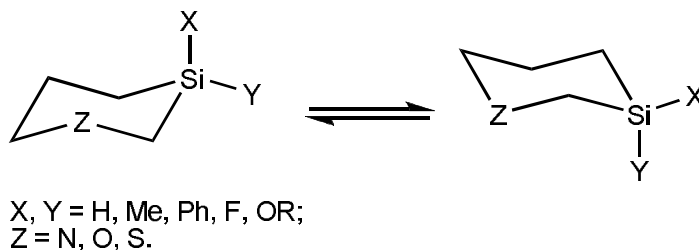


Conformational analysis of silaheterocyclohexanes versus their carbon analogues

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Conformational analysis of 3-silathianes,¹ 3-silapiperidines,² 3-silatetrahydropyran³ in gas phase and solution by LT NMR, FTIR spectroscopy, gas phase electron diffraction showed principal differences in the conformational behavior of silaheterocyclohexanes as compared to their carbon analogues, as partly summarized in.⁴ Energetically, the main differences are much lower conformational energies (Δ) of the substituents at silicon resulting in appearance or even predominance of the axial conformers and lower barriers to ring inversion with respect to cyclohexanes, thianes, piperidines, tetrahydropyranes. Structurally silaheterocyclohexanes are characterized by the longer Si–C vs. C–C bonds and less folding of the “Si-part” of the ring than of the “C-part” or “Z-part”, which is responsible for the observed energetic differences.



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