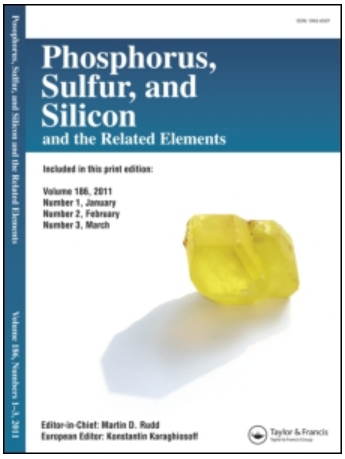

Phosphorus, Sulfur, and Silicon and the Related Elements
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713618290

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To cite this Article He, Liang-Nian , Zhuo, Ren-Xi , Liu, Xiao-Peng and Cai, Fei(1999) 'The Quantitative Structure-Herbicidal Activity Relationship of 1-Alkyl-1,3,2-Diazaphospholidin-4-Thione-2-Sulfides', Phosphorus, Sulfur, and Silicon and the Related Elements, 144: 1, 453 — 456
To link to this Article: DOI: 10.1080/10426509908546279
URL: http://dx.doi.org/10.1080/10426509908546279

Phosphorus, Sulfur and Silicon, 1999, Vol. 144-146, pp. 453-456
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The Quantitative Structure-Herbicidal Activity Relationship of 1-Alkyl-1,3,2-Diazaphospholidin-4-Thione-2-Sulfides

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A number of 1-alkyl-1,3,2-diazaphospholidin-4-thione-2-sulfides(**2**) have been synthesized by the cyclization reaction of Lawesson's reagent with 3- alkyl- glycinamides(**1**). The bioassay indicates that some of compounds prepared have good selective herbicidal activity and the quantitative structure- herbicidal activity relationship (QSAR) of compounds(**2**) has also been studied.

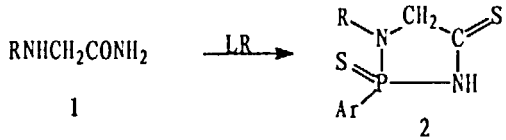
Keywords: Lawesson's reagent; 1,3,2-diazaphospholidin-2-sulfides; herbicidal activity; QSAR

INTRODUCTION

In our previous work[1-4], a number of 1,4,2-diazaphospholidines and 1,3,2 -diazaphosphlidinthiones were synthesized by a Mannich-type reaction and heterocyclization reaction of Lawesson's reagent with bifunctional substrates. Glycinamides are known as biologically active materials, for example , herbicides, plant-growth regulators. We have found that the reaction of 3-aryl glycinamides with Lawesson's reagent lead to 1-aryl-1,3,2-diazaphospholidin-4-thione-2-sulfide, which possess good selective herbicidal activity against rape[5,6].For the purpose of making sure the relationship between the strcture and the properties. 1-Alkyl-1,3,2-diazaphospholidin-4-thione-2-sulfide(**2**) were synthesized. The quantitative structure- herbicidal activity relationship (QSAR) of compounds(**2**) is described in this paper[7] .

RESULT AND DISCUSSION

The title compounds **2** were synthesized by the reaction of Lawesson's reagent with 3-alkyl glycinamides **1** in dry benzene at 70℃ in moderate yield, as shown in Scheme 1.



1 2

Ar = *p*-$CH_3OC_6H_4$, R = H, alkyl,

Scheme 1

The herbicidal activity of conpounds **2** was tested . A set amount of each sample was dissolved in acetone to which a drop of an emulsifier

was added. Then, the solution was diluted with water until it reached the concentration required. Some herbs such as rape, oats ,flax and barnyard grass were subjected to the leaf treatment. Preliminary bioassay indicatedthat some of them displayed good selective herbicidal activity against rape. The results are given in Table 2 in terms of activity indicator (D):

$$D = \lg [a/(100-a)] + \lg MW$$

Where a refers to inhibition percertage against rape at 100ppm. MW is the molecular weight.Determination of a was repeated for at least three runs and averaged.

TABLE 2 The Herbicidal Activity of Compounds(2) against rape

No.	2a	2b	2c	2d	2e	2f
R	Me	Et	n-Pr	i-Pr	n-Bu	i-Bu
Ar	*P*-MeOPh	*P*-MeOPh	*P*-MeOPh	*P*-MeOPh	*P*-MeOPh	*P*-MeOPh
D	3.76	4.23	4.03	4.25	3.26	3.86

2g	2h	2i	2j	2k	2l	2k
Pentyl	Me	Et	n-Pr	i-Pr	n-Bu	i-Bu
P-MeOPh	PhS	PhS	PhS	PhS	PhS	PhS
3.05	4.29	4.16	4.04	4.18	3.62	3.92

The quantitative relationship between the structure of **2** and their herbicidal activity on the rape was analyzed, using the physico-chemical parameter of the substituents in the benzene ring by regression analysis.The following regression equation could be established:

$$D = 2.980\,\pi + 2.035\,\sigma - 0.150Es + 2.947$$

$$n=13,\ r=0.872, s=0.211$$

The equation indicates that the relationship between the hydrophobic parameter (π)[6], steric parameter (Taft constant: Es) and electronic effect parameter(σ) of substitutent and herbicidal activity with a significant regression coeffient. Although the steric parameter also affected herbicidal activity but the contribution was much smaller than that of the hydrophobic property and electronic parameter.The results were used in guiding the synthesis of higher active compounds.

Acknowledgment

We gratefully acknowledge support for this work by the National Natural Science Foundation of China and the NSF of Hubei Province and the Dawn Plan of Science and Technology for Young Scienists of Wuhan City.

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