

Experimental and Theoretical Conformation Analysis of Eight-Membered Silocines with Planar Fragments

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Abstract—The dipole moments of 6-thia-4,5:6,7-dibenzo-1,3,2-dioxasilocines were determined experimentally and calculated at the DFT B3LYP/6-31G* level of theory and by the additivity scheme. The experimental and theoretical (DFT B3LYP/6-31G*) conformation analysis of eight-membered 1,3,2-dioxasilocines having planar fragments showed that these compounds in solution exist as *boat-chair*, *boat-boat*, or *twist-boat* conformers, depending on the presence of unsaturated planar fragment, nature of the heteroatom in position 6 of the eight-membered ring, and substituents on the silicon atom.

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