

Steric structure of heterocycles containing phosphorus - 51. Conformational heterogeneity of 4,5;7,8-dibenzo- 2-thiono-1,3,2-dioxaphosphocenes

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Abstract

¹H and ³¹P dynamic NMR, vibrational spectroscopy, and consideration of dipole moments have shown that 2-chloro-2-thiono-4,5;7,8-dibenzo(4,4'-dimethyl-6,6'-di-tert-butyl)-1, 3,2-dioxaphosphocene and its 2-ethoxy derivative are conformationally heterogeneous. The former exists as a three-component equilibrium mixture, and the latter as a two-component equilibrium mixture. In the chlorothiophosphate the boat-chair conformation predominates, with equatorial location of thiophosphoryl; next in frequency is boat-chair with axial orientation of P=S, and third is the deformed boat form. In the ethyl thiophosphate the preponderant form is the deformed boat with thiophosphoryl in the equatorial position. © 1991 Plenum Publishing Corporation.

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