

PL-21**RESENT ADVANCES IN THE CHEMISTRY OF MACROCYCLES****Andrei K. Yudin***University of Toronto**Department of Chemistry, 80 St. George St., Toronto, ON, M5S 3H6 Canada*

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Abstract. Knowledge of the thermally accessible ensemble of conformers is useful in many applications because the corresponding conformations define the shape of the molecule, which determines its physical and biological properties. For instance, a cyclohexane ring typically prefers the chair over the twist-boat conformation. Although the barrier for interconversion can be readily overcome at ambient temperature, the energy difference of approximately 5.5 kcal mol⁻¹ makes the high-energy twist-boat conformation challenging to observe. The introduction of bulky substituents into the cyclohexane structure, however, can remodel the energy landscape and allow the twist-boat conformation to be detected. Apart from such rare exceptions in small rings, there is currently no easy way to access the less common conformations of complex molecules under fast exchange. We refer to such rarely observed metastable states as the ‘dark conformational space’.



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