Unique Selectivity in Iodohydroxylation Reaction of Allenyl Phenyl Sulfoxides.

A Stereodefined Synthesis of (*E*)-2-Iodo-3-hydroxy-1-alkenyl Sulfoxides

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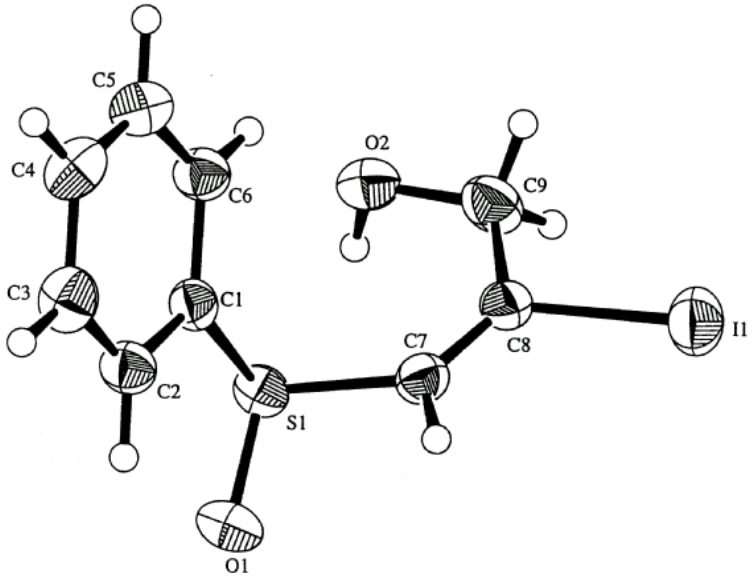
Supporting Information

Iodohydroxylation Reactions of Allenyl Phenyl Sulfoxides.

(a) (*E*)-2-Iodo-3-(phenylsulfinyl)-2-propen-1-ol (*E*-2a): solid, m.p. 115.5-116.5^{o}C (dichloromethane-hexane); ^{1}H NMR δ 7.60-7.74 (m, 2H), 7.44-7.60 (m, 3H), 6.89 (s, 1 H), 4.69 (d, *J* = 5 Hz, 1H), 4.56 (d, *J* = 5 Hz, 1H), 3.98 (bs, 1H); EI-MS, *m/z* 308 (M^{+}, 100); IR (KBr) 3219, 1589, 1473, 1012 cm^{-1}.



ORTEP presentation of ***E*-2a**

(b) (*E*)-2-Iodo-3-phenyl-3-(phenylsulfinyl)-2-propen-1-ol (*E*-2b): solid, m.p. 147-148°C (dichloromethane/hexane); ^{1}H NMR δ 6.89-7.56 (m, 8H), 6.49-6.89 (s, 2H), 5.13 (d, *J* = 3.5 Hz, 1H), 5.02 (d, *J* = 5 Hz, 1H), 3.40 (bs, 1H); SCI-MS, *m/z* 385 (MH^+, 56.04), 131 (100); IR (KBr) 3356, 1616, 1017 cm^{-1}; Anal. Calcd for $C_{15}H_{13}IO_2S$: C, 46.89; H, 3.41. Found: C, 46.70; H, 3.22.

(c) (*E*)-2-Iodo-3-(phenylsulfinyl)-2-hepten-1-ol (*E*-2c): solid, m.p. 83-84°C (dichloromethane/hexane); ^{1}H NMR δ 7.40-7.68 (m, 5H), 4.94 (d, *J* = 3.5 Hz, 1H), 4.87 (d, *J* = 5 Hz, 1H), 2.90 (bs, 1H), 2.37-2.52 (m, 1H), 2.08-2.22 (m, 1H), 1.33-1.53 (m, 2H), 1.09-1.33 (m, 2H), 0.77 (t, *J* = 7.3 Hz, 3H); SCI-MS, *m/z* 365 (MH^+, 100); IR (KBr) 3324, 1615, 1042 cm^{-1}; Anal. Calcd for $C_{13}H_{17}IO_2S$: C, 42.87; H, 4.70. Found: C, 43.04; H, 4.61.

(d) (*E*)-2-Iodo-4,4-dimethyl-1-(phenylsulfinyl)-1-penten-3-ol (*E*-2d): solid, m.p. 163.5-164.5°C (dichloromethane/hexane); d.e. ratio: 93:7; ^{1}H NMR δ 7.65-7.73 (m, 2H), 7.47-7.59 (m, 3H), 7.21 (s, 1H), 4.36 (s, 1H), 4.00 (bs, 1H), 1.07 (s, 9H); The following data are discernible for the other diastereoisomer: 7.08 (s, 1H), 4.41 (s, 1H); SCI-MS, *m/z* 365 (MH^+, 11.7), 57 (100); IR (KBr) 3422, 1626, 1032 cm^{-1}; Anal. Calcd for $C_{13}H_{17}IO_2S$: C, 42.87; H, 4.70. Found: C, 42.73; H, 4.76.

(e) (*E*)-3-Iodo-2-methyl-4-(phenylsulfinyl)-3-buten-2-ol (*E*-2e): solid, m.p. 147.5-148.5°C (ethyl actate/hexane); ^{1}H NMR δ 7.73-7.87 (m, 2H), 7.42-7.60 (m, 3H), 6.73 (s, 1H), 2.90 (bs, 1H), 1.66 (s, 3H), 1.44 (s, 3H); EI-MS, *m/z* 336 (M^+, 0.71), 43 (100); IR (KBr) 3262, 1626, 1021 cm^{-1}; Anal. Calcd for $C_{11}H_{13}IO_2S$: C, 39.30; H, 3.90. Found: C, 39.13; H, 3.70.

(f) 1-[(*E*)-1'-Iodo-2'-(phenylsulfinyl)ethenyl]-1-cyclohexanol (2f): solid, m.p. 173-174^{o}C (dichloromethane/hexane); ^{1}H NMR δ 7.72-7.87 (m, 2H), 7.42-7.58 (m, 3H), 6.77 (s, 1H), 4.20 (bs, 1H), 1.13-2.25 (m, 10H); SCI-MS, *m/z* 377 (MH^{+}, 11.12), 359 (100); IR (KBr) 3235, 1029 cm^{-1}; Anal. Calcd for $C_{14}H_{17}IO_2S$: C, 44.69; H, 4.55. Found: C, 44.45; H, 4.40.

(g) (*E*)-3-Iodo-2-methyl-4-(phenylsulfinyl)-3-octen-2-ol (*E*-2g): solid, m.p. 150-152^{o}C (dichloromethane /hexane); ^{1}H NMR δ 7.84-7.87 (m, 2H), 7.74-7.50 (m, 3H), 3.95 (bs, 1H), 2.55-2.65 (m, 1H), 2.38-2.48 (m, 1H), 1.81 (s, 3H), 1.71 (s, 3H), 1.43-1.54 (m, 1H), 1.20-1.34 (m, 2H), 0.94-1.03 (m, 1H), 0.826 (t, *J* = 7.3 Hz, 3H); SCI-MS, *m/z* 393 (MH^{+}, 27.84), 375 (100); IR (KBr) 3218, 1673, 1029 cm^{-1}; Anal. Calcd for $C_{15}H_{21}IO_2S$: C, 45.93; H, 5.40. Found: C, 45.81; H, 5.32.