

Supporting Information

Visible-light induced phenylchalcogenyl-oxygenation of activated allenes with ambient air as sole oxidant

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General information:

All reactions were conducted under open air atmosphere. Apparatus used for reactions were oven dried. THF was distilled over sodium benzophenone ketyl before use. MeCN purchased directly from the commercial suppliers and used without further purification. Starting materials (**1a**, **8a**, **4m-q**),¹ **8c**,² **4j**, **4k**, **4l**, **6a**, **10a**,³ **4b**,⁴ **4c**⁵ **4d**,⁶ **4e**,⁷ **4f-g**,⁸ and **4q**⁹ were prepared according to the reported procedure. All other chemicals used were commercially available. Progress of the reactions was monitored by TLC on pre-coated silica gel 60 F-254. Evaporation of solvents was performed at reduced pressure on a rotary evaporator. Column chromatography was carried out with silica gel grade 60-120 and 100-200 mesh. ¹H NMR spectra were recorded at 300, 400 & 500 MHz and ¹³C NMR 75, 100 & 125 MHz in CDCl₃. Chemical shifts (δ) are reported in ppm. Tetramethylsilane (δ = 0.00 ppm for ¹H) and CDCl₃ (δ = 77.00 ppm for ¹³C) were used as the internal standard. Scalar coupling constants (J) are reported in hertz (Hz). The following abbreviations are used to designate the multiplicities: s = singlet, d = doublet, t = triplet, dd = doublet of doublet, ddd = doublet of doublet of doublet, m = multiplet, br.s = broad singlet. Mass spectral data were compiled using MS (ESI), and High resolution mass spectra (HRMS) were recorded by ESI probe in positive mode using ORBITRAP analyzer.

Electrochemical measurements were performed on a PC-controlled CH instruments model CHI 620C electrochemical analyzer. The experiments were performed in a 1 mM phenyl allene solution in CAN at scan rate of 100 mV s⁻¹ using 0.1 M tetrabutyl ammonium perchlorate (TBAP) as supporting electrolyte. The working electrode was glassy carbon, a standard calomel electrode (SCE) was the reference electrode and platinum wire was an auxiliary electrode. After a cyclic voltammogram (CV) had been recorded, ferrocene was added, and a second voltammogram was measured.

The UV spectrum was recorded on a HITACHI U-2910 double beam UV/VIS spectrophotometer.

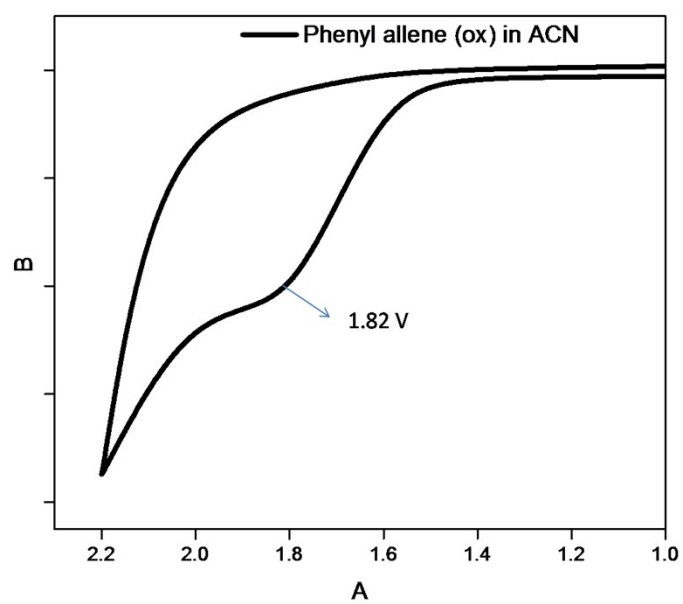


Figure 1. 3-Phenyl propa-1,2-diene **1a** oxidation potential in MeCN

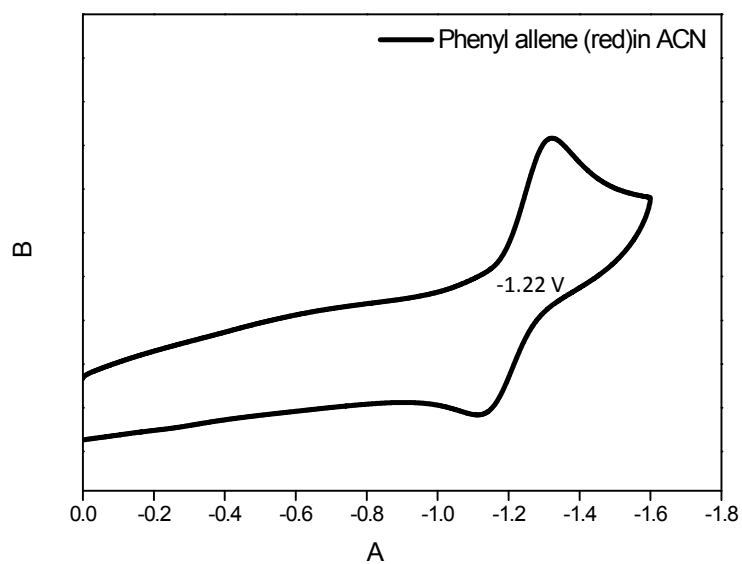
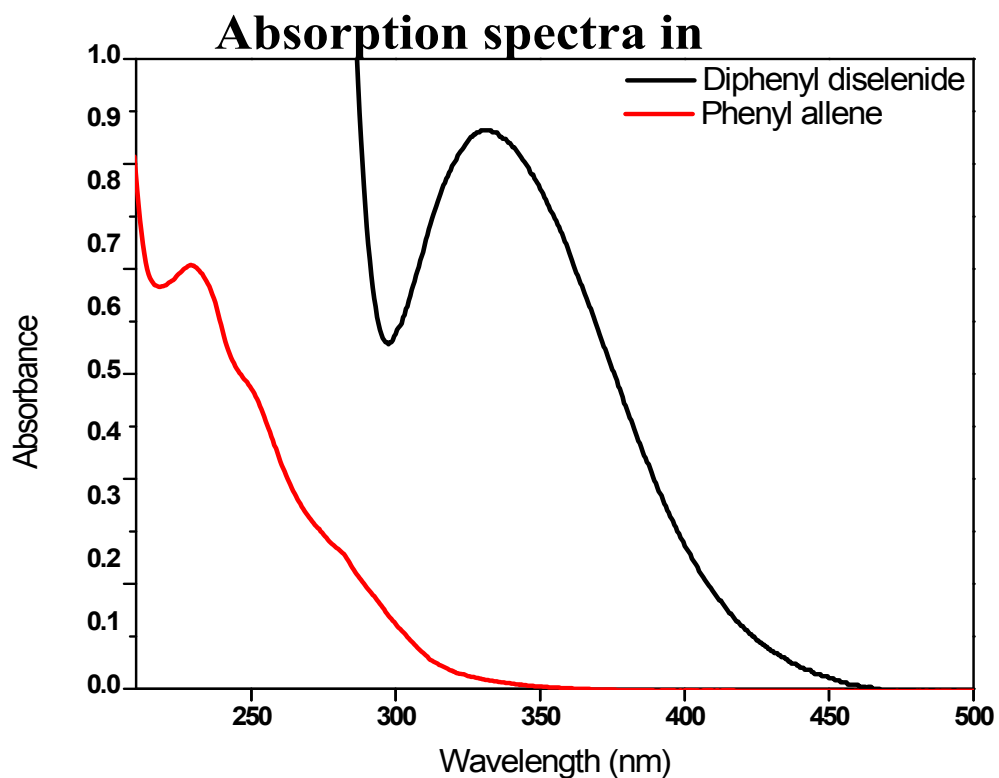


Figure 2. 3-Phenyl propa-1,2-diene **1a** reductive potential in MeCN



Absorption spectra in

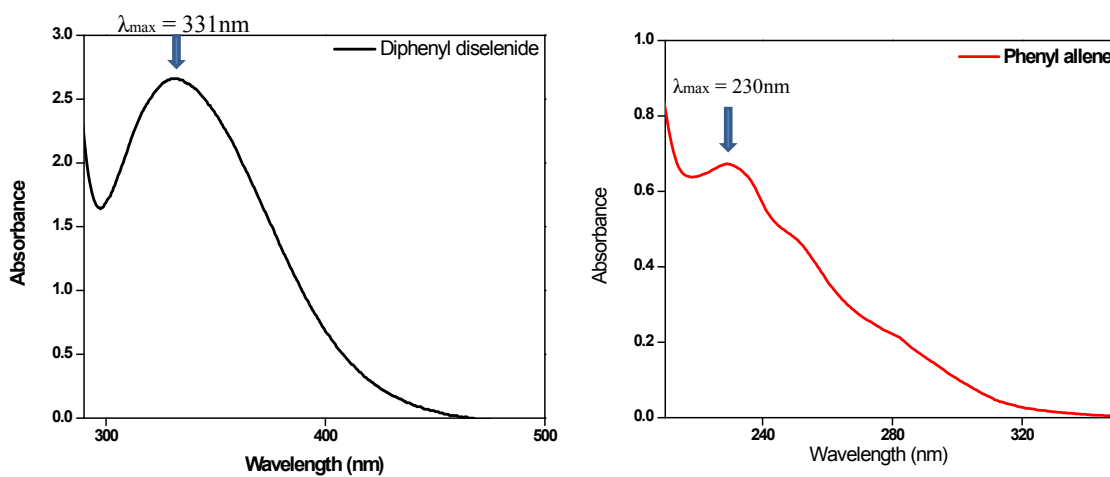


Figure 3. UV spectrum of 3-phenyl propa-1,2-diene **1a** and PhSeSePh, **2a** in MeCN

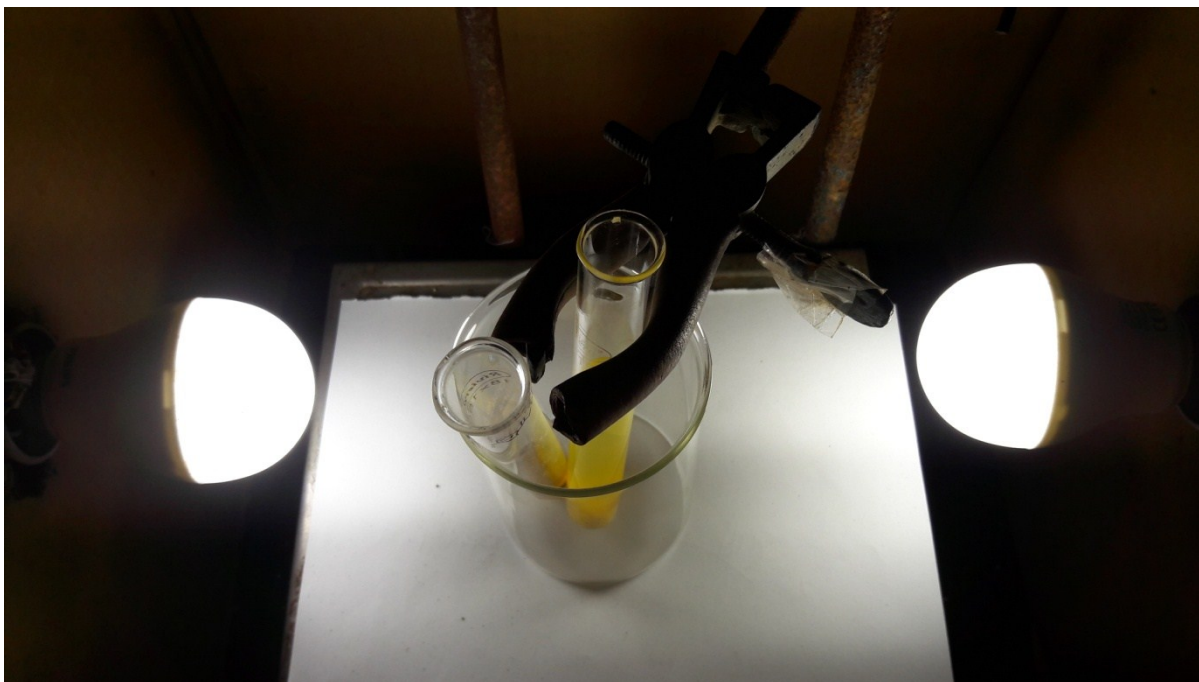
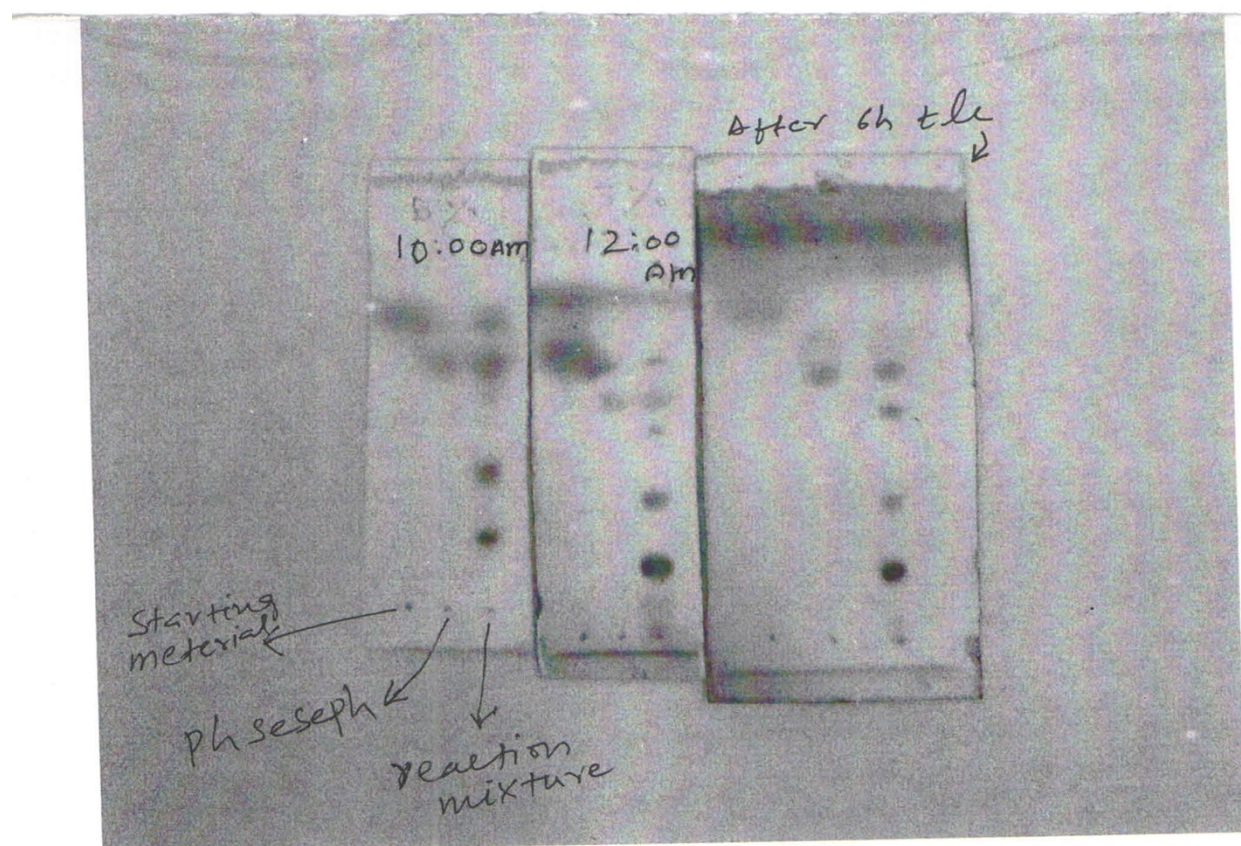


Figure 4. Irradiation of reaction mixture with two 7W Day light white LED bulbs [6500K, 42mA (220-240Vac 50Hz) PHILIPS, Made in India]

References:

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TLC images of **3a** with different intervals:



3a
Z:E mixture spectra (crude)

