

This article was downloaded by:

On: 28 January 2011

Access details: *Access Details: Free Access*

Publisher *Taylor & Francis*

Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK



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>

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

Marina Balakina^a; Mikhail Zuev^a

^a A.E. Arbuzov Institute of Organic & Physical Chemistry, Kazan Scientific Center, Russian Academy of Sciences, Kazan, Russia

To cite this Article Balakina, Marina and Zuev, Mikhail(1996) 'The Study of Electronic and Spatial Structure of Some Derivatives of 5-Phosphoranylidenbarbituric Acid and 5-Phosphoranylidenthioarbituric Acid', *Phosphorus, Sulfur, and Silicon and the Related Elements*, 111: 1, 134

To link to this Article: DOI: 10.1080/10426509608054763

URL: <http://dx.doi.org/10.1080/10426509608054763>

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: <http://www.informaworld.com/terms-and-conditions-of-access.pdf>

This article may be used for research, teaching and private study purposes. Any substantial or systematic reproduction, re-distribution, re-selling, loan or sub-licensing, systematic supply or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

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

MARINA BALAKINA, MIKHAIL ZUEV

A.E.Arbuzov Institute of Organic & Physical Chemistry, Kazan Scientific
Center, Russian Academy of Sciences, Kazan, Russia

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-phosphoranylidenebarbituric acid (I) and 5-phosphoranylidenthioarbituric 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 nitrogen¹. The ability of molecules of type I to self-association with vertical π -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 4.3 Å. 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 π -orbitals of donor centers of one molecule with acceptor centers of the other is impossible.

REFERENCE

1. M.Yu.Balakina, M.B.Zuev, *Izv.Acad.Nauk, Ser. Khim.*, (1995), in press.