

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>

Theoretical Investigation of Interaction of Hydrogen Dithiophosphate with 2-Phenyl-2H-1,2,3-diazaphosphole

Narkis Khusainova^a; Vladislav Zverev^b; Goulmara Garipova^a; Rafael Cherkasov^a; Arkady Pudovik^a

^a Kazan State University, Russia ^b A. E. Arbuzov Institute of Organic and Physical Chemistry, Russia

Online publication date: 27 October 2010

To cite this Article Khusainova, Narkis , Zverev, Vladislav , Garipova, Goulmara , Cherkasov, Rafael and Pudovik, Arkady(2002) 'Theoretical Investigation of Interaction of Hydrogen Dithiophosphate with 2-Phenyl-2H-1,2,3-diazaphosphole', Phosphorus, Sulfur, and Silicon and the Related Elements, 177: 8, 2229

To link to this Article: DOI: 10.1080/10426500213307

URL: <http://dx.doi.org/10.1080/10426500213307>

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.



THEORETICAL INVESTIGATION OF INTERACTION OF HYDROGEN DITHIOPHOSPHATE WITH 2-PHENYL-2H-1,2,3-DIAZAPHOSPHOLE

Narkis Khusainova,^a Vladislav Zverev,^b Goul'nara Garipova,^a
Rafael Cherkasov,^a Arkady Pudovik^a
Kazan State University, Russia;^a and A. E. Arbuzov Institute
of Organic and Physical Chemistry, Russia^b

(Received July 29, 2001; accepted December 25, 2001)

We showed previously that the cyclic two-coordinate phosphorus derivative—5-methyl-2-acetyl(phenyl)-2H-1,2,3-diazaphosphole—takes up O,O'-dialkyl hydrogen phosphorothio- and dithioates across the $\sigma^2\lambda^3\text{P}=\text{C}$ bond; the anionic moiety of the thio and dithio acid was directed toward the two-coordinate phosphorus atom.¹ In the ³¹P NMR spectra of the resulting 3-(dialkoxyphosphinoyldithio)-2-phenyl-1,2,3-diazaphospholines **1** the chemical shifts of the three and four—coordinate phosphorus atoms were equivalent owing to intramolecular interaction of the P(III) atom with the thione sulfur atom in the adduct. As a continuation of these studies, the electron and molecular structure of adduct of hydrogen dimethyl dithiophosphate with 2-phenyl-5-methyl-2H-1,2,3-diazaphosphole, containing P=C bond, have been studied by the methods of quantum chemical calculations (MNDO, PM3, ab initio) with the usage of the photoelectron spectroscopy. It has been shown, that the equality of the shifts of P(III) and P(IV) in ³¹P NMR spectra of the adduct **1** probably takes place in the results of the real of the structure with nearly equal lengths of four P—S bonds.

REFERENCE

- [1] N. G. Khusainova, T. A. Zyablikova, G. G. Reshetkova, and R. A. Cherkasov, *Zh. Gen. Chem. Rus.*, **66**, 416 (1996).

This work was supported by grant of the Russian Foundation for financial Support of the Leading Scientific School, by the program "The Universities of Russia—Basic Researches" and by the joint program of CRDF and Russian Ministry of Education (REC-007).

Address correspondence to Narkis Khusainova, Department of Chemistry, Kazan State University, Kremlevskaya str. 18, Kazan, 420008, Russia.