

*Dedicated to Full Member of the Russian Academy of Sciences
B.A. Trofimov on the 65th Anniversary of His Birth*

Quantum-Chemical Study of the Mechanism of Formation of 1- and 2-(Trimethylsilylmethyl)benzotriazoles

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Abstract - Quantum-chemical study of the mechanism of formation of 1- and 2-(trimethylsilylmethyl)benzotriazoles, including the reaction of 1,2,3-benzotriazole with sodium methoxide, showed that the predominant formation of the 1-substituted isomer is determined by favorable combination of the thermodynamic and kinetic parameters of the process.