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Phosphorus, Sulfur, and Silicon and the Related Elements

Publication details, including instructions for authors and subscription information: http://www.informaworld.com/smpp/title~content=t713618290

Pyrimidinic Cyclic Thiophosphorylic Esthers with Biological Activity

O. Musat^a; I. Penesan^a; M. Horn^a; S. Musat^b; M. Culea^b; A. Hantz^a

^a Institute of Chemistry, Entreprise of Chemical Drugs "Terapia", Romania ^b Institute of Isotopic and Molecular Technology, Cluj-Napoca, Romania

To cite this Article Musat, O. , Penesan, I. , Horn, M. , Musat, S. , Culea, M. and Hantz, A.(1990) 'Pyrimidinic Cyclic Thiophosphorylic Esthers with Biological Activity', Phosphorus, Sulfur, and Silicon and the Related Elements, 51:1,388 To link to this Article: DOI: 10.1080/10426509008040915

URL: http://dx.doi.org/10.1080/10426509008040915

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PYRIMIDINIC CYCLIC THIOPHOSPHORYLIC ESTHERS WITH BIOLOGICAL ACTIVITY

O.MUSAT, I.PENESAN, M.HORN, S.MUSAT*, M.CULEA*, and A.HANTZ

Institute of Chemistry, Entreprise of Chemical Drugs "Terapia", Romania

*Institute of Isotopic and Molecular Technology, 3400 Cluj-Napoca, Romania

Pyrimidinic derivates of dioxaphosphorinan-2-thione (I) have been synthesized by substituting the chlorine atom in 2-chloro-2-thiono-5,5'-dimethyl-1,2,2-dioxaphosphorinane by 2'-substituted-6'-methyl-4'-hydroxypyrimidine

$$X = SCH_{3}, NH_{2}, N(CH_{3})_{2}, N(CH_{3})_{2}, N(CH_{3})_{2}$$

$$X = SCH_{3}, NH_{2}, N(CH_{3})_{2}, N(CH_{3})_{2}$$

Crystal structure by X-ray diffractometry and physico--chemical characteristics were established.

IR spectra show bands characteristic to the basic functional groups of the molecule. ^{31}P NMR spectra show high shielding of the thionic phosphorus atom. ^{1}H NMR spectra reveal the P-H coupling phenomenon with the 5'-CH and 4,6-CH $_{2}$ protons. The difference between the values of the chemical shifts of axial and equatorial 5-CH $_{3}$ protons can be explained with the existence of a conformational equilibrium.

The mass spectra reveal the molecular ion being basic. The fission of P-O bond(pyrimidinyl) and elimination of X radical was demonstrated.

The fungicide effect of the compounds X was established by the biological tests.