

## Synthesis, spectroscopic and computational investigation of bis (3-methoxyphenylthio) ethyl naphthalene

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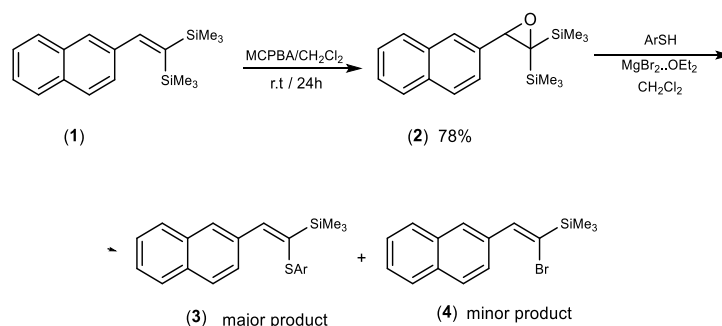
## ABSTRACT

In this study, we report an interesting combined experimental and theoretical studies on the molecular structure of 2-(2,2-bis(3-methoxyphenylthio)ethyl)naphthalene (**5**). The compound **5** was unexpectedly synthesized and characterized by FT-IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR, mass spectrum, and elemental analyses. The optimized geometry and Mulliken charge density on atoms of **5** were calculated by RM062X and PBE1PBE methods using a 6-31+G(d) basis set. The experimental obtained IR spectra of **5** was compared to the theoretical results at the RM062X/PBE1PBE/6-31+G(d) level which explained in terms of potential energy distribution (PED) analysis. The scaled theoretical vibrational wavenumber displayed very good agreement with experimental data. The calculated proton and carbon chemical shifts show almost a nice correlation with experimental data using RM062X/6-31+G(d) level. Theoretical investigations of frontier molecular orbitals, mapped molecular electrostatic potential (MEP), thermodynamic properties and physico-chemical characteristics of **5**, were also acquired.

## 1. Introduction

2,2-Bis(trimethylsilyl)oxirans are very significant compounds that used to production of organosilicon compounds [1,2]. Cleavage reaction of epoxide rings with thiols is very beneficial in pharmaceutical and natural product chemistry [3]. Commonly, thiolysis of epoxides can be performed by a base [4] or a Lewis acid [5], or in the existence of a heterogeneous catalysts [6]. Ring opening reactions of epoxides having organosilicon group with the attack of the nucleophiles has been extensively investigated [7-9]. These compounds react with various types of reactants *via* cleavage reaction of epoxide ring. The cleavage reaction of epoxide ring in alkyl silicon compounds has generally led to produce 1-trimethylsilylvinyl sulfides, **3**, as a major product and 1-bromovinyl silane, **4**, as a minor product through reaction between (3-(naphthalen-2-yl)-2,2-bis(trimethylsilyl) oxiran, **2**, with ArSH/MgBr<sub>2</sub> (Scheme 1). In this study, however, cleavage reaction of (3-(naphthalene-2-yl)-2,2-bis(trimethylsilyl) oxiran, **2**, surprisingly produces **5** as a major product and 1-bromovinyl silane, **4**, as a minor product in the presence of magnesium bromide catalyst and 3-methoxythio phenol (Scheme 2). In this study, we proposed an interesting mechanism for the synthesis of **5**

(Scheme 3). Also, the structural explanations for **5** such as geometrical optimization is scrutinized using both experimental and theoretical methods including M062X and PBE1PBE methods using 6-31+G(d) basis set. Vibrational wavenumber, proton and carbon NMR chemical shifts, energy gaps and HOMO-LUMO orbitals were performed with same methods using 6-31+G(d) basis set.



**Scheme 1.** Preparation of 1-trimethylsilylvinyl sulfides, **3**, in major product and 1-bromovinyl silane, **4**, in minor product.

## 2. Experimental

## 2.1 General method

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