OP-19

SILACYCLOHEXANES: CONFORMATIONAL PREFERENCES IN GAS AND SOLUTION

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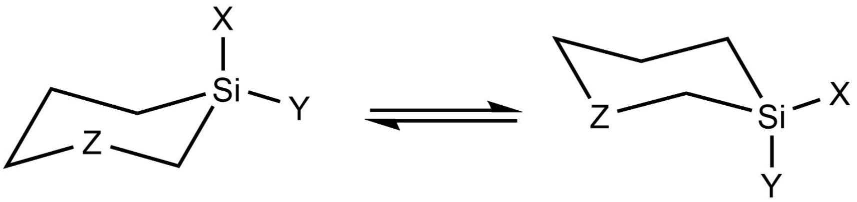
Conformational preferences of silacyclohexanes possessing different substituents at silicon, as well as of their heteroanalogues with N, O, S atoms in the ring will be outlined including recent theoretical and experimental research in gas and solution. The reasons of principal differences between the title compounds and their carbon analogues are established; the main factor is the decisive role of the bulkiness of the substituent at carbon, which can often be neglected for the substituents at silicon, and the dominant role of electrostatic effects in silacyclohexanes, which is a very subordinate effect in cyclohexanes.

Two other discriminating factors are (i) much lower conformational energies (*A*) of the substituents at silicon resulting in appearance or even predominance of the axial conformers and (ii) much lower barriers to ring inversion in silacyclohexanes as compared to those in cyclohexanes, piperidines, tetrahydropyranes or thianes, that makes the title compounds conformationally very flexible. Specific role is played also by stereoelectronic interactions of heteroatoms in the ring with highly polar Si–X bonds, especially for electronegative groups X. All these issues will be discussed in the lecture summarizing research up to 2019.



X, Y = H, Me, Ph, F, Cl, Br, OR, CN;
Z = CH_2, NR, O, S.