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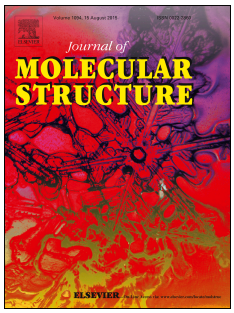

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Synthesis and characterization of sulfolane-based amino alcohols: a combined experimental and computational study

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Abstract

Aminolysis of 3,4-epoxysulfolane in aqueous media leads to a very complex mixture of products with unresolved stereochemistry. Herein, we report a detailed theoretical and experimental mechanistic investigation of this reaction along with extensive spectroscopic characterization of the resulting amino alcohols, using 1D and 2D NMR techniques (^{1}H, ^{13}C, NOE, NOESY, COSY, HSQC, HMBC) as well as XRD analysis. In addition to simple amines such as ammonia and benzylamine, our study also employed the more sterically hindered *endo*-bicyclo[2.2.1]hept-5-en-2-ylmethanamine. The mechanism of the aminolysis of 3,4-epoxysulfolane by aqueous ammonia was studied in more detail using quantum chemical calculations at the MO6-2X/6-31++G** level of theory. The computational results led us to conclude that the most probable way of initial epoxide transformation is base-catalyzed rearrangement to a corresponding allylic alcohol. Subsequent formation of vicinal amino alcohols and diols proceeds *via* addition of ammonia or hydroxy-anions to activated double C=C bond with some preference of a *cis*-attack. Detailed analytical data obtained in the course of our work will be useful for the stereochemical identification of new sulfolane derivatives.

Keywords amino alcohols, rearrangement, quantum chemical calculations, XRD analysis, 2D NMR investigation