to form the very acid-sensitive chiral carbinol 5[6] in 95% isolated yield.

4 5

The reactivity of Tbs ethers toward DIBAL-H at room temperature should be kept in mind when reductions are carried out with this reagent on O-silylated substrates.[7]

Experimental Section

The following experimental procedure is representative.

Desilylation of *trans*-4-*tert*-Butylcyclohexyl *tert*-Butyldimethylsilyl Ether by Diisobutylaluminum Hydride. A solution of 17 mg (0.063 mmol) of the Tbs ether of *trans*-4-*tert*-butylcyclohexanol in methylene chloride (3 mL) was treated at 0 °C with a 1.0 M solution of diisobutylaluminum hydride in toluene (0.18 mL, 0.18 mmol) under nitrogen with stirring. After 2 h at 23 °C, 0.5 g of crushed ice was added, and the mixture was washed with 1 mL of 0.5 M hydrochloric acid. The organic layer was dried (K_2CO_3), filtered through a small plug of silica gel, and concentrated under reduced pressure to give 9 mg of *trans*-4-*tert*-butylcyclohexanol (87%) which was identified and shown to be pure by 500-MHz ^1H NMR and TLC analyses and comparison with an authentic sample.[5,7]

Registry No. 1 (R = hexyl), 80033-60-9; 1 (R = benzyl), 21862-63-5; 1 (R = Ph), 18052-27-2; 1 (R = 4-*tert*-butylcyclohexyl), 71009-16-0; 2, 29681-57-0; 4, 137655-10-8; 5, 124563-11-7; hexanol, 111-27-3; phenol, 108-95-2; benzyl alcohol, 100-51-6; diisobutylaluminum hydride, 1191-15-7.

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Reactions of α,β-Epoxy Carbonyl Compounds with Methanethiolate: Regioselectivity and Rate

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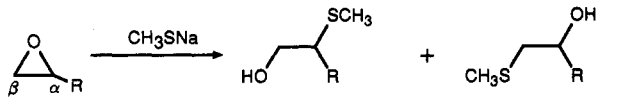
Reactions between epoxides and biogenic thiols are biologically important in several respects.[1] Potentially toxic xenobiotic epoxides[2] and endogenous epoxides[3] form adducts with glutathione. Epoxides alkylate active-site cysteine residues of certain enzymes.[4] Potent enzyme inhibitors, known to alkylate cysteine residues, include structurally diverse α,β-epoxy carbonyl and related compounds.[5]

Under physiological conditions, the thiolate of cysteine (pK_a 8.2) is actually the significant nucleophile.[1] As a nonpeptidic model, we were therefore interested in the reactivity of α,β-epoxy carbonyl compounds (i.e. **1a–c,e**) toward simple thiolate anions to afford β-hydroxy-α-thio carbonyl compounds (**2**) and α-hydroxy-β-thio carbonyl compounds (**3**). A primary question was whether the carbonyl would increase the reactivity of these epoxides. Although reactions of epoxides[6] including α,β-epoxy ketones,[7] α,β-epoxy esters,[2c,8] α,β-epoxy carboxylic acids,[9] and α,β-epoxy amides[10] with thiols and (occasionally) thiolates have been reported, reaction rates have not been measured and a comprehensive understanding of regioselectivity and relative reactivity does not emerge from the literature due to differences in the reagents, solvents, and temperatures employed. Retro-aldol reactions of the β-hydroxy-α-thio carbonyl regioisomers (i.e. **2**) also complicate comparisons. Catalysis by Lewis acids and mineral acids provides dif-

Table I. Pseudo-First-Order Rates and Regioselectivities in Reactions of CH_3S^- with Epoxides (1) at pD 9.84[a]

epoxide	R	k (min^{-1})	2:3	k_α (min^{-1})	k_β (min^{-1})
1a	$COCH_3$	1.45[b]	>95:5	1.45[b]	
1b	CO_2CH_3	0.44	57:43	0.25	0.19
1c	$CONH_2$	0.166	22:78	0.037	0.13
1d	CH_2CH_3	0.086	<5:95		0.086
1e	CO_2^-	0.010	36:64	0.0036	0.0064

[a] Reactions of 1 (0.097 M) with CH_3S^- (0.0145 M) were conducted in D_2O at 19.4 °C. [b] Extrapolated from rate at pD 9.21.



1 2 3

a; R = $COCH_3$
b; R = CO_2CH_3
c; R = $CONH_2$
d; R = CH_2CH_3
e; R = CO_2^-

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ferent regioselectivity than attack by thiolates.[10a,b,11]

Results and Discussion

In order to determine the relative importance of the opposing steric[6] and electronic[12] factors under biologically relevant conditions, we have studied the rate and regioselectivity of reactions between methanethiolate and a series of comparable, sterically unincumbered, water-soluble α,β-epoxy carbonyl compounds (1). Reactions were followed by NMR spectroscopy in D_2O at pD 9.84. The logarithms of the reaction rates of **1a** increase linearly with pD between pD 7.3 and 9.2, suggesting that methanethiolate (pK_a 10.3[13]) is the active nucleophile.

1,2-Epoxybutane (**1d**) was used as a standard to demonstrate the effect of steric hindrance alone. As shown in Table I, methanethiolate exclusively attacks the less substituted[6] β-carbon of **1d**, affording **3d**.[14] In contrast, methanethiolate attacks the α-carbon of all of the α,β-epoxy carbonyl substrates significantly (**1b,c,e**) or exclusively (**1a**), despite steric hindrance. Evidently the carbonyl groups activate the α-carbon toward nucleophilic substitution. The analogous high reactivity of α-halo carbonyl compounds has been attributed to bridging of the incoming nucleophile between the α-carbon and the carbonyl carbon, or alternatively to resonance delocalization of partial bonds from the nucleophile and nucleofuge into the carbonyl group.[12]

An improved analysis results when each rate constant is multiplied by the mole fractions of products **2** and **3**. Rates of attack on the α- and β-carbons, k_α and k_β, respectively, are obtained (Table I). The rates of α-substitution, k_α, decrease in the order $COCH_3 > CO_2CH_3 > H > CONH_2 > CO_2^- > CH_2CH_3$. This order of reactivity is similar to that observed for S_N2 reactions of α-chloro carbonyl compounds.[12] The low rate of substitution α to the carboxylate of **1e** is probably due to unfavorable development of additional negative charge in the transition state. As expected, the rates of β-substitution, k_β, are similar for **1b–d**, indicating that ester or amide groups have little influence on the β-carbon. However, attack on **1e** is slowed β to the carboxylate anion, again indicating charge development in the transition state.

These results may aid the understanding of epoxide reactivity, toxicity, and metabolism and may be applicable to the design of improved enzyme inhibitors.

Experimental Section

Epoxides **1a**,[15a] **1b**,[15b] and **1c**,[15c] were prepared according to literature procedures. Hydrolysis of **1b** with KOH in methanol afforded the potassium salt of **1e**.[9b] $NaDCO_3$ was prepared from $NaHCO_3$ by exchange with D_2O, followed by lyophilization.

Kinetics. A freshly prepared solution (1.00 mL) of $NaSCH_3$ (0.0145 M), $NaDCO_3$ (0.618 M), Na_2CO_3 (0.132 M), and sodium 3-(trimethylsilyl)propanoate-d_4 (TSP, 0.005 M) in D_2O was mixed with the epoxide (0.097 ± 0.002 mmol) in a capped NMR tube which was placed in an NMR spectrometer (300 MHz) at 19.4 ± 0.1 °C. The observed pH (9.43), measured with a combination electrode, was constant throughout reaction. Therefore pD = 9.84.[16] The reaction of **1a** at pD 9.84, which was too fast to measure accurately, was extrapolated from the following data at lower pD: pD 7.28 phosphate buffer, $k = 0.0479$ min^{-1}; pD 8.27 phosphate buffer, $k = 0.165$ min^{-1}; pD 9.21 carbonate buffer, $k = 0.614$ min^{-1}, log k increases linearly with pD. Reactions were generally followed by integration of the CH_3S NMR signals vs the TSP standard. Kinetics were pseudo-first-order over >3 half-lives. Product distributions (2:3) were determined by integration after >4 half-lives.

Preparative Reactions. In a typical procedure, the epoxide (3 mmol) was added to a solution of $NaHCO_3$ (660 mg, 7.86 mmol) in water (7 mL) at 0 °C. $NaSCH_3$ (300 mg, 4.29 mmol, 143 mol %) was added in portions over 2 min, and the capped mixture was stirred at 0 °C for 0.5 h (8 h in the case of **1e**). In the reactions of **1a**, **1b**, and **1d**, the products were extracted into EtOAc. The extract was dried over $MgSO_4$, and the solvent was evaporated in vacuo to afford crude product. In the reactions of **1c** and **1e**, HCl was added to pH 2. The water was removed by lyophilization or evaporation. The residue was extracted with ethanol, and the filtrate was evaporated to afforded the crude product.

4-Hydroxy-3-(methylthio)-2-butanone (2a) was purified by Kugelrohr distillation (155–165 °C, 30 Torr) to afford a pale yellow oil (91% yield): ^{1}H NMR (D_2O) δ 2.04 (3 H, s), 2.42 (3 H, s), 3.72 (1 H, t), 3.84 (1 H, dd), 3.94 (1 H, dd); ^{1}H NMR (D_2O, Na_2CO_3) δ 2.04 (3 H, s), 2.42 (3 H, s), 3.84 (1 H, d), 3.94 (1 H, d); IR (neat) 3417, 2924, 1703, 1427, 1358, 1038 cm^{-1}. Anal. Calcd for $C_5H_{10}O_2S$: C, 44.75; H, 7.51; S, 23.89. Found: C, 44.37; H, 7.48; S, 23.89.

Methyl 3-hydroxy-2-(methylthio)propanoate (2b) and methyl 2-hydroxy-3-(methylthio)propanoate (3b) (71% yield) were separated by chromatography on silica gel with ethyl ether–hexanes (2:1).

2b:[17] ^{1}H NMR ($CDCl_3$) δ 2.15 (3 H, s), 2.52 (1 H, t, OH), 3.39 (1 H, dd), 3.77 (3 H, s), 3.82 (1 H, m), 3.90 (1 H, m); IR (neat) 3446, 1734 cm^{-1}. Anal. Calcd for $C_5H_{10}O_3S$: C, 39.98; H, 6.71; S, 21.35. Found: C, 39.33; H, 6.52; S, 21.45.

3b:[17] ^{1}H NMR ($CDCl_3$) δ 2.18 (3 H, s), 2.85 (1 H, dd), 2.96 (1 H, dd), 3.11 (1 H, d, OH), 3.81 (3 H, s), 4.44 (1 H, dd); IR (neat) 3447, 1741 cm^{-1}. Anal. Calcd for $C_5H_{10}O_3S$·0.25H_2O: C, 38.82; H, 6.84. Found: C, 38.85; H, 6.66.

3-Hydroxy-2-(methylthio)propanamide (2c) and 2-Hydroxy-3-(methylthio)propanamide (3c) (91% crude yield). Chromatography on silica gel with EtOAc–EtOH (90:10) afforded **2c**: mp 73–74 °C. Recrystallization from EtOAc afforded **3c**: mp 76–78 °C.

2c: ^{1}H NMR (D_2O) δ 2.18 (3 H, s), 3.51 (1 H, t), 3.84 (1 H, dd), 3.93 (1 H, dd); IR (neat) 3333, 3187, 2909, 1667, 1590, 1418, 1306, 1051 cm^{-1}. Anal. Calcd for $C_4H_9NO_2S$: C, 35.54; H, 6.71; N, 10.36. Found: C, 35.01; H, 6.12; N, 10.06.

3c: ^{1}H NMR (D_2O) δ 2.16 (3 H, s), 2.84 (1 H, dd), 2.97 (1 H, dd), 4.36 (1 H, dd); IR (neat) 3392, 3312, 2919, 1651, 1412, 1328, 1108, 1089 cm^{-1}. Anal. Calcd for $C_4H_9NO_2S$: C, 35.54; H, 6.71; N, 10.36; S, 23.70. Found: C, 35.40; H, 6.36; N, 10.24; S, 23.34.

1-(Methylthio)-2-butanol (3d)[14] (100 % yield) did not require purification. Colorless oil: ^{1}H NMR (D_2O) δ 0.95 (3 H, t), 1.58 (2 H, m), 2.15 (3 H, s), 2.60 (1 H, dd), 2.74 (1 H, dd), 3.76 (1 H, m).

3-Hydroxy-2-(methylthio)propanoic acid (2e) and 2-hydroxy-3-(methylthio)propanoic acid (3e) (121% crude yield) were separated by chromatography on silica gel with chloroform–methanol–AcOH (87:10:3). Treatment with diazomethane (methanol–ethyl ether) afforded methyl esters **2b** and **3b**.

2e: colorless oil; ^{1}H NMR (D_2O) δ 2.17 (3 H, s), 3.53 (1 H, t), 3.84 (1 H, dd), 3.92 (1 H, dd); IR (neat) 3412, 2927, 1714 cm^{-1}. Anal. Calcd for $C_4H_8O_3S$·0.1$CHCl_3$: C, 33.25; H, 5.51. Found: C, 33.03; H, 5.87.

3e: amorphous solid, mp 66–72 °C; ^{1}H NMR (D_2O) δ 2.16 (3 H, s), 2.84 (1 H, dd), 2.97 (1 H, dd), 4.35 (1 H, dd); IR (neat) 3392, 3210, 1719, 1584, 1426 cm^{-1}. Anal. Calcd for $C_4H_8O_3S$·0.1$CHCl_3$: C, 33.25; H, 5.51. Found: C, 33.00, H, 5.51.

Acknowledgment is made to Dr. P. W. Erhardt for his support and interest in this investigation.

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Registry No. **1a**, 4401-11-0; **1b**, 4538-50-5; **1c**, 5694-00-8; **1d**, 106-88-7; **1e**, 137946-04-4; **2a**, 137946-05-5; **2b**, 42998-10-7; **2c**, 137946-07-7; **2d**, 137946-09-9; **2e**, 137946-10-2; **3a**, 137946-06-6; **3b**, 54864-75-4; **3c**, 137946-08-8; **3d**, 76137-53-6; **3e**, 137946-11-3; $NaSCH_3$, 5188-07-8; $NaDCO_3$, 21254-75-1.

The Simplest Cyclic Polyacene. A Semiempirical (MNDO) Study of *cyclo*-Anthracene

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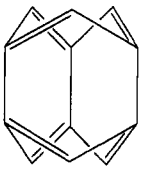
Introduction

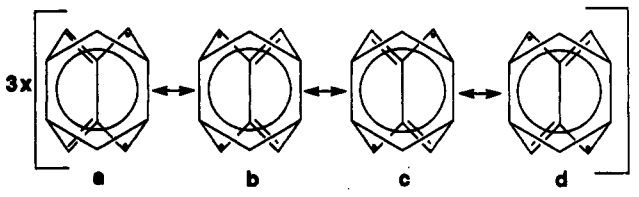
In 1983, Kivelson and Chapman[1] proposed the possibility of cyclic polyacenes in their computational study of infinite linear polyacenes as potential one-dimensional conductors. Although we find these cyclic polyacenes to be inherently interesting, they have apparently not been studied since this original report.[2]

The smallest and simplest possible cyclic polyacene contains three fused hexagonal rings, **1**. Drawn as **1**, the molecule does not contain any aromatic sextets[3] and is, in fact, a Hückel $4n$ system with 12 π electrons.



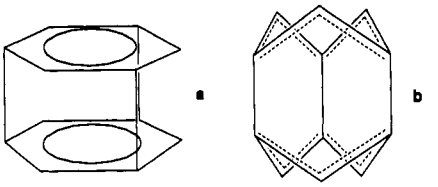
1

If the presence of an aromatic sextet is of greatest importance to the stability of this cyclic triacene (*cyclo*-anthracene), **1** could be envisioned as containing one (but only one) lateral aromatic ring. Such a structure, **2**, must be a diradical with the unpaired electrons conjugated with both the aromatic system and the two alkene moieties, as in **2a** and **2b**. Other possibilities, **2c** and **2d**, place the radicals in adjacent rings. (There are two additional sets of four equivalent structures in which the aromatic system is permuted into the other two lateral hexagonal rings.) A total of 12 "resonance structures" for such a small molecule, albeit all diradicaloid, might allow the molecule some stability. However, the extremely distorted nonplanar nature of the central carbon atoms and the subsequent unfavorable orbital overlaps may make the conjugation effects unlikely and, therefore, somewhat less important.



2

There is yet a third possible representation of **1**. The molecule could be described as a "1,3,5-face-fused"-cyclophane, as in **3a**. If *cyclo*-anthracene were constructed in this manner, **3** would contain two probably extremely distorted aromatic systems, but delocalized bonds might be expected on the molecular "top" and "bottom", as in **3b**. The delocalized systems would be connected by isolated single bonds.



3

We have developed an interest in moderately strained systems composed of benzene-like hexagons.[4] The cyclic polyacenes certainly meet this strain criterion, and **1** would probably be expected to exceed the term "moderately". Herein we report our computational investigation of **1** using the MNDO (modified neglect of diatomic overlap) method.[5]

Methods

The MOPAC Version 5.0 package[6] of semiempirical molecular calculational programs, which incorporates MNDO, was used. All minimization calculations were carried out on an Apollo/Hewlett-Packard DN4600 workstation under the Domain O/S operating system. For calculations involving force constant determinations, an Apollo/Hewlett-Packard DN10000 computer was employed due to the long times involved for these calculations.

For the successful[7] initial trial geometries (ITGs), and the Z matrices, all carbon–carbon distances were set at either 1.3, 1.4, or 1.5 Å, while carbon–hydrogen distances were set at either 1.1 or 1.0 Å. All hexagons were considered to be regular, with angles of 120°. Each hexagon was considered to be individually planar, and the plane torsion angle between two adjacent hexagons was set to 60° so as to produce an overall system with a triangular cross-section. All $3n$–6 degrees of freedom were allowed to minimize fully under the MNDO conditions. The keyword PRECISE was used to automatically increase the gradient norm and self consistent field criteria by a factor of 100. This increase resulted in individual distance, angle, and torsion gradients of less than 0.01 kcal/Å or kcal/radian.

Results and Discussion

The simplest cyclic polyacene, *cyclo*-anthracene, is formally constructed from three cyclically fused hexagons. This molecule minimizes on the MNDO potential energy

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(7) Only ITGs in which all hexagons were regular and planar, producing a molecule with a triangular cross-section, resulted in an output optimized molecule which exhibited real vibrational, rotational, and translational frequencies after a force constant calculation. Other ITGs, in which the input geometry appeared to be a better approximation of the successfully minimized geometry, resulted in molecules with imaginary translational frequencies after force constant calculations, and were, therefore, not considered further. The input geometry with carbon–carbon distances of 1.4 Å and carbon–hydrogen distances of 1.0 Å resulted in the optimized molecule with the least positive (most stable) heat of formation.

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