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Dynamic ^{1}H-NMR demonstration of anomeric effect and structure: conformational and configurational analysis of N-2-(1,4-dioxane)-N'-(p-methylbenzenesulfonyl)- O-(p-methylphenoxy) İsourea

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Abstract: The conformational and configurational behavior and the structure of N-2-(1,4-dioxane)-N'-(p-methylbenzenesulfonyl)-O- (p-methylphenoxy) isourea (1) were studied using dynamic NMR. The endo-anomeric effect, hydrogen bonding, temperature, and polarity of solvent control the population of dioxane ring conformers or anomers but not the configuration interconversion of the imine of the imidoyl moiety. Dynamic ^{1}H-NMR, Δ H°, Δ S°, Δ G°, and Δ G‡ analysis of 1 demonstrates that the dioxane ring adopts the chair conformation, that the imidoyl amino group prefers axial conformation, and that the tosyl and tolyl groups about the C=N bond retain the E configuration.

Key Words: Anomeric effect, dynamic NMR, conformational analysis, configurational analysis, hydrogen bonds, dioxane, aminoimidoyl.

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