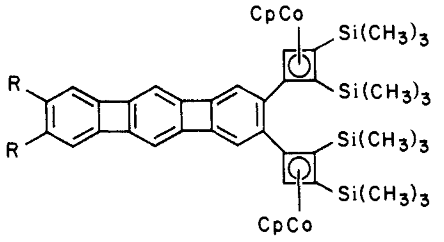
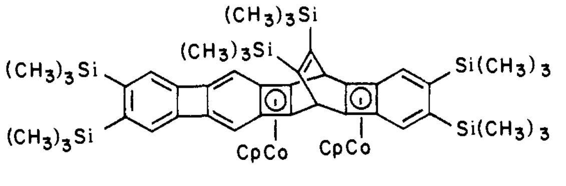


6 (R = H)
7 [R = $(CH_3)_3Si$]



8

The structural assignment of **8** is based on analytical and spectral data, particularly comparison of the ^1H NMR spectrum with that of model compounds.[6,9,10,12] Compound **8** constitutes the first example of a (formal) Diels–Alder-type addition to the phenylene nucleus, signaling increasing reactivity along the series, as in the acenes.[2,11] This conclusion is corroborated by the tenacity with which the [4]phenylene nucleus holds on to complexed CpCo, both desired cyclization products emerging initially attached to the metal. On the basis of models[10a,12] and symmetry (for **3b**–CpCo) the cobalt unit must be complexed to the central ring, maximizing aromatic character[13] in the system. Decomplexation with CO (Schemes I and II) furnished **3** as deep red-brown, very air-sensitive solids which decomposed on attempted melting point determination.

On cyclobutabenzoannulation of [3]phenylene **1** (N = 3) the UV spectrum[9] experiences strong bathochromic shifts ($\Delta\lambda_{max}$ = 52 nm for the highest wavelength band) as predicted by theory[2,14] and clearly indicative of through-conjugation. Particularly instructive are the ^1H NMR spectra of **3a** and **3b**[9] in comparison with those of its analogue **1** (N = 3).[1] While the outside benzene ring hydrogens have approximately the *same* chemical shifts, their inside counterparts experience a noticeable upfield movement when going from the [3]- to the [4]phenylene nucleus. A possible interpretation of this finding is that the outside benzenes attempt to maximize their aromatic character at the expense of that in the other two. In support of this conclusion, the chemical shift of H^3 in 1,2-bis(trimethylsilyl)benzocyclobutadiene (**9**)[10a] is δ 5.75, almost identical with those of H^5 and H^6 in **3a**. Striking is the effect of CpCo complexation on the chemical shift of the hydrogens in **3**,[9] all nuclei undergoing deshielding in increments ranging from 0.32 to 0.99 pm, pointing to substantial "aromatization" of the system[13] as also observed for **9**.[10a] Unprecedented is the remote effect on the outside rings, the molecule now appearing to adopt a "double biphenylenoid" electronic structure.[15] It thus appears that in the phenylenes, the properties of local π-electronic circuits override those expected based on the total π-electron count.[16] The preparation of [5]phenylene, currently under way, is necessary to clarify this point.

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Registry No. 1 (N = 2; $R^1 = R^2$ = H; $R^3 = R^4 = C_2H$), 87710-28-9; 1 (N = 3; $R^1 = R^2$ = H; $R^3 = R^4$ = Sn), 101471-34-5; **1** (N = 2; $R^1 = R^2 = R^3 = R^4$ = Br), 62754-84-1; **3a**, 101471-35-6; **3b**, 101471-37-8; **4**, 101471-38-9; **5**, 101471-36-7; **6**, 101471-39-0; **7**, 101471-40-3; **8**, 101471-41-4; $(CH_3)_3SnC{\equiv}CSn(CH_3)_3$, 2117-50-2; $CpCo(CO)_2$, 12078-25-0; $(CH_3)_3SiC{\equiv}CH$, 1066-54-2; $PdCl_2(PPh_3)_2$, 13965-03-2.

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Triphenylsilyl Cation

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We wish to report the preparation and characterization in solution of the triphenylsilyl cation, the silicon analogue of the trityl cation. Although numerous attempts have been made to prepare this species,[2] all have met with failure. The only silylenium ion prepared to date is tris(2-propylthio)silyl, an esoterically substituted species in which the sulfur atoms serve to stabilize the electron deficient silicon center through polarization and resonance.[3]

We now report that the triphenylsilyl cation[4] may be prepared by the Corey method[5] as the ion pair in dichloromethane or 1,2-dichloroethane and as the free ion in acetonitrile or sulfolane. The reaction involves hydride transfer from the silane to the trityl cation (eq 1).

$$Ph_3SiH + Ph_3C^+\ ClO_4^- \rightarrow Ph_2Si^+\ ClO_4^- + Ph_3CH \quad (1)$$

The ^1H and ^{13}C spectra of a solution from the reaction of equimolar amounts of triphenylsilane and trityl perchlorate in CD_2Cl_2 show the clean production of a single species. Thus the ^{13}C aromatic region contains only one set of four resonances from the product (plus the peaks from triphenylmethane at known positions).

Solutions have been examined in a number of solvents with high polarity (to promote ionization) but with low nucleophilicity or donor number (to avoid complexation with solvent). The molar conductance (mho cm^2 mol^{-1}) is only 1.13 in CH_2Cl_2 or 0.28 in 1,2-dichloroethane but 179.5 in acetonitrile and 12.0 in sulfolane.[6] A log–log plot of molar conductance vs. concentration indicates whether the formed species exists as an ion pair or as free ions. For acetonitrile and sulfolane, the plot is linear and horizontal, as expected for free ions (the increase in conductance at higher

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[1] This work was supported by the National Science Foundation (Grant CHE83-12285).

[2] For a review, see: Corriu, R. J. P.; Henner, M. *J. Organomet. Chem.* **1974**, *74*, 1-28.

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[4] With some trepidation we suggest the name *sityl* (rhymes with *trityl*) for this cation.

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[6] The apparently low value in sulfolane is caused by its very high viscosity (9.87) in comparison with acetonitrile (0.325) and dichloromethane (0.393), since conductivity is inversely proporational to viscosity.

Table I. Carbon-13 Chemical Shifts

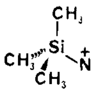
		solvent	additive[a]	δ_i[b]	Δ_i[c]	δ_p[d]	Δ_p[e]
1	Ph_3SiH	CH_2Cl_2		133.73	0.00	130.16	0.00
2	$Ph_3SiOSiPh_3$	CH_2Cl_2		135.51	1.78	130.27	0.11
3	Ph_3SiOH	CH_2Cl_2		135.30	1.57	130.49	0.33
4	$Ph_3Si^+ClO_4^-$	CH_2Cl_2		128.70	−5.03	132.43	2.27
5	$Ph_3Si^+ClO_4^-$	CH_2Cl_2	CH_3CN	128.70	−5.03	132.41	2.25
6	$Ph_3Si^+ClO_4^-$	CH_2Cl_2	sulfolane	128.70	−5.03	132.43	2.27
7	$Ph_3Si^+ClO_4^-$	CH_2Cl_2	pyridine	125.72	−8.01	133.64	3.48
8	$Ph_3Si^+ClO_4^-$	CH_2Cl_2	DMF	128.08	−5.65	132.71	2.55
9	$Ph_3Si^+ClO_4^-$	CH_2Cl_2	Me_2SO			132.92	2.76
10	$Ph_3Si^+ClO_4^-$	CH_2Cl_2	NMI	127.08	−6.65	132.95	2.79
11	Ph_3SiH	CH_3CN		134.23	0.00	130.95	0.00
12	Ph_3SiOH	CH_3CN		137.16	2.93	130.92	−0.03
13	$Ph_3Si^+ClO_4^-$	CH_3CN		128.73	−5.50	133.30	2.35
14	$Ph_3Si^+ClO_4^-$	CH_3CN	pyridine			134.03	3.08
15	Ph_3SiH	sulfolane		133.42	0.00	130.59	0.00
16	Ph_3SiOH	sulfolane		136.60	3.18	130.57	−0.02
17	$Ph_3Si^+ClO_4$	sulfolane		128.03	−5.34	133.00	2.41

[a] Equimolar to $Ph_3Si^+ClO_4^-$; DMF is dimethylformamide; Me_2SO is dimethyl sulfoxide; NMI is *N*-methylimidazole. [b] Shift of the ipso carbon. [c] Difference from the ipso shift of Ph_3SiH in the same solvent. [d] Shift of the para carbon. [e] Difference from the para shift of Ph_3SiH in the same solvent.

concentration is offset through division by concentration in *molar* conductance). In contrast, the plot in dichloromethane or 1,2-dichloroethane is linear with a substantial negative slope, as expected for an ion pair (molar conductance increases at lower concentrations since ion pairs dissociate more easily).[7]

Molecular weight measurements were carried out cryoscopically in sulfolane. With the assumption of two particles, expected for the silylenium ion, the observed molecular weight was 381.2 (6.3% deviation from the expected 358.5). With the assumption of one particle, expected for a covalent species, the observed molecular weight was 190.6 (46.8% deviation from 358.5). With the assumption of three particles, expected for a bridged dimer (which carries two positive charges on bridging phenyl rings and requires 2 mol of anion), the observed molecular weight was 571.9 (20.2% deviation from 717.0). Thus the molecular weight measurements eliminate the covalent form and the dimer and are in agreement with a two-particle, ionic form.

These results indicate that the single species formed on reaction of triphenylsilane with trityl perchlorate is a free ion in acetonitrile or sulfolane and an ion pair in dichloromethane or 1,2-dichloroethane. Conductance and molecular weight measurements eliminate the covalent, one-particle structure and the dimeric, three-particle structure. Thus the two-particle silylenium perchlorate is best in accord with the data. It is difficult, however, to eliminate the presence of a coordinating solvent molecule on the basis of molecular weight measurements alone. Bassindale and Stout have obtained considerable data on complexes between trimethylsilyl perchlorate and various nucleophiles.[8] The complexes have structures of the type **1**, in which N is a nucleophile



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such as dimethylformamide or pyridine. Indeed the crystal structure of the stable complex with pyridine has been reported.[9] Bassindale's measurements were carried out in dichloromethane or acetonitrile, implying that these solvents do not complex with the silyl group.

In the present case of triphenylsilyl we have been able to eliminate the solvent complex as a structural alternative by NMR experiments. Table I presents ^{13}C data on the shifts of the phenyl carbons. Entries 4, 13, and 17 show that there is very little variation of the ipso and para shifts for sityl perchlorate in the three solvents. The effects of complexation are shown very clearly for the addition of pyridine and other strong nucleophiles to sityl perchlorate in CH_2Cl_2 (entries 7–10). Addition of acetonitrile or sulfolane (entries 5 and 6) has no effect. A plot of the difference between the para and meta shifts[10] vs. the Taft β parameter is linear (correlation coefficient 0.94) for six nucleophilic additives (entries 7–10 plus HMPA and (dimethylamino)pyridine), whereas the points for acetonitrile and CH_2Cl_2 lie far off the correlation. These results indicate that for the solvents we are using coordination does not take place but that complexes of the type **1** form when stronger nucleophiles are present. The data of Table I also demonstrate that the species formed are not the result of hydrolysis to the silanol or disilyl ether, whose shifts (entries 2, 3, 12, and 16) are quite different from those of the perchlorates (entries 4, 13, and 17). Measurement of water levels in the three solvents by the Karl Fischer method showed that water was present at 1% or less of the level of perchlorate in the NMR experiments. The ^{29}Si spectrum contained no clear peaks, presumably because of slow relaxation.

An even more sensitive NMR test is provided by the chemical shifts of the nucleophile. To a solution of the sityl ion pair in dichloromethane we added an equimolar amount of acetonitrile. If acetonitrile acts as a nucleophile, its ^{13}C and ^{15}N chemical shifts should be altered predictably. The nitrile carbon, however, changed negligibly from free acetonitrile (δ 117.0) to acetonitrile in the presence of sityl (δ 117.3). The nitrile carbon of protonated acetonitrile moves to δ 106.8. The ^{15}N atom provides an even more sensitive probe, since complexation, like protonation, removes the nitrogen lone pair. The ^{15}N shift should move about 100 ppm upfield since the n–π transition is no longer present to cause the large paramagnetic (downfield) shift of nitriles. We found the ^{15}N shift of free acetonitrile at δ 244.2 and of acetonitrile in the presence of sityl at δ 245.7 in CH_2Cl_2 and similar values in $ClCH_2CH_2Cl$. Even if 6 equiv of acetonitrile is present, the shift is only δ 244.8. This observation permits essentially no interaction between acetonitrile and sityl, so the ionic species cannot be complexed with solvent in dichloromethane, 1,2-dichloroethane, or acetonitrile. Similar ^{13}C observations were made in sulfolane. By way of a control, we placed 1 mol of pyridine in the presence of sityl in CH_2Cl_2. Whereas free pyridine has an ^{15}N resonance at δ 314.0, pyridine in the presence of sityl resonates at δ 216.8. This shift of 100 ppm is consistent with complexed pyridine of the type **1**. The ^{13}C chemical shifts of pyridine also changed appropriately. Thus the stronger nucleophilicity of pyridine

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(7) For a discussion of conductance plots, see: Kraus, C. A. *J. Chem. Educ.* **1958**, *35*, 324–337.

(8) Bassindale, A. R.; Stout, T. *J. Organomet. Chem.* **1982**, *238*, C41–C45. Bassindale, A. R.; Stout, T. *Tetrahedron Lett.* **1985**, *26*, 3403–3406.

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(10) Batchelor, R. J.; Birchall, T. *J. Am. Chem. Soc.* **1983**, *105*, 3848–3852.

(11) Moreover, addition of pyridine instantly decolorizes the light yellow solution of sityl perchlorate in dichloromethane, whereas acetonitrile has no effect on the color.

permits it to react with sityl to form the tetrahedral complex.[10] The absence of such shifts for the less nucleophilic acetonitrile confirms that sityl lacks the fourth coordination partner and is a true silylenium ion in solvents of low nucleophilicity. We do not claim that the ion is unsolvated but that it is nonspecifically solvated in the same way that trityl is under the same conditions.

Pentacoordinate Carbon in Trigonal-Bipyramidal Symmetry. The Eight-Membered Ring X-ray Structure of Tetrakis(benzylsodium-*N*,*N*,*N'*,*N'*-tetramethylethylenediamine)

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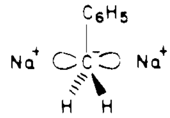
Unlike organolithium compounds,[1] relatively few structures of the synthetically important organic derivatives of the heavier alkali metals have been reported.[2] A new hexane-soluble butylsodium reagent[3] facilitates the preparation of crystalline organosodium compounds.[3b] Thus, metalation of toluene in hexane at -18 °C in the presence of *N*,*N*,*N'*,*N'*-tetramethylethylenediamine (TMEDA) gave yellow needles of $(NaCH_2C_6H_5{\cdot}TMEDA)_4$.[4a] The X-ray structure[4b] (a stereoview is shown in Figure 1) represents the first organoalkali metal tetramer that prefers an eight-membered ring over a tetrahedral arrangement.[1,2] Each α-benzyl carbon is pentacoordinate (**1**) and possesses the trigonal-bipyramidal geometry first suggested by calculations on MCH_3M^+ (M = Li, Na, etc.) models.[5] The predicted preference for pentacoordinate carbon to adopt D_{3h} (**2**) over C_s (**3**) symmetry when at least two metals are present[5] (in contrast to CH_5^+)[6] has now been verified experimentally in other instances as well.[7]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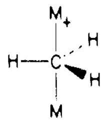
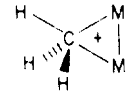

2. D_{3h}


3. C_s

	E_{rel}, kcal/mol	
	2	3
M = H (MP4/6-311G**//6-31G*)[6]	10 8	0 0
M = Li (MP4/6-31G*//6-31G*)[5]	0 0	3 4
M = Na (MP4/6-31G*//6-31G*)[5]	0 0	4 4

The benzylsodium-TMEDA complex (Figure 1) is a tetramer with approximate D_{2d} symmetry. The four sodium atoms define a square, each edge of which is intersected by a benzyl α-carbon. The resulting eight-membered ring puckers into a crown conformation, presumbly to alleviate crowding. The phenyl rings exhibit short carbon contacts to the methyl groups of neighboring TMEDA ligands in the 3.48-3.70-Å range and bend, in alternation, up and down out of the Na_4 plane. The benzyl groups (including the hydrogens) are exactly planar, but because of the ring puckering the coordination of two sodiums with each benzyl α-CH_2 group (as in **1**) is not exactly perpendicular. However, the deviation from linearity is small (the mean NaCNa angle is 146.5°). The average geometry of the benzyl groups shows nearly exactly the same variations in CCC angles and CC bond lengths (see caption, Figure 1), due to π-electron delocalization, as reported by Power et al.[7c] for benzyllithium; Stucky's 1970 values deviate a little more.[8] The average C-Na distances, 2.64 Å to the α-carbon and 2.76 Å to the ipso carbons, indicate that the sodiums bridge these positions to some extent. The situation in the two benzyllithium structures is similar, but there are greater variations.[7c,8] Two coordination sites on each sodium are occupied by the nitrogen atoms of a TMEDA ligand. Like the C-Na distances, the N-Na distances (around 2.50 Å) are quite normal for sodium compounds.[2] These are about 0.4 Å larger than the corresponding C-Li and N-Li values[1] due to the larger ionic radius of sodium.

The structure of $(\text{benzylsodium-TMEDA})_4$ differs significantly from those of related polar metallic benzyl derivatives. In

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[2] For a review of the crystal structures of organoalkali compounds of Na, K, Rb, and Cs, see: Schade, C.; Schleyer, P. v. R. *Adv. Organomet. Chem.*, in press. Note, in particular, the tetrahedral structure of $[NaCH_3]_4$: Weiss, E.; Sauermann, G.; Thirase, G. *Chem. Ber.* **1983**, *116*, 74-85.

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[4] (a) **NMR Data in Tetrahydrofuran-d_8 (THF-d_8)**: ^{23}Na (-95 °C, 105 MHz; reference $NaCl/H_2O$) δ +1.15; ^{1}H (-75 °C, 400 MHz; reference THF-d_8, δ 3.58 from Me_4Si) δ 6.08 (dd, 6.5, 7.7 Hz; meta H), 5.77 (d, J = 7.7 Hz; ortho H), 4.94 (t, J = 6.5 Hz, para H), 2.28 (s, TMEDA-CH_2), 2.13 (s, TMEDA-CH_3), 1.87 (s, CH_2Na); ^{13}C (-95 °C, 100.5 MHz; reference THF-d_8, δ 67.4 from Me_4Si) δ 157.0 (ipso), 128.8 (meta), 113.2 (ortho), 98.8 (para), 58.6 (TMEDA-CH_2), 46.4 (TMEDA-CH_3), 42.3 (CH_2Na). (b) **Crystal Data.** Monomer = $C_{13}H_{23}N_2Na$, M = 230.332, monoclinic, space group $P2_1/n$, a = 14.176 (3) Å, b = 15.011 (5) Å, c = 27.368 (7) Å, β = 90.82 (2)°, V = 5823 Å^3, Z = 16, D_x = 1.051 g/cm^3 (at 117 K) with one tetramer in the asymmetric unit. Graphite monochromated Mo Kα radiation, λ = 0.71069 Å. Two crystals of dimension 0.13 × 0.2 × 0.25 and 0.15 × 0.33 × 0.23 mm^3, respectively, were measured in order to improve the accuracy, especially in the range above the diffraction angle of about 18°, where the diffracted intensities fade out rapidly due to disorder in the structure. A total of 162650 reflection profiles ($2° < \theta < 25°$) were measured at 117 K. Averaging yielded a unique set of 10250 structure factors; 6011 of these were stronger than 2σ. The averaging R value $R_{av} = \sum|F_o^2 - F_{av}^2|/\sum F_o^2$ was 0.102 for the 55103 measurements above 2σ and 0.077 for the 39628 measurements above 3σ. The structure was solved by direct methods (MULTAN 76: Main, P.; Hull, S. E.; Lessinger, L.; Germain, G.; Declecq, F.; Woolfson, M. M. MULTAN 76, Universities of York, England, and Louvain, Belgium, 1976) and refined by large block matrix least-squares methods (X-ray 76: Steward, J. M.; Machin, P. A.; Dickinson, C. W.; Ammon, H. L.; Heck, H.; Flack, H. X-RAY 76, Technical Report TR 446, 1976; Computer Science Center, University of Maryland, College Park, MD) by using weights $1/\sigma^2 (F_o^2)$ and including all hydrogen atoms (1063 variables in six blocks). All non-nitrogen atoms of the TMEDA groups are disordered. In case of the methyl groups this disorder was approximated adequately by the anisotropic tempertaure parameters, but each ethylene group had to be divided into two alternative positions, whose populations were chosen so that the mean "vibrations" of the carbon atoms were about equal. All hydrogen atoms of the benzyl groups and most of the TMEDA groups were refined with isotropical vibration parameters; 16 of the lower populated (disordered) methylene hydrogens were given the anisotropic vibration parameters obtained for their mother carbon atoms and refined only with respect to their positional parameters. The R values, based on the 6011$F_o^2 > 2\sigma$ (of the average values), converged to $R(F^2)$ = 0.069, $R_w(F^2)$ = 0.058. The biggest peak and the lowest hole in the final difference map are 0.55 and --0.57 e/Å^3, respectively.

[5] (a) Jemmis, E. D.; Chandrasekhar, J.; Schleyer, P. v. R. *J. Am. Chem. Soc.* **1979**, *101*, 527-533, and unpublished calculations on $CH_3Na_2^+$. (b) Jemmis, E. D.; Chandrasekhar, J.; Würthwein, E.-U.; Schleyer, P. v. R.; Chinn, B.; Pople, J. A. *Ibid.* **1982**, *104*, 4275-4276. (c) Schleyer, P. v. R.; Tidor, B.; Jemmis, E. D.; Chandrasekhar, J.; Würthwein, E.-U.; Kos, A. J.; Luke, B. T.; Pople, J. A. *Ibid.* **1983**, *105*, 484-488. (d) For experimental verifications of the predicted stability of the $CH_3Li_2^+$ cation, see: Chinn, J. W., Jr.; Lagow, R. J. *Organometallics* **1984**, *3*, 75-77. Lagow, R. J. *J. Organomet. Chem.* **1983**, *249*, 1-9.

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[7] Examples of pentacoordinate trigonal-bipyramidal carbon in X-ray structures: (a) A near planar methyl group bridging two zirconium atoms: Waymouth, R. M.; Santarsiero, B. D.; Grubbs, R. H. *J. Am. Chem. Soc.* **1984**, *106*, 4050-4051. There are linear B-CH_3-Li arrangements in the $LiB(CH_3)_4$ aggregate, but neutron diffraction shows the methyl groups to have local C_{3v} rather than D_{3h} symmetry: Rhine, W. E.; Stucky, G.; Petersen, S. W. *J. Am. Chem. Soc.* **1975**, *97*, 6401-6406. (b) The Li_2CH_2R grouping in the "Y-conjugated dianion", $[(C_6H_5CH)_2CCH_2Li_2{\cdot}2TMEDA]$: Wilhelm, D.; Schleyer, P. v. R.; Clark, T.; Dietrich, H.; Mahdi, W., unpublished results. (c) Polymeric $[C_6H_5CH_2Li{\cdot}Et_2O]_n$ (see text): Beno, M. A.; Hope, H.; Olmstead, M. M.; Power, P. P. *Organometallics* **1985**, *4*, 2117-2121. These results are pertinent to the mechanisms of S_E2 reactions which proceed with inversion of configuration: Fukuto, J. M.; Jensen, F. R. *Acc. Chem. Res.* **1983**, *16*, 177.

[8] Patterman, S. D.; Karle, I. L.; Stucky, G. D. *J. Am. Chem. Soc.* **1970**, *92*, 1150-1157.

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