CONFORMATIONAL ANALYSIS OF 1,3-DIOXA-2-BORACYCLOALKANES

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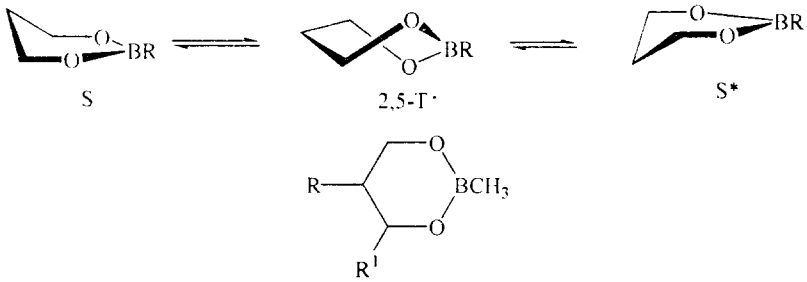
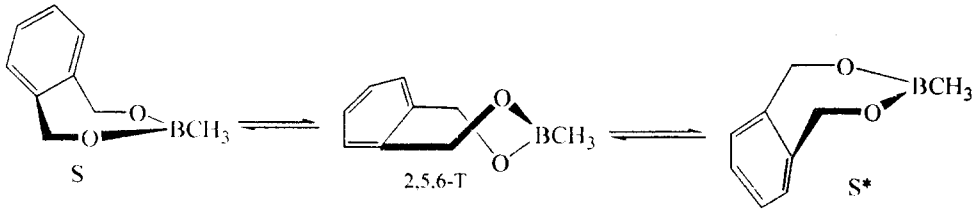
In accordance with NMR ^1H results together with empirical (MM+) and quantum-chemical *ab initio* computations the potential energy surface of 1,3-dioxa-2-boracycloalkanes (the energy differences between axial and equatorial forms [ΔE, kcal/mol] and barriers of ring inversion [$\Delta E^{\neq}$, kcal/mol]) has been described. The conformational behavior of six-membered rings includes axial-equatorial equilibrium between two forms of *sofa* (S and S*) over 2,5-*twist*-form (2,5-T).



R	R^1	method	ΔE	$\Delta E^{\neq}$
CH_3	H	MM+	0.9	7.7
		MP2/6-31G*	0.6	9.1
		MP2/6-31G**	0.6	9.1
H	CH_3	MM+	0.8	7.0
		MP2/6-31G*	0.9	8.8
		MP2/6-31G**	0.9	8.7
		MP2/6-311G**	1.0	8.3
		MP2/D95**	0.8	7.9

The conformational behavior of seven-membered rings also includes equilibrium between two forms of *sofa*.



The theoretical $\Delta E^{\neq}$ of this process lays between 6.3 (MM+) and 9.0 (STO-3G) kcal/mol.