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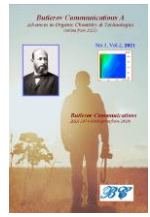

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Nitrogen and sulfur-containing heterocycles – potential antioxidant additives in mineral and synthetic lubricating oils

Vladimir N. Koshelev,* **Olga V. Primerova**,[+] and **Anna S. Stupnikova**
Department of Organic Chemistry and Petroleum chemistry. National University of Oil and Gas «Gubkin University. Lenin Ave., 65-1. Moscow, 119991. Russia. Phone: +7 (499) 507-81-11. E-mail: primerova92@yandex.ru

*Supervising author; [+]Corresponding author

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Abstract

This review summarizes the literature and our own data on the structure of *N*,*S*-heterocycles, which improve the thermal-oxidative stability of synthetic and mineral oils, published over the past 20 years. Compounds of this series as promising additives for lube oils: antioxidant or polyfunctional additives with antioxidant action, capable to replace zinc dialkyldithiophosphate. Among the nitrogen-containing hete-rocycles exhibiting antioxidant properties, derivatives of 1,2,4-, 1,2,3-triazole, imidazole, benzimidazole, benzotriazole, triazine were found. Derivatives of thiadiazole, thiazolidine, thiazolone, thiazole, benzothiazole were found among sulfur-containing heterocycles – promising antioxidants. The classification and mechanism of action of antioxidants depending on their structures are discussed: ability to break chain reactions, to decompose hydroperoxides, to deactivate the catalytic action of metals during oxidation. The influence of the structure of antioxidants on the mechanism of their action and efficiency is analyzed. Examples of promising antioxidants, which include in their structure a phenolic or amine fragment and a heterocycle and are capable to act by several mechanisms are given. The main directions in the development of this type of antioxidants have been identified. The most effective approaches to predicting the antioxidant properties of complex molecules by computer chemistry methods are analyzed, including calculation of the energy of homolysis of the ArO-H bond in phenols or ArN-H in amines, analysis of the structure of the transition state, and calculation of the energy barrier for the reaction of an antioxidant with alkylperoxyradicals. Examples of the QSPR (Quantitative Structure-Activity Relationship) method, as well as molecular dynamics methods application, for the analysis and prediction of the antioxidant properties of compounds are given.

Contents

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