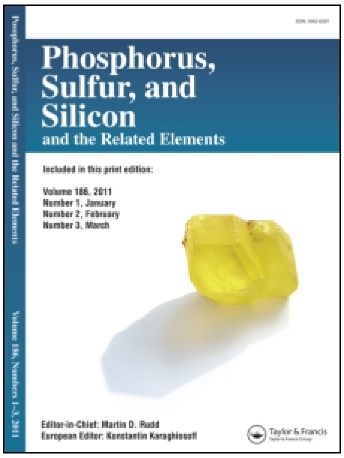

Phosphorus, Sulfur, and Silicon and the Related Elements
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713618290

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To cite this Article Erchak, Nikolai(1999) 'Theoretical Aproach to Electrostatic Stabilization of Molecules. Sulfur Compounds', Phosphorus, Sulfur, and Silicon and the Related Elements, 153: 1, 355 — 356

To link to this Article: DOI: 10.1080/10426509908546468

URL: http://dx.doi.org/10.1080/10426509908546468

Phosphorus, Sulfur and Silicon, 1999, Vol. 153-154, pp. 355-356
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Theoretical Aproach to Electrostatic Stabilization of Molecules. Sulfur Compounds

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The main application perspectives of the Theory of Electrostatic Stabilization of Molecules have been suggested.

Keywords: Theory; aromaticity; thiophene; furan; acidity; sulfur

Any molecule can be presented as a sphere of infinite number of points, the electrical field of which changes according to some laws depending on the character of a molecule. For the compounds of Td (tetrahedron) symmetry the space round the central atom can be divided up into four equal volumes (or the so called lodgings). This division can be done in following ways:(I) The system of coordinates is directed along the bonds of a molecule and a lodging takes the positions between three axes (See Figure 1). (II) All the lodgings are mirror-reflected in the planes, which are perpendicular to bonds and pass through the central atom (See Figure 2). In this case the four bonds are lying on the axes of symmetry of the 3rd-order lodgings.

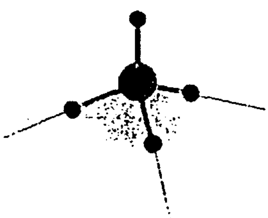

FIGURE 1

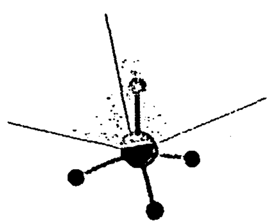

FIGURE 2

It is shown, that the electrical field produced by one functional group is limited by the volume of one lodging and can be presented with a summary R-vector. The direction of R-vector coincides with the direction of the chemical bond.

It proved to be useful for the analysis of chemical systems and compounds of all kinds to present the electrical field of functional groups of lodgings by means of R-vector. It has been shown, that one and the same molecule (for example MR_4) can be represented by several boundary or transitional forms, stabilization energy of which may differ greatly. It has been determined, that the flat form of a molecule (with the angle of 90° between bonds) is more power-profitable. The molecules of most organic and elements-organic compounds can exist in this form only at temperatures close to absolute zero. The central atom will be situated in the electrical field, which stabilizes the system by quantity proportional to ~ 4R̲ . Each functional group will have its own R̲-value.

With the increase of temperature as a result of heat motion of molecules and the deviation of angle between bonds from 90° the stabilizing effect will decrease up to $2\sqrt{2}$ R̲. The following increase of temperature will cause the departure of substitutes from the plane and formation of molecules of tetrahedron structure. The stabilizing effect of substitutes decreases up to ~ 2R̲.

The R-vector presentation of the electrical field of molecules allows us to look anew at the mechanism of reactions of nucleophilic substitution. It is revealed that for reactions of nucleophilic substitution there's no need in activation energy for transfer of a molecule into the flat transitional complex. Transitional forms of molecules in reactions of nucleophilic substitution can exist under certain conditions for a long period of time.

By means of the Theory of Electrostatic Stabilization of Molecules it is possible to explain the specific behavior of the 3rd period elements in chemical reactions, why sulfur compounds with two double bonds and phosphoric compounds with one double bond are stable, why there are no stable silicon compounds with double bonds.

Explanations of differences in strength of some inorganic (sulfuric, sulfurous, hydrogen sulfide, hydrochloric, carbonic, etc.) acids have been received.

A new interpretation of the Resonance Energy in aromatic systems has been received as well. Differences in stabilization of aromatic systems of furan and thiophene have been explained.