Supporting Information

Electron Transfer Promoted Regioselective Ring-Opening Reaction of Cyclopropyl Silyl Ethers
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General Experimental Procedures. NMR spectra were recorded in CDCl3 with Me4Si as an internal standard at 200 MHz and 270 MHz for 1H NMR, and 50 MHz and 68 MHz for 13C NMR. Uncorrected melting points are reported. Oxidation and reduction potentials in MeCN were measured with cyclic voltammetry using platinum electrodes as working and counter electrodes, Ag/0.01 M AgNO3 as a reference electrode, and 0.1 M Et4NClO4 as a supporting electrolyte at the scan rate of 100 mV/s. Sample solutions were purged with N2 before measurements. Ferrocene was used as a reference.1 Reported standard potentials of ferrocene/ferrocenium couple against Ag/AgNO3 and SCE were employed.2 Then, peak potentials of cyclopropyl silyl ethers were
converted to those against SCE. Half-wave potentials were obtained from these peak potentials by subtracting or adding 0.029 V (see below). Photoreactions were conducted in a Pyrex test tube (1.5 cm diameter) immersed in a water bath at room temperature with either a 500 W Xe–Hg lamp as a light source. Column chromatography was performed with silica gel (Wakogel C-200). Preparative TLC was performed on 20 cm x 20 cm plates coated with silica gel (Wakogel B-5F). MeCN was distilled over P2O5 and subsequently with K2CO3. Tris-p-bromophenylaminium hexachloroantimonate was prepared according to the literature procedure. 4 9,10-dicyanoanthracene and biphenyl were purchased and recrystallized twice from pyridine and ethanol, respectively. Other reagents and solvents were purchased and used without further purification.

Preparations of cyclopropyl silyl ethers. Compound 1a could be prepared from 2-methyl-1-tetralone, that is obtained through several steps described in Scheme 1, either by method A5 or method B6 described in Scheme 2 and Scheme 3, respectively. Compounds 1b, 1c and 1d were similarly prepared by method A. Known compound 18 was prepared according to the literature procedure. 7 Experimental details will be reported in a full paper.

Scheme 1

Scheme 2 (method A)

Scheme 3 (method B)

Spectral data of 1a, 1b, 1c and 1d are reported below.

6-Methyl-1-trimethylsilyloxy-2,3-benzobicyclo[4.1.0]heptane (1a): colorless oil; IR (Neat) 2920, 2848, 1290, 886 cm⁻¹; 1H-NMR (270 MHz) δ 0.25 (s, 9H), 0.86 (d, J = 5.7 Hz, 1H), 1.25 (d, J = 5.9 Hz, 1H), 1.37 (s, 3H), 1.59 (td, J = 13.0, 5.9 Hz, 1H), 1.91 (dd, J = 13.0, 5.9 Hz, 1H), 2.40 (td, J = 15.9, 5.9 Hz, 1H), 2.58 (dd, J = 15.9, 4.9 Hz, 1H), 6.98-7.01 (m, 1H), 7.04–7.10 (m, 1H), 7.18-7.23 (m, 1H); 13C NMR (68 MHz) δ 1.5, 19.8, 22.0, 25.7, 26.6, 27.4, 60.9, 124.7, 125.0, 125.8, 128.0, 133.0, 140.9. LRMS (EI) m/z (relative intensity) 246 (M⁺, 40), 73 (100).

7-Methyl-1-trimethylsilyloxy-2,3-benzobicyclo[5.1.0]octane (1b): colorless oil; IR (Neat) 2936,
2860, 864, 842 cm\(^{-1}\); \(^1\)H-NMR (270 MHz) \(\delta = -0.02\) (s, 9H), 0.28-0.41 (m, 1H), 0.69 (d, \(J = 5.1\) Hz, 1H), 0.81 (d, \(J = 5.1\) Hz, 1H), 1.22 (s, 3H), 1.33-1.46 (m, 1H), 1.76 (dd, \(J = 14.3, 5.7\) Hz, 1H), 1.85-2.00(m, 1H), 2.54 (dd, \(J = 13.0, 4.9\) Hz, 1H), 3.05-3.15 (m, 1H), 7.08–7.11 (m, 1H), 7.19-7.23 (m, 2H), 7.41–7.44 (m, 1H); \(^{13}\)C NMR (68 MHz) \(\delta = 1.4, 15.7, 21.2, 22.9, 26.3, 30.1, 32.5, 62.9, 125.9, 127.8, 128.3, 129.6, 140.1, 140.8.\) LRMS (EI) \(m/z\) (relative intensity) 260 (M\(^+\), 8), 73 (100).

\(6\)-(3'-butenyl)-1-trimethylsilyloxy-2,3-benzobicyclo[4.1.0]heptane (1c):\) colorless oil; IR (Neat) 2948, 2920, 1252, 838 cm\(^{-1}\); \(^1\)H-NMR (270 MHz) \(\delta = 0.27\) (s, 9H), 0.91 (d, \(J = 5.9\) Hz, 1H), 1.27 (d, \(J = 5.1\) Hz, 1H), 1.45-1.89 (m, 3H), 2.12 (ddd, \(J = 13.0, 6.2, 1.9\) Hz, 1H), 2.15-2.42 (m, 3H), 2.65 (dd, \(J = 16.2, 3.5\) Hz, 1H), 4.96-5.10 (m, 2H), 5.85-6.00 (m, 1H), 7.02–7.05 (m, 1H), 7.08-7.14 (m, 1H), 7.21-7.26 (m, 1H), 7.51–7.54 (m, 1H); \(^{13}\)C NMR (68 MHz) \(\delta = 1.5, 21.2, 23.6, 27.3, 29.4, 31.5, 32.4, 60.9, 114.1, 124.7, 125.1, 126.0, 127.9, 133.0, 139.1, 141.0.\) LRMS (EI) \(m/z\) (relative intensity) 286 (M\(^+\), 7), 83 (100).

\(6\)-(4'-pentenyl)-1-trimethylsilyloxy-2,3-benzobicyclo[4.1.0]heptane (1d):\) colorless oil; IR (Neat) 2920, 2852, 1252, 838 cm\(^{-1}\); \(^1\)H-NMR (270 MHz) \(\delta = 0.25\) (s, 9H), 0.86 (d, \(J = 6.2\) Hz, 1H), 1.23 (d, \(J = 6.2\) Hz, 1H), 1.48-1.73 (m, 5H), 1.98 (ddd, \(J = 11.0, 6.1, 2.0\) Hz, 1H), 2.08-2.15 (m, 2H), 2.40 (td, \(J = 16.0, 6.2\) Hz, 1H), 2.62 (ddd, \(J = 16.1, 5.3, 1.9\) Hz, 1H), 4.94-5.07 (m, 2H), 5.77-5.92 (m, 1H), 7.00–7.03 (m, 1H), 7.05-7.11 (m, 1H), 7.19-7.25 (m, 1H), 7.49–7.52 (m, 1H); \(^{13}\)C NMR (68 MHz) \(\delta = 1.5, 21.2, 23.6, 26.5, 27.3, 29.6, 32.5, 34.3, 61.0, 114.4, 124.7, 125.0, 125.9, 127.9, 133.0, 138.9, 141.0.\) LRMS (EI) \(m/z\) (relative intensity) 300 (M\(^+\), 87), 231 (100).

Reaction of cyclopropyl silyl ethers with tris-p-bromophenylaminium hexachloroantimonate (TBPA), To a solution of 1 (0.40 mmol) in MeCN (8 mL) was added TBPA (0.81 mmol) under N\(_2\). The resulting mixture was stirred until the consumption of 1 was confirmed by TLC analysis, 2 h for 1a and 1b, 1 h for 1c, and then it was concentrated. The residue was dissolved in CH\(_2\)Cl\(_2\) and followed by filtration. The filtrate was concentrated and subjected to column chromatography using CH\(_2\)Cl\(_2\)/n-C\(_6\)H\(_{14}\) (1/1) to give the mixture of 2a and 3a. Formation of 3a was confirmed by comparing its \(^1\)H-NMR with that of 3a obtained in FeCl\(_3\) promoted reaction of 1a.\(^8\) Subsequently, without separation, this mixture was dissolved in MeOH (8.0 mL) with NaOAc (2.0 mmol) and refluxed for 2 h. After addition of water, the resulting mixture was extracted with Et\(_2\)O. The extract was treated with sat. aqueous NaHCO\(_3\), sat. aqueous NaCl, and dried over anhydrous MgSO\(_4\) and then concentrated. The residue was subjected to TLC (CH\(_2\)Cl\(_2)/n-C\(_6\)H\(_{14}\) = 1/2) and enone 2 was obtained. Same treatment of 18 with TBPA gave the complicated mixture. Spectral data of 2a, 2b, 2c and 3a are described below.

\(3\)-methyl-2,3-\(\text{H}\) benzosuberone (2a): colorless oil; IR (Neat) 1642, 1304 cm\(^{-1}\); \(^1\)H-NMR (270 MHz) \(\delta = 2.01\) (s, 3H), 2.54 (t, \(J = 6.0\) Hz, 2H), 3.04 (t, \(J = 6.0\) Hz, 2H), 6.23 (s, 1H), 7.15–7.18 (m, 1H), 7.29-7.32 (m, 1H), 7.36-7.42 (m, 1H), 7.73–7.76 (m, 1H); \(^{13}\)C NMR (68 MHz) \(\delta = 27.0, 33.7, 34.8, 126.4, 128.2, 129.1, 129.3, 131.6, 139.0, 139.4, 158.6, 192.9.\) LRMS (EI) \(m/z\) (relative
intensity) 172 (M⁺, 61), 129 (100). HRMS (EI) calcd for C₁₂H₁₂O 172.0888, found 172.0888.

3-methyl-7,8-benzocyclooct-2-en-1-one (2b): pale yellow oil; IR (Neat) 1620, 1304 cm⁻¹; ¹H-NMR (200 MHz) δ 1.76-1.86 (m, 2H), 2.00 (s, 3H), 2.14 (t, J = 6.5 Hz, 2H), 2.83 (t, J = 6.3 Hz, 2H), 6.44-6.46 (m, 1H), 7.09–7.13 (m, 1H), 7.25-7.32 (m, 1H), 7.37-7.41 (m, 1H), 7.64–7.68 (m, 1H); ¹³C NMR (50 MHz) δ 26.8, 29.0, 29.9, 30.5, 126.5, 129.0, 129.5, 131.6, 132.3, 139.0, 142.0, 154.3, 190.7. LRMS (EI) m/z (relative intensity) 186 (M⁺, 94), 158 (100). HRMS (EI) calcd for C₁₃H₁₄O 186.1045, found 186.1048.

3-(3'-butenyl)-2,3-2H benzosuberone (2c): colorless oil; IR (Neat) 1638, 1304 cm⁻¹; ¹H-NMR (200 MHz) δ 2.22-2.39 (m, 4H), 2.54 (t, J = 5.9 Hz, 2H), 3.03 (t, J = 5.9 Hz, 2H), 4.95-5.09 (m, 1H), 5.68-5.86 (m, 1H), 6.21-6.22 (m, 1H), 7.14-7.17 (m, 1H), 7.25-7.43 (m, 2H), 7.75-7.80 (m, 1H); ¹³C NMR (50 MHz) δ 31.9, 33.6, 34.1, 40.0, 115.5, 126.7, 128.5, 129.4, 129.6, 131.9, 136.9, 139.1, 139.9, 161.4, 193.3. LRMS (EI) m/z (relative intensity) 212 (M⁺, 36), 128 (100). HRMS (EI) calcd for C₁₅H₁₆O 212.1201, found 212.1197.

3-chloro-3-methyl-2,3-benzosuberone (3a): white solid: mp 56.2-60.3 ºC; IR (Nujol) 1676, 758 cm–¹; ¹H-NMR (200 MHz) δ 1.78 (s, 3H), 2.02 (ddd, J = 15.4, 10.3, 1.2 Hz, 1H), 2.55 (ddt, J = 15.4, 8.1, 1.2 Hz, 1H), 3.05 (dd, J = 17.0, 7.9 Hz, 1H), 3.12 (dd, J = 11.7, 1.4 Hz, 1H), 3.41 (dd, J = 17.8, 10.8 Hz, 1H), 3.53 (d, J = 11.7 Hz, 1H), 7.24–7.46 (m, 3H), 7.79 (m, 1H); ¹³C NMR (50 MHz) δ 31.4, 32.4, 44.9, 57.6, 69.3, 126.6, 129.0, 130.3, 132.0, 137.8, 143.8, 198.0. LRMS (CI) m/z (relative intensity) 208 (M⁺, 69), 210 (M+2, 22), 118 (100%).

Photoreaction of cyclopropyl silyl ethers with 9,10-dicyanoanthracene (DCA) and biphenyl (BP). A solution of 1 (0.40 or 0.10 mmol), DCA (0.04 or 0.01 mmol) and BP (0.48 or 0.12 mmol) in an appropriate volume (4 or 1 mL) of solvent (MeCN, MeOH, 1,4-cyclohexadine) in the presence or absence of Cu(OAc)₂ (0.48 mmol) was purged with N₂ for 10 min prior to irradiation. The resulting mixture was irradiated with the light (λ > 340 nm) using a cut-off glass-filter for an appropriate irradiation time. While a photolysate was usually concentrated, a photolysate containing Cu(OAc)₂ was subjected to the extraction with Et₂O and water. Organic layer was treated with water, sat. aqueous NaHCO₃, sat. aqueous NaCl, and dried over anhydrous MgSO₄ and then concentrated. In both cases, the residues were subjected to TLC separation to obtain unreacted 1 and products. When column separation using n-C₆H₁₄ was performed before TLC, it was possible to recover BP (above ~90%). Characterization of product 5 was previously reported. Because purification of photo-produced 6 (2 : 1 mixture of two diastereomers, isomer 6a and 6b) could not be completed, 6 (6a : 6b = 1 : 2) was independently obtained by the hydrogenation of 17 using H₂-Pd/C. Photoreaction of 18 was similarly performed. Product 19 is a known compound. Spectral data of products 4, 6, 15, 16, and 17 are described below.

3-Propyl-3-methyl-1-indanone (4): pale yellow oil; IR (Neat) 1604 cm⁻¹; ¹H-NMR (270 MHz) δ 0.85 (t, J = 7.1 Hz, 3H), 0.89-1.01 (m, 1H), 1.21-1.33 (m, 1H), 1.41 (s, 3H), 1.43-1.75 (m, 2H),
2.44 (d, \( J = 18.9 \) Hz, 1H), 2.68 (d, \( J = 18.9 \) Hz, 1H), 7.33-7.39 (m, 1H), 7.44–7.47 (m, 1H), 7.58-7.64 (m, 1H), 7.68-7.71 (m, 1H); \(^{13}\)C NMR (68 MHz) \( \delta \) 14.6, 18.4, 28.4, 42.1, 44.7, 50.3, 123.2, 123.7, 127.3, 134.7, 135.9, 162.8, 205.9. LRMS (EI) \( m/z \) (relative intensity) 188 (M\(^+\), 72), 145 (100). HRMS (EI) calcd for C\(_{13}\)H\(_{16}\)O 188.1201, found 188.1206.

1-Benzosuberone-3-spiro-2'-methylocyclopentane (6): colorless oil: IR (Neat) 2944, 1676 cm\(^{-1}\); \(^{1}\)H-NMR (270 MHz) \( \delta \) 0.94 (d, \( J = 6.8 \) Hz, 3H, 6\( a \)), 0.97 (d, \( J = 6.5 \) Hz, 3H, 6\( b \)), 1.26-2.00 (m, 9H), 2.49 (d, \( J = 12.2 \) Hz, 1H, 6\( b \)), 2.62 (d, \( J = 11.9 \) Hz, 1H, 6\( a \)), 2.83-3.14 (m, 3H), 7.19-7.29 (m, 2H), 7.34–7.40 (m, 1H), 7.78-7.86 (m, 1H); \(^{13}\)C NMR (68 MHz) \( \delta \) 15.2 (6\( a \)), 15.5 (6\( b \)), 20.8 (6\( a \)), 21.2 (6\( b \)), 32.4 (6\( a \)), 32.7 (6\( b \)), 38.4, 39.1 (6\( a \)), 39.7 (6\( b \)), 44.2 (6\( a \)), 45.2 (6\( b \)), 45.7 (6\( a \)), 46.0 (6\( b \)), 47.2, 53.4, 126.1, 128.5 (6\( b \)), 128.7 (6\( a \)), 130.0 (6\( b \)), 130.1 (6\( a \)), 131.6, 138.6, 143.9 (6\( b \)), 144.8 (6\( a \)), 202.5 (6\( a \)), 203.6 (6\( b \)). LRMS (EI) \( m/z \) (relative intensity) 228 (M\(^+\), 70), 210 (100). HRMS (EI) calcd for C\(_{16}\)H\(_{20}\)O 228.1514, found 228.1521.

2,2-Dimethyl-1-tetralone (15): colorless oil: IR (Neat) 1684 cm \(^{-1}\); \(^{1}\)H-NMR (200 MHz) \( \delta \) 1.22 (s, 6H), 1.98 (t, \( J = 6.3 \) Hz, 2H), 2.98 (t, \( J = 6.3 \) Hz, 2H), 7.20-7.33 (m, 2H), 7.41–7.49 (m, 1H), 8.02-8.06 (m, 1H); \(^{13}\)C NMR (50 MHz) \( \delta \) 24.3, 25.7, 36.6, 41.6, 126.5, 127.9, 128.6, 131.4, 132.9, 143.3, 202.9. LRMS (EI) \( m/z \) (relative intensity) 174 (M\(^+\), 59), 118 (100). HRMS (EI) calcd for C\(_{12}\)H\(_{12}\)O 174.1045, found 174.1047.

1-Tetralone-2-spiro-3'-cyclopentylidene (16): colorless oil: IR (Neat) 1680, 1600 cm \(^{-1}\); \(^{1}\)H-NMR (270 MHz) \( \delta \) 1.67-1.77 (m, 1H), 2.04-2.59 (m, 6H), 2.84-3.07 (m, 3H), 4.89 (broad s, 2H), 7.21-7.33 (m, 2H), 7.50–7.84 (m, 1H), 8.03-8.05 (m, 1H); \(^{13}\)C NMR (68 MHz) \( \delta \) 26.4, 31.1, 33.6, 34.2, 42.0, 52.9, 106.2, 126.5, 127.8, 128.5, 131.6, 133.0, 143.3, 150.5, 201.1. LRMS (EI) \( m/z \) (relative intensity) 212 (M\(^+\), 39), 197 (100). HRMS (EI) calcd for C\(_{15}\)H\(_{16}\)O 212.1201, found 212.1197.

1-Benzosuberone-3-spiro-2'-cyclopentylidene (17): colorless oil: IR (Neat) 1676, 1598 cm \(^{-1}\); \(^{1}\)H-NMR (270 MHz) \( \delta \) 1.60-1.84 (m, 5H), 2.04 (dd, \( J = 14.6 \), 8.6 Hz, 1H), 2.45-2.50 (m, 2H), 2.64 (d, \( J = 10.8 \) Hz, 1H), 2.93-3.02 (m, 2H), 3.17 (dd, \( J = 16.5 \), 9.5 Hz, 1H), 4.86 (broad s, 1H), 4.92 (broad s, 1H), 7.22-7.30 (m, 2H), 7.36–7.41 (m, 1H), 7.81-7.84 (m, 1H); \(^{13}\)C NMR (68 MHz) \( \delta \) 21.9, 32.0, 32.9, 39.4, 40.2, 46.4, 52.1, 104.8, 126.2, 128.7, 130.1, 131.5, 138.3, 144.3, 158.6, 202.0. LRMS (EI) \( m/z \) (relative intensity) 226 (M\(^+\), 87), 131 (100). HRMS (EI) calcd for C\(_{16}\)H\(_{18}\)O 226.1358, found 226.1354.

Discussion on photoinduced electron transfer processes involving cyclopropyl silyl ethers, DCA and BP. Oxidation potentials (\( E_{\text{ox}1/2} \) V vs. SCE) were obtained to be +1.53, +1.80, +1.36, +1.36, and 1.84 for 1\( a \), 1\( b \), 1\( c \), 1\( d \) and 18, respectively. Reduction potential of the singlet excited state of DCA (\(^{1}\)DCA\(^*\)) is reported to be +1.97 on the basis of reduction potential (\( E_{\text{red}1/2} = -0.89 \) V vs. SCE) and the excitation energy (\( E_{00} = 66 \) kcal/mol) of DCA.\(^9\) Therefore, single electron transfer (SET) from 1 and 18 to \(^{1}\)DCA\(^*\) should be feasible. On the other hand, SET from 1\( a \), 1\( c \) and 1\( d \) to
the radical cation of BP (BP⁺) is exoergonic while that from 1b and 18 to BP⁺⁺ are slightly endoergonic on the basis of the reported oxidation potential of BP (\(E_{\text{ox1/2}}^{\text{BP}} = +1.77 \text{ V vs. SCE})\). However, the radical ion pair generated by SET between electron-donating substrate and 1DCA* has a tendency to undergo unproductive back electron transfer to give starting substrate. Therefore, in the reaction systems reported in this paper, BP⁺⁺ appeared to act as more effective catalyst than 1DCA* although SET processes for 1b and 18 with BP⁺⁺ are energetically less favorable.

References
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9
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![Chemical Structure](attachment:image.png)