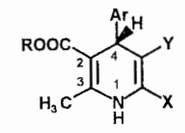
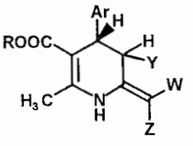
A series of 1,4-dihydropyridines (**1**), 1,4,5,6-tetrahydropyridines (**2**) 1,4-dihydro-1,6-naphthyridines (**3**) 1,4,5,6-tetrahydro-1,6-naphthyridines (**4**) have been synthesized as potential calcium antagonists and analyzed by X-ray diffraction.
In the solid state the unsymmetrically substituted 4-aryl group is always in axial position oriented either toward the C-4 hydrogen (synperiplanar) or away from the C-4 hydrogen (antiperiplanar). The orientation of the aryl group might influence receptor binding (G. Rovnyak et al., *J. Med. Chem.*, **1988**, *31*, 936).



1



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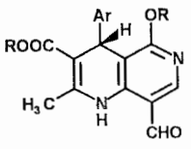

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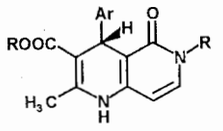
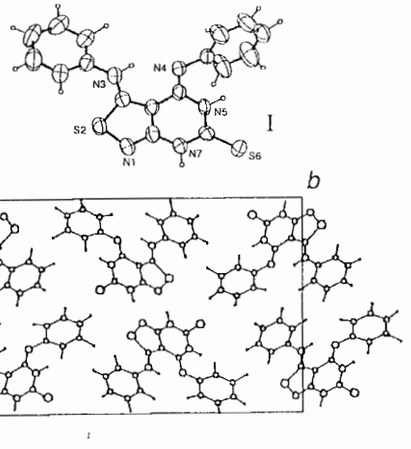


4

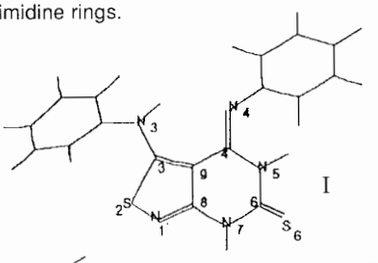
PS-06.05.11 CRYSTAL STRUCTURE OF 3-PHENYLAMINO-4-PHENYLIMINOISOTHIAZALO-[3,4-d] PYRIMIDINE-6(5H-7H)-THIONE. P. Phavanantha*, C. Katarapanich°, S. Akarapanichkorn° and T. Taga+. * Chulalongkorn Univ., Crystallography Lab, Bangkok 10330, Thailand. + Kyoto Univ., Faculty of Pharmaceutical Sciences, Kyoto, Japan.

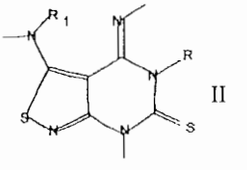
3-phenylamino-4-phenyliminoisothiazalo-[3,4-d] pyrimidine-6(5H-7H)-thione, $C_{17}H_{13}N_5S_2$, M_r =351.45, monoclinic, $P2_1/a$, a = 15.590(4), b = 22.176(4), c = 4.724(2) A°, β = 92.68(2), V = 1631.3 A°^{3}, Z=4, D_m(297K) = 1.400, D_x=1.431 g cm^{-3}, CuKα, λ = 1.54178 A°, μ = 29.72 cm^{-1}, F(000) = 728, T =298 K, R = 0.061 for 1474 reflections.

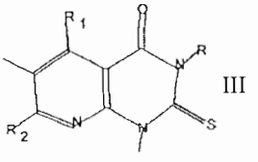


The compound (I) was formed as a reaction product in the preparation of an isothiazalolpyrimidine analog (II) based on isosterism with sulfur atom replacing ethylenic moieties of some pyridopyrimidinethione derivatives (III) reported to possess significant antimicrobial and antihistaminic activities [Dave, Shah, Desai, Srinivasan (1982). *Ind. J. Pharm. Sci.* **44(4)**, 83]. The compound is possibly a rearrangement product of the isothiazalopyrimidine analog (II), and may be similar to the rearrangements reported in several other ring systemss [Brown (1961). *Nature* **189**, 828].

The intramolecular hydrogen-bond may be formed by the amino-hydrogen atom and imino-nitrogen atom between N(3)H...N(4). The molecules in the crystal form dimers by two intermolecular N(7)H...N(1) hydrogen bonds bridging the pyrimidine rings.







PS-06.05.12 CRYSTAL STRUCTURES OF (I) 2,10-DICHLORO 6-ETHOXY-DIBENZO [d,g] [1,3,6,2] DIOXA THIAPHOSPHOCIN 6-OXIDE and(II) 8-(PHENOXY)-16H -DINAPTHO [2,1-d; 1',2'-g] (1,3,6,2) DIOXATHIA PHOSPHOCIN 8-OXIDE: CONFORMATION OF 8-MEMBERED HETEROCYCLIC RING:
M.KRISHNAIAH, S.MANI NAIDU, N.JAGADEESH KUMAR, Department of Physics, College of Engineering, Sri Venkateswara University, TIRUPATI-517 502, INDIA.

Biologically the cyclic forms of organophosphorus compounds containing phosphoryl units react rapidly with proteins and nucleic acids in the cell to alkylate carboxyl, sulfhydroxyl and amino groups. Suitably substituted phosphoryl units in the molecule exhibit significant physiological activity (Schrader, 1963). These molecules play an important role as insecticides, pesticides, nerve gases, etc. Dioxaphosphocin derivatives have applications as bactericides, fungicides, lubricants, insecticides, etc. The structures of the title compounds have been investigated to know the effect of the substituents on the conformation of the hetero ring.

(I) Crystals of the first compound are colourless transparent from methanol and toluene, $C_{14}H_{11}O_3PSCl_2$, Mr=377.18; Orthorhombic Pnma, a=15.331(3), b=11.253(2) and c=8.973(4)Å V=1548.0(8)Å^3; Z=4; ϱ=1.615 and ϱ=1.618gmcm^{-3}; μ(CuKα)=62.32cm^{-1}; F(000)=768; Final R=0.051 & Rw=0.059 for 1293 ($I \geq 3\sigma(I)$) significant reflections.

