

Reactions of Heterocumulenes with Organometallic Reagents: XXII.* Quantum Chemical Study of Structural Transformations of Benzylsulfanyl-Substituted 2-Aza-1,3,5-triene by the Action of Superbases. Concurrent Formation of 4,5-Dihydro-3*H*-azepine and 4,5-Dihydro-1,3-thiazole

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Abstract—The formation of 4,5-dihydro-3*H*-azepine and/or 4,5-dihydro-1,3-thiazole structures in the reaction of 1-(benzylsulfanyl)-2-methoxy-*N*-(propan-2-ylidene)buta-1,3-dien-1-amine (2-aza-1,3,5-triene) with potassium *tert*-butoxide or lithium diisopropylamide has been analyzed by B3LYP/6-31G(*d,p*) quantum chemical calculations. According to the calculations, the reaction with potassium *tert*-butoxide gives 4,5-dihydro-3*H*-azepine and 4,5-dihydro-1,3-thiazole derivatives with almost equal probabilities, whereas lithium diisopropylamide clearly favors the formation of thiazole ring.

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