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Effect of the medium on the equilibrium between stereoisomeric six- and seven-membered cyclic chair-like acetals. Role of nonspecific and specific interactions

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Abstract

Principles for establishing the nature of solvation effects in stereoisomeric equilibria have been formulated. Using ¹H NMR spectroscopy, the equilibrium constants have been determined in 12 solvents for the endo and exo isomers of 1,9,10,11,12,12-hexachloro-4-6-dioxatricyclo[7.2.1.0^{2,8}]dodec-10-ene which is characterized by a high barrier to stereoisomeric transformations. The results of correlation analysis have shown that solvation of the conformers with dissimilar orientations of the hexachloronorbornene fragment with respect to the chair-like acetal moiety is determined by the polarity and proton-acceptor properties of the medium. Comparison with the data on solvent effect on the equilibrium between 2-isopropyl-5-methoxy-1,3-dioxane epimers suggests that the formation of H-complexes is controlled by electronic and conformational factors.

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