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Three-dimensional structure of phosphorus-containing heterocycles. 48. 2-methoxy-5,6-benz-1-3,2-dioxaphosphepine oxide and sulfide

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Abstract

Using PMR spectroscopy and the dipole moment and Kerr effect methods it has been shown that 2-methoxy-5,6-benzo-1,3,2-dioxaphosphepine oxide and sulfide are characterized by solution equilibria involving two chair-like (C) conformers e-C \rightleftharpoons a-C, which are shifted in favor of the e-C form; in the case of an equatorial orientation of the methoxy group equilibrium involves the gauche and anti rotamers, while in the case of an axial orientation (of the methoxy group) the gauche rotamer of the methyl group relative to P=O or P=S bond is stabilized. The presence of a twist conformer in the case of the oxide cannot be precluded from consideration. © 1989 Plenum Publishing Corporation.

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