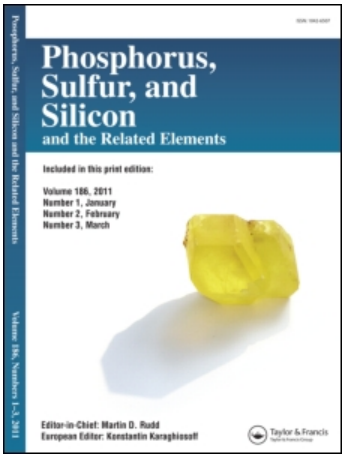


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# The Study of Electronic and Spatial Structure of Some Derivatives of 5-Phosphoranylidenbarbituric Acid and 5-Phosphoranylidenthiobarbituric Acid

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# THE STUDY OF ELECTRONIC AND SPATIAL STRUCTURE OF SOME DERIVATIVES OF 5-PHOSPHORANYLIDENBARBITURIC ACID AND 5-PHOSPHORANYLIDENTHIOBARBITURIC ACID

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## INTRODUCTION

Barbituric acid derivatives are known to participate in formation of ordered supramolecular structures with other pyrimidine derivatives.The properties of such species are determined by the structure and specific features of molecules which are the building blocks of such arrangements. Here, the results of MNDO study of spatial and electronic structure of a number of derivatives of 5-phosphoranylidenbarbituric acid (I) and 5-phosphoranylidenthiobarbituric acid (II) are presented (the substituents at P are: H, Me, Et, Ph; the substituents at N are: H, t-Bu, OH).

## RESULTS AND CONCLUSIONS

All molecules under consideration are shown to have nearly planar configuration of heterocycle, the deviation from planarity being essentially dependent on the size and nature of substituents at phosphorus and nitrogen[1].The ability of molecules of type I to self-association with vertical $\pi$-bonding is considered. The formation of weak van der Waals complex is shown to be possible, the energy of formation being estimated as $\cong$ 4 kcal/mole. In this structure heterocycles retain their planarity, the distance between the planes being 4.3A. The attempt to stabilize this structure by means of $(CH_2)_n$-bridges, so that the formed structure may have parallel-plane arrangement of heterocycles, is undertaken. The structures with various length of bridges (n=2,3) are studied. The heterocycles in the resulting structures are shifted relative to each other; therefore, the overlap between $\pi$-orbitals of donor cen-ters of one molecule with acceptor centers of the other is impossible.

## REFERENCE

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