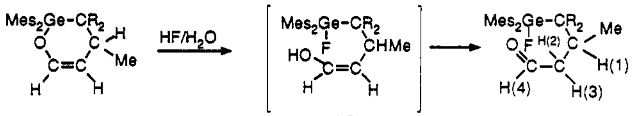
Derivatives 2–7 have also been characterized by IR spectroscopy, which shows, besides the expected ν(C=C), strong bands generally round 1020 cm^{-1} attributable to the Ge–O valence vibration (see Table IV).

The structure of the adducts 2–7 also is supported by some of their chemical conversion. For example, hydrolysis of 3 leads to the corresponding aldehyde 8, whereas ketone 9 is obtained from 5.



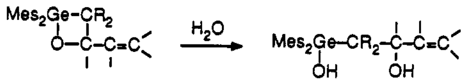
The ^1H NMR spectrum of 9 (see Table V), shows very different chemical shifts for the methyl (1.10 ppm) and methylene (3.31–3.49 ppm) groups bonded to the carbon of the carbonyl group. This phenomenon can be explained by the existence of a pseudocyclic structure due to a hydrogen bond between carbonyl oxygen, and the hydrogen of germanol, involving very different positions of these two groups particularly toward the fluorenyl. This hypothesis is confirmed by the IR spectrum, which shows both free and associated OH bands. This pseudocyclic structure can also be postulated for 8, which presents the same type of IR spectrum between 3400 and 3700 cm^{-1} and also ^1H NMR spectrum with a rather low-field CH_2 signal (3.00–3.19 ppm).

Heterocycles 2, 4, 6, and 7 are less sensitive to hydrolysis. For example, in the case of 2, the germanium–oxygen bond is only cleaved by hydrofluoric acid, leading to the corresponding aldehyde 11, via the enolic form intermediate 10.



2 10 11

The hydrolysis reaction provides good proof for the six-membered-ring structure, since with germaoxetanes I, only β-diols would be obtained:



Experimental Section

Solutions of germene 1 are highly air and moisture sensitive, so the synthesis and the handling of 1 require high-vacuum line techniques and use of carefully deoxygenated solvents which must be freshly distilled over sodium benzophenone. ^1H NMR spectra were recorded on Bruker AC 80, AC 200, and AM 300 WB instruments, respectively, at 80.1, 200.1, and 300.1 MHz. ^{13}C NMR spectra were recorded on Bruker AC 200 and AC 250 instruments, respectively, at 50.3 and 62.9 MHz (TMS internal standard). IR

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spectra were recorded on a Perkin-Elmer 1600 instrument (FT). Mass spectra were measured on a Nermag R 10 010 spectrometer by EI at 70 eV. Melting points were determined on a Reichert apparatus. Elemental analyses were performed by the "Service de microanalyse de l'Ecole de Chimie de Toulouse" (Toulouse, France).

Germene 1 was synthesized as previously described[5] by addition of 1 molar equiv of *tert*-butyllithium (1.7 N in pentane) to a solution of the fluorogermane $Mes_2Ge(F)CHR_2$ in Et_2O, cooled at −78 °C. Warming to room temperature afforded an orange solution of the germene, which is nearly quantitatively produced in this reaction along with a precipitate of lithium fluoride. The reactions with aldehydes and ketones can be performed with the crude solution of 1 without further purification or also with the pure germene, which can be obtained after filtration of LiF and recrystallization from pentane.

In both cases the final yields are about the same, but reactions from pure germene are generally slightly cleaner.

Reaction of 1 with Acrolein. A solution of acrolein (0.26 g, 4.62 mmol) in pentane (3 mL) was added slowly to an orange solution of germene (2.20 g, 4.62 mmol) in Et_2O (20 mL) cooled at −78 °C. The reaction mixture rapidly turned red but became colorless after being warmed to room temperature. After removal of solvents in vacuo, crude **3** was recrystallized from pentane to give 1.82 g of white crystals of **3** (74%), mp 210–211 °C.

Anal. Calcd for $C_{34}H_{34}GeO$: C, 76.87; H, 6.45. Found: C, 76.61; H, 6.38.

Hydrolysis of 3. A 1.10-g sample of **3** (2.02 mmol) was dissolved in 5 mL of THF. After addition of a stoichiometric amount of water, the reaction mixture was stirred for 1 week. NMR analysis showed complete hydrolysis of **3**. THF was removed in vacuo, giving crude **8**, which was recrystallized from pentane to give 0.90 g of white crystals (mp 199–200 °C), 79%.

Anal. Calcd for $C_{34}H_{36}GeO_2$: C, 74.35; H, 6.61. Found: C, 74.30; H, 6.56.

Reaction of 1 with Methacrolein. To a solution of germene 1 (1.25 g, 2.62 mmol) in Et_2O (15 mL) cooled at −78 °C was added via a syringe a solution of methacrolein (0.18 g, 2.62 mmol) in Et_2O (5 mL). The reaction mixture turned brown and then, after 3 h at room temperature, nearly colorless. After removal of Et_2O in vacuo, recrystallization from pentane afforded 1.18 g of white crystals of **4** (83%), mp 195–196 °C.

Anal. Calcd for $C_{35}H_{36}GeO$: C, 77.03; H, 6.66. Found: C, 77.27; H, 6.71.

Reaction of 1 with Crotonaldehyde. A solution of crotonaldehyde (0.20 g, 2.83 mmol) in Et_2O (15 mL) was added slowly to a solution of germene 1 (1.35 g, 2.83 mmol) cooled at −78 °C. The solution turned violet and then gradually became yellow on stirring at room temperature. After 3 h, Et_2O was removed in vacuo. White crystals of **2** (0.78 g) were obtained by crystallization from pentane, mp 209–210 °C, 69%.

Anal. Calcd for $C_{35}H_{36}GeO$: C, 77.09; H, 6.66. Found: C, 77.32; H, 6.78.

Reaction of 2 with Hydrofluoric Acid. To a solution of **2** (0.70 g, 1.25 mmol) in THF (5 mL) was added a 10% excess of a solution of 40% hydrofluoric acid in water (70 mg). The reaction mixture was heated for 1 h at reflux, and then the solvent was eliminated in vacuo and replaced by pentane. After drying over Na_2SO_4, crystallization from pentane gave 0.46 g of white crystals of **11** (64%), mp 176–177 °C.

^1H NMR (C_6D_6): δ 0.78 (d, $^3J_{HH} = 6.6$ Hz, 3 H, Me), 1.67 (ddd, $^2J_{H(2)H(3)} = 17.5$ Hz, $^3J_{H(2)H(1)} = 10.2$ Hz, $^3J_{H(2)H(4)} = 2.0$ Hz, 1 H, H(2)), 1.95 (s, 3 H, *p*-Me), 1.97 (s, 3 H, *p*-Me), 2.07 (s, 6 H, *o*-Me), 2.11 (s, 6 H, *o*-Me), 2.47 (dd, $^2J_{H(3)H(2)} = 17.5$ Hz, $^3J_{H(3)H(1)} = 1.7$ Hz, 1 H, H(3)), 4.07 (qdd, $^3J_{H(1)Me} = 6.6$ Hz, $^3J_{H(1)H(2)} = 10.2$ Hz, $^3J_{H(1)H(3)} = 1.7$ Hz, 1 H, H(1)), 6.54 (s, 2 H, arom Mes), 6.56 (s, 2 H, arom Mes), 6.98–7.74 (m, 8 H, CR_2), 9.13 (d, $^3J_{H(4)H(2)} = 2.0$ Hz, 1 H, CH=O). IR: ν(C=O) 1720 cm^{-1}.

Anal. Calcd for $C_{35}H_{37}FGeO$: C, 74.37; H, 6.60. Found: C, 74.50; H, 6.68.

Reaction of 1 with Methyl Vinyl Ketone. Methyl vinyl ketone (0.22 g, 3.15 mmol) in solution in Et_2O (5 mL) was added to a solution of germene 1 (1.50 g, 3.15 mmol) cooled at −78 °C. After warming of the mixture to room temperature, the starting orange solution gradually turned colorless. Recrystallization from Et_2O afforded 1.41 g of white crystals of **5** (82%), mp 290 °C.

Anal. Calcd for $C_{35}H_{36}GeO$: C, 77.09; H, 6.66. Found: C, 76.79; H, 6.38.

Hydrolysis of 5. A stoichiometric amount of water was added to a solution of **5** (1.30 g, 2.38 mmol) in 50/50 THF/Et_2O. After 1 h of stirring at room temperature, solvents were removed in vacuo. Crystallization from pentane afforded 0.89 g (66%) of white crystals of **9**, mp 205–206 °C.

Anal. Calcd for $C_{35}H_{38}GeO_2$: C, 74.63; H, 6.80. Found: C, 74.41; H, 6.61.

Reaction of 1 with Mesityl Oxide. To a solution of germene 1 (2.10 g, 4.41 mmol) in Et_2O was added a solution of mesityl oxide (0.43 g, 4.41 mmol). The reaction mixture immediately turned from orange to dark brown. Five hours of stirring were necessary for the completion of the reaction. Removal of solvent in vacuo from the light yellow solution afforded crude **6**. Recrystallization from pentane gave 2.01 g of white crystals (66%) of **6**, mp 234–235 °C.

Anal. Calcd for $C_{37}H_{40}GeO$: C, 77.51; H, 7.03. Found: C, 77.38; H, 6.91.

Reaction of 1 with Tetraphenylcyclopentadienone. To 1.20 g (2.52 mmol) of germene 1 in Et_2O (10 mL) was added 1 equiv of tetraphenylcyclopentadienone (0.97 g). The reaction mixture was refluxed for 1 h and became red. After removal of Et_2O in vacuo, crystallization in pentane afforded 1.75 g of white crystals of **7** (80%), mp 197–198 °C.

Anal. Calcd for $C_{60}H_{50}GeO$: C, 83.83; H, 5.86. Found: C, 83.82; H, 6.03.

Registry No. 1, 108946-03-8; 2, 138152-29-1; 3, 138152-30-4; 4, 138152-31-5; 5, 138152-32-6; 6, 138152-33-7; 7, 138152-34-8; 8, 138152-35-9; 9, 138152-36-0; 11, 138152-37-1; HC(O)CH=CHMe, 4170-30-3; HC(O)CH=CH_2, 107-02-8; HC(O)C(Me)=CH_2, 78-85-3; MeC(O)CH=CH_2, 78-94-4; MeC(O)CH=CMe_2, 141-79-7; tetraphenylcyclopentadienone, 479-33-4.