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RESEARCH ARTICLE

The effect of ureas and their sulfur- and selenium-containing analogs on the vulcanization and thermo-oxidative resistance of elastomers based on nitrile butadiene rubber

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Abstract

Objectives. The study set out to investigate the effect of ureas and their sulfur- and selenium-containing analogs on the vulcanization of elastomeric materials based on nitrile butadiene rubber and their resistance to thermo-oxidative aging.

Methods. The properties of the molecules of ureas under study were calculated by the MM+ quantum chemical method of molecular mechanics and PM3 semiempirical method using the HyperChem 8.0 software. Vulcanization of rubbers and total crosslink density were studied using the rotorless vulcanization method with a MonTech MDR 3000 Professional rheometer. The dynamic characteristics of vulcanized rubbers were investigated in accordance with ASTM D6601-02 and D5992-96 standards. The efficiency of the studied antioxidants against thermo-oxidative aging was evaluated in accordance with GOST 9.024-74. Infrared (IR) spectra of samples were recorded with an FT-801 Fourier-transform IR spectrometer (Russia) according to the attenuated total reflection method.

Results. For the first time, a study was conducted on the efficiency of 1-(3-chlorophenyl)-3-phenylurea, 1-(3-chlorophenyl)-3-phenylthiourea, and 1-(3-fluorophenyl)-3-phenylselenourea as antioxidants for elastomers under conditions of thermo-oxidative aging. The effect of these substances on the vulcanization characteristics and total crosslink density of materials based on nitrile butadiene rubber was investigated.

Conclusions. The values of electron affinity energy and its sign were shown to accurately predict the possibility of using individual molecules as accelerators of the vulcanization process or antioxidants. With a change in the electron affinity energy from 0.051 (urea) to −1.115 (thiourea) and −1.365 eV (selenourea), the time to the start of vulcanization was shown to change from 15 to 3 and 2 min, respectively. As a result of thermo-oxidative aging of rubbers based on BNKS-28 AN rubber without a stabilizer and with 1-(3-chlorophenyl)-3-phenylurea, 1-(3-chlorophenyl)-3-phenylthiourea, and 1-(3-fluorophenyl)-3-phenylselenourea, the total crosslink density changes by 33%, 23%, 25%, and 29%, respectively. In this connection, the use of 1-(3-chlorophenyl)-3-phenylurea somewhat improves the stability of rubbers to thermo-oxidative aging, whereas 1-(3-chlorophenyl)-3-phenylthiourea and 1-(3-fluorophenyl)-3-phenylselenourea do not worsen this property when introduced into the rubber compound.

Keywords

elastomers, urea, thiourea, selenourea, nitrile butadiene rubber, vulcanization, thermo-oxidative resistance

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НАУЧНАЯ СТАТЬЯ

Исследование влияния мочевин и их серо- и селенсодержащих аналогов на вулканизацию и термоокислительную стойкость эластомеров на основе бутадиен-нитрильного каучука

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Аннотация

Цели. Исследование влияния мочевин и их серо- и селенсодержащих аналогов на вулканизацию эластомерных материалов на основе бутадиен-нитрильного каучука и на их стойкость термоокислительному старению.

Методы. Квантово-химическими методами молекулярной механики ММ+ и с помощью полуэмпирического метода РМ3 проведен расчет исследуемых молекул мочевины и ее аналогов в программном комплексе HyperChem 8.0. Вулканизацию резин и оценку общей плотности сшивки изучали методом безроторной вулканометрии на реометре MonTech MDR 3000 Professional. Исследование динамических характеристик вулканизованных резин проводили в соответствии с ASTM D6601-02 и D5992-96. Эффективность исследуемых противостарителей к термоокислительному старению проводили по ГОСТ 9.024-74. Инфракрасные (ИК) спектры образцов получены на ИК-Фурье спектрометре ФТ-801 (Россия) методом нарушенного полного внутреннего отражения.

Результаты. Впервые проведено исследование эффективности действия 1-(3-хлорфенил)-3-фенил мочевины, 1-(3-хлорфенил)-3-фенил тиомочевины и 1-(3-фторфенил)-3-фенил селеномочевины в качестве антиоксидантов для эластомеров в условиях термоокислительного старения. Изучено влияние указанных соединений на вулканизационные характеристики и общую плотность сшивки материалов на основе бутадиен-нитрильного каучука.

Выводы. Установлено, что значения энергии сродства к электрону и ее знак позволяют прогнозировать возможность использования отдельных молекул в качестве ускорителей процесса вулканизации или антиоксидантов. Показано, что при изменении энергии сродства к электрону от 0.051 (мочевина) до −1.115 (тиомочевина) и −1.365 эВ (селеномочевина) время до начала вулканизации изменяется от 15 до 3 и 2 мин соответственно. В результате термоокислительного старения резин на основе каучука БНКС-28 АН без стабилизатора с 1-(3-хлорфенил)-3-фенил мочевиной, 1-(3-хлорфенил)-3-фенил тиомочевиной и 1-(3-фторфенил)-3-фенил селеномочевиной значение общей плотности сшивки изменяется в ряду 33%, 23%, 25% и 29% соответственно. В этой связи сделан вывод, что применение 1-(3-хлорфенил)-3-фенил мочевины несколько улучшает стабильность резин при термоокислительном старении, а 1-(3-хлорфенил)-3-фенил тиомочевина и 1-(3-фторфенил)-3-фенил селеномочевина не ухудшают данный показатель при введении в резиновую смесь.

Ключевые слова

эластомеры, мочевина, тиомочевина, селеномочевина, бутадиен-нитрильный каучук, вулканизация, термоокислительная стойкость

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INTRODUCTION

Exposure to high temperatures and oxygen changes the initial properties of elastomers depending on the composition of their ingredients [1, 2]. Aromatic amines, substituted phenols, phosphorous acid esters, and organosilicon compounds are widely used in industry as antioxidants for elastomeric materials [3–6]. However, the above-mentioned groups of antioxidants have fairly high values of saturated vapor pressure and are poorly soluble in rubber, which limits their use in the food and medical industries. As a rubber stabilizer for the food industry, 2,2-methylene-bis(4-methyl-6-*tert*-butylphenol), better known as Agidol 2[1], is commonly used. The use of D,L-camphor anils as heat stabilizers was studied in [7]. Other potentially interesting options for use as heat stabilizers may include compounds of sulfur- or selenium-containing carboxyalkylphenols based on selenium-containing analogs of phenozan (3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)propionic acid) [8] and compounds based on 2,3-camphorquinone.

Modern computational systems allow one to evaluate compatibility and predict interactions between polymer macromolecules under the action of various aggressive factors [9]. A method was developed for selecting components of elastomer compositions based on quantum-chemical modeling [10]. The relationship of the total energy of the system, which was determined by quantum-chemical calculation methods, including dynamic testing methods, with relaxation parameters allows the effect of additives on the properties of whole elastomer compositions to be predicted.

The aim of this work was to investigate the influence of ureas and their sulfur- and selenium-containing analogs on the vulcanization of elastomeric materials based on nitrile butadiene rubber and on their resistance to thermo-oxidative aging.

EXPERIMENTAL

Figure 1 presents the structural formulas of the studied compounds obtained by the syntheses described in the literature [11–13], as well as their notation.

The objects of the study comprised two groups of samples:

(1) Samples of rubber compounds based on BNKS-28 AN synthetic nitrile butadiene rubber (Specification TU 38.30313-2006) that was obtained by suspension polymerization at low temperatures (A) and contained a noncoloring antioxidant (N), without additives of the compounds shown in Fig. 1. Such objects have the letter ***K*** in the notation. Rubber samples containing 4 parts by weight (pbw) of 1-(3-chlorophenyl)-3-phenylurea, 1-(3-chlorophenyl)-3-phenylthiourea, or 1-(3-fluorophenyl)-3-phenylselenourea per 100 pbw of rubber are designated as ***KO***, ***KS***, and ***KSe***, respectively.

(2) Samples of rubber compounds based on BNKS-28 AN commercial rubber that do not contain a filler. They were produced on laboratory rollers 320 160/160 (*Yarpolimermash*, USSR) by sequential introduction of the recipe ingredients. The vulcanization activator was a combination of zinc oxide (4 pbw) and stearic acid (2 pbw). The crosslinking agent was sulfur (2 pbw). The vulcanization accelerator was *N*-cyclohexyl-2-benzothiazole sulfenamide (1.5 pbw). Such samples have the letter ***P*** in their notation. In turn, elastomers containing 1-(3-chlorophenyl)-3-phenylurea, 1-(3-chlorophenyl)-3-phenylthiourea, or 1-(3-fluorophenyl)-3-phenylselenourea in an amount of 4 pbw per 100 pbw of rubber are assigned the notation ***PO***, ***PS***, and ***PSe***, respectively. The objects of comparison were rubbers containing the standard antiaging agent *N*-isopropyl-*N'*-phenyl-1,4-phenylenediamine (4 pbw) and the vulcanization accelerator *N*-cyclohexyl-2-benzothiazole sulfenamide (1.5 pbw) with the notation ***IPPD*** and ***CBS***, respectively. The dosage of the studied compounds was selected in such a way as to obtain differences in the exhibited properties of rubbers while taking into account the fact that ***IPPD*** has a low saturated vapor pressure (0.00046 kPa at 90°C) and a boiling point (166°C) close to the vulcanization temperature (150°C). Further increase is impractical since it leads to migration of the antiaging agent from the rubber matrix [14]. For better dispersion, the antiaging agents were introduced first, and then the remaining ingredients of the rubber mixture were added in the order they are mentioned in the text.

The preliminarily obtained chemical compounds were characterized using quantum-chemical methods for calculating the properties of molecules in the HyperChem 8.0 software[2] (*Hypercube Inc*, USA). The geometry of the molecules was optimized using the MM+ molecular mechanics method, and then the PM3 (Parameterized Model, revision 3) semiempirical method was used to calculate the diagrams of energy levels, the lowest unoccupied molecular orbital (LUMO),

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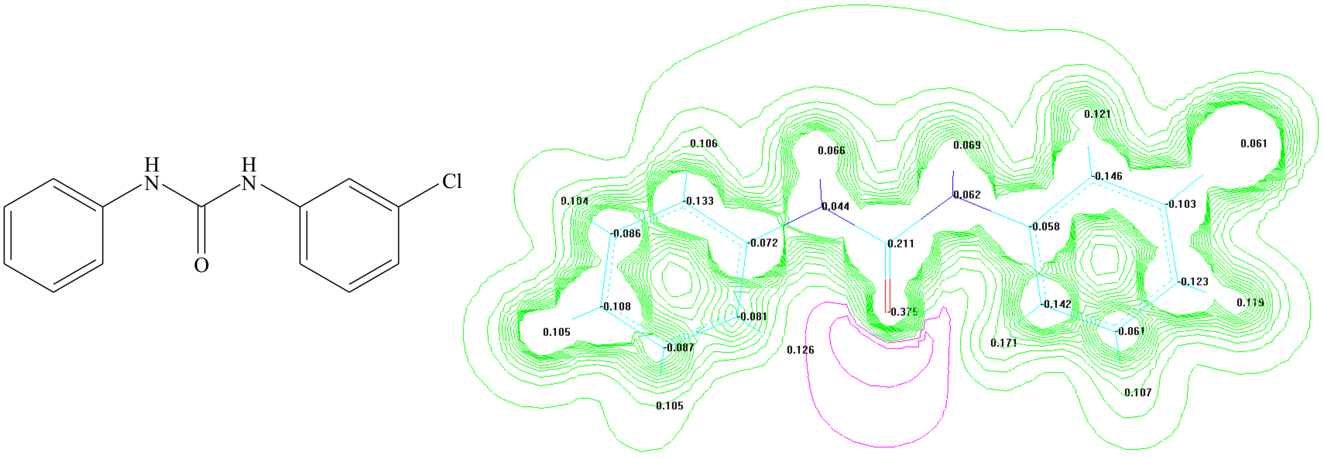
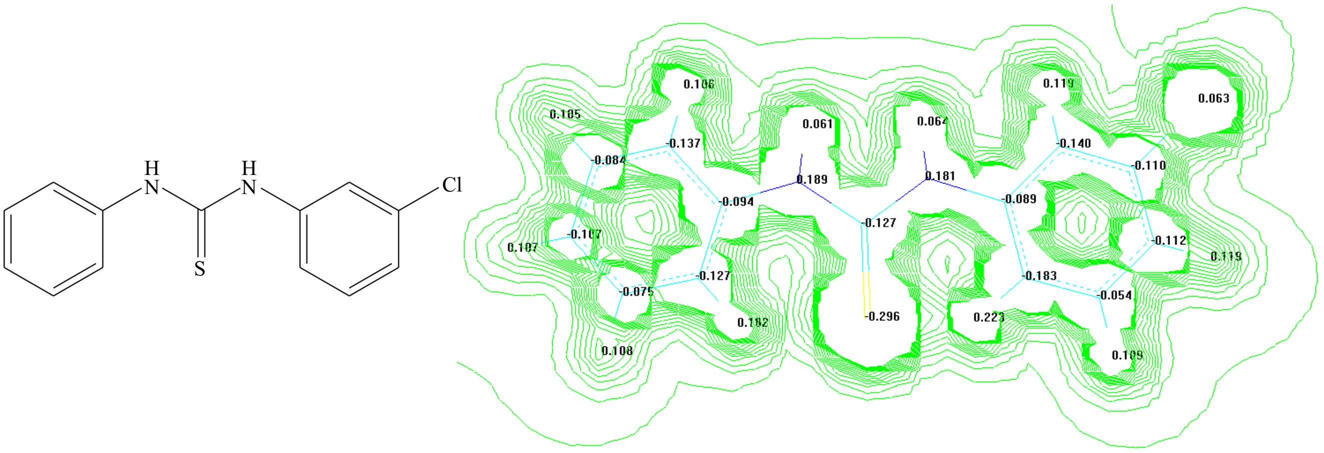
[1] Technical Information. Vulkanox BKF / Lanxess. 2004. http://www.symtake.com/tw/uploads/filelist/1000/2/1382580948_c0a80afd82d4d906.pdf. Accessed April 10, 2024.

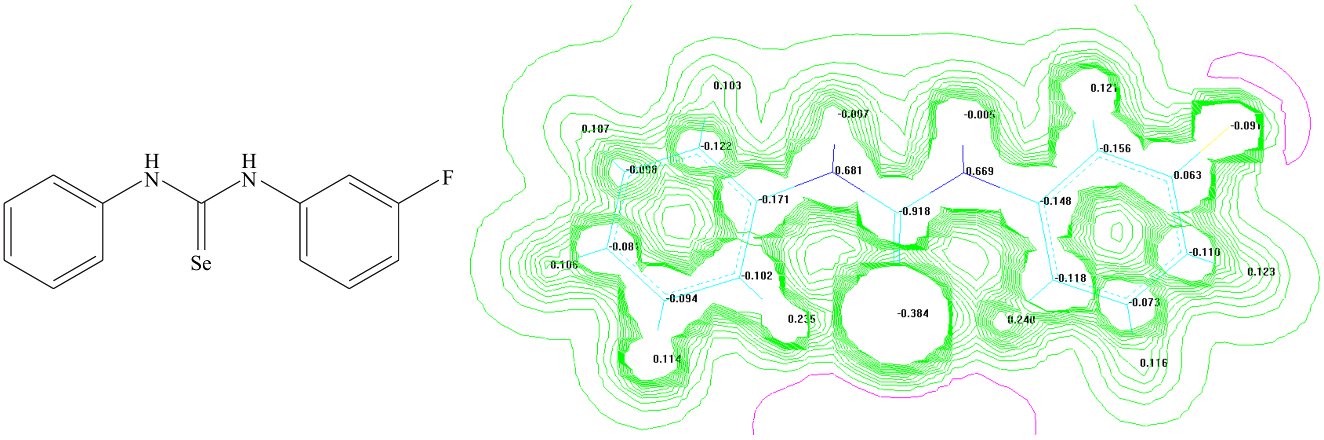
[2] HyperChem Professional 8.0. http://www.hypercubeusa.com/. Accessed February 25, 2025.



1-(3-Chlorophenyl)-3-phenylurea (***O***) [12]



1-(3-Chlorophenyl)-3-phenylthiourea (***S***) [13]



1-(3-Fluorophenyl)-3-phenylselenourea (***Se***) [14]

(a) (b)

Fig. 1. (a) Structures, and (b) charge distributions and electronic densities of the studied molecules

and the highest occupied molecular orbital (HOMO), as well as the thermodynamic parameters: enthalpy, entropy, and heat capacity of the compounds. By comparing the shapes and excitation energies ΔE_{exc} of these frontier molecular orbitals, a conclusion can be drawn about the nucleophilicity or electrophilicity of the molecules under study. Characteristics were also calculated for the system of the molecules under study together with nitrile butadiene rubber to assess their compatibility from the changes in the total energies of the system and individual substances.

The vulcanization of rubbers was investigated by the rotorless vulcanization method with a MonTech MDR 3000 Professional rheometer

(*MonTech*, Germany) at a temperature of 150°C in accordance with GOST R 54547-2011[3]. Using this rheometer, the total crosslink density ν_{tot} of vulcanized rubber samples was found under shear deformation conditions at 100°C from the change in the storage modulus depending on the shear strain in accordance with the ASTM D6601-02[4] standard and the described procedure [15]. In this case, the relationship between the parameter ν_{tot} and the equilibrium dynamic modulus is determined in accordance with the kinetic theory of rubber elasticity [16] using the equation

$$\nu_{tot} = \frac{G_\infty}{3RT}, \tag{1}$$

where ν_{tot} is the total crosslink density, mol/cm^3; G_∞ is the equilibrium dynamic modulus, Pa; R is the universal gas constant (R = 8.314 J/(mol·K)); T is the test temperature (373.15 K).

The dynamic characteristics of vulcanized rubbers were studied in accordance with ASTM D6601-02 and ASTM D5992-96[5] using a MonTech MDR 3000 Professional rheometer in dynamic moving die rheometer mode. The conditions for conducting dynamic tests were selected from those recommended by the standard: temperature 100°C and oscillation frequency 10 Hz. The change in dynamic moduli after thermal-oxidative aging at 90°C for 72 h in an oven was also assessed. In this case, the corresponding temperature was added to the notation, e.g., ***PO90***.

The physical and mechanical characteristics of vulcanized rubbers were evaluated in accordance with GOST 270-75[6]. The efficiency of the studied antioxidants to thermo-oxidative aging was determined at a temperature of 100°C for 72 h according to GOST 9.024-74[7].

IR spectra of the samples were recorded with an FT-801 Fourier transform infrared (FTIR) spectrometer (*NPF SIMEKS*, Russia) by the attenuated total reflection method on a ZnSe crystal in the wavelength range λ = 550–4000 cm^{-1} with a resolution of 4 cm^{-1}.

RESULTS AND DISCUSSION

Tables 1 and 2 present the results of calculations of the properties of ureas and their ***S***- and ***Se***-containing analogs by the PM3 semiempirical method in comparison with standard compounds used as vulcanization accelerators and antioxidants.

The obtained values of the energies of the LUMO molecular orbital were used to find the electron affinity energies, which are related by density functional theory, as well as to determine such parameters as the dipole moment and the charge distribution and electron density on the amine groups. The presence of reaction sites of the synthesized compounds can be assumed based on these parameter values. These parameters are also of interest due to the vulcanization of nitrile butadiene rubber during thermos-oxidative aging due to the lone pair of electrons on the nitrogen atom. At the same time, by varying the functional groups in the urea molecule to obtain ***S***- and ***Se***-containing analogs with the same number of electrons on the outer energy levels (ns^2, np^4) and different energies of the levels, it is possible to influence the mobility of hydrogen atoms at the amino group. Note that, for antiaging agents and antiozonants (Agidol-2 and ***IPPD***), the electron affinity energy is positive; i.e., the addition of an electron is accompanied by the release of energy, whereas the vulcanization accelerator ***CBS*** demonstrates a negative value. It can be assumed that the ***S*** and ***Se*** compounds, for which the energies are −1.115 and −1.365 eV, respectively, will accelerate vulcanization, with the latter acting to a greater extent. In addition, these compounds can have canonical mesomeric thio- and selenoamide forms, carrying a negative charge on the sulfur atom and a positive charge on the nitrogen atoms of the amidine fragment. In turn, the sulfur/selenium atom is a strong nucleophilic site, which allows these compounds to act as sulfur/selenium donors and consequently as a crosslinking agent [17]. At the same time, the compound ***O*** has an electron affinity energy of 0.051 eV and does not exhibit nucleophile properties; therefore, it will not react with the nitrile group. The electronic

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[3] GOST R 54547-2011. National Standard of the Russian Federation. Rubber compounds. Measurement of vulcanization characteristics using rotorless cure meters. Moscow: Standartinform; 2018.

[4] ASTM D6601-02. Standard Test Method for Rubber Properties—Measurement of Cure and After-Cure Dynamic Properties Using a Rotorless Shear Rheometer. https://www.astm.org/d6601-02.html. DOI: 10.1520/D6601-02. Accessed February 25, 2025.

[5] ASTM D5992-96(2018). Standard Guide for Dynamic Testing of Vulcanized Rubber and Rubber-Like Materials Using Vibratory Methods. https://www.astm.org/d5992-96r18.html. DOI: 10.1520/D5992-96R18. Accessed February 25, 2025.

[6] GOST 270-75. Interstate Standard. Rubber. Method of the determination elastic and tensile stress-strain properties. Moscow: IPK Izdatelstvo standartov; 1978.

[7] GOST 9.024-74. State Standard of the USSR. Unified system of corrosion and ageing protection. Rubbers. Methods of heat ageing stability determination. Moscow: Izdatelstvo standartov; 1986.

structure shows (Fig. 1) that this compound has a lone pair of electrons, which prevents any reaction with the nitrile group. However, during heating with sulfur, such an electron-pair donor can react with it to form thiourea, which will affect the vulcanization rate.

Calculation of the properties of the model of the rubber–molecule system begins with finding the state with the minimum potential energy, which usually corresponds to the equilibrium geometry of the atoms. Figure 2 presents the results of calculating the minimum energies of the compounds under study in comparison with the standard antioxidant ***IPPD*** using molecular dynamics methods.

Various physicochemical parameters of the rubber–molecule system can be calculated on the basis of the determination of the electron density distribution in the molecules together with the bond force constants. From Fig. 2, which depicts the change in the kinetic and potential energy with time for the compounds under study in the BNKS rubber environment, it can be seen that the values of the change in the potential energy of the ***O*** compound are similar to those of the standard antiaging agent ***IPPD***. Replacing the heteroatom with sulfur and selenium in the compounds leads to a decrease in this parameter. First of all, we note that high-molecular-weight compounds have limited molecular mobility. The formation of a transition complex is accompanied by rehybridization of the carbon atoms of the rubber backbone from sp^3 to sp^2 hybridization state, which is limited by structural relaxation. Higher values of the potential energy show that an activated complex having an optimal energetically favorable structure does

Table 1. Results of quantum-chemical calculation of the enthalpy H, entropy S, heat capacity C_p, and energies of molecular orbitals HOMO and LUMO of molecules*

Compound	H, kJ/mol	S^{298}, kJ/(mol·K)	C_p, kJ/(mol·K)	LUMO, eV	HOMO, eV	ΔE_{exc}, eV	Dipole moment D	Nitrogen atom charge
BNKS-28 AN	284.8	0.9823	0.4959	0.664	−9.657	10.32	–	−0.077
Urea	−171.7	0.2724	0.0586	1.061	−9.618	10.68	4.071	−0.017
O	67.2	0.4676	0.2026	0.051	−8.921	8.97	2.512	0.045
S	344.3	0.5526	0.2872	−1.115	−8.614	7.49	4.376	0.189
Se	158.0	0.4631	0.2095	−1.365	−8.234	6.86	4.493	0.277
IPPD	148.9	0.5122	0.2473	0.224	−8.179	8.40	2.116	0.031
Agidol-2	−278.0	0.4945	0.2583	0.397	−8.723	9.12	1.425	–
CBS	143.5	0.5152	0.2440	−0.878	−8.911	8.03	2.025	−0.105

* HOMO is the highest occupied molecular orbital, LUMO is the lowest unoccupied molecular orbital, and $\Delta E_{\text{exc}} = E_{\text{LUMO}} - E_{\text{HOMO}}$ is the difference of the energies of the orbitals.

Table 2. Estimation of changes in the total energy of rubber–compound systems

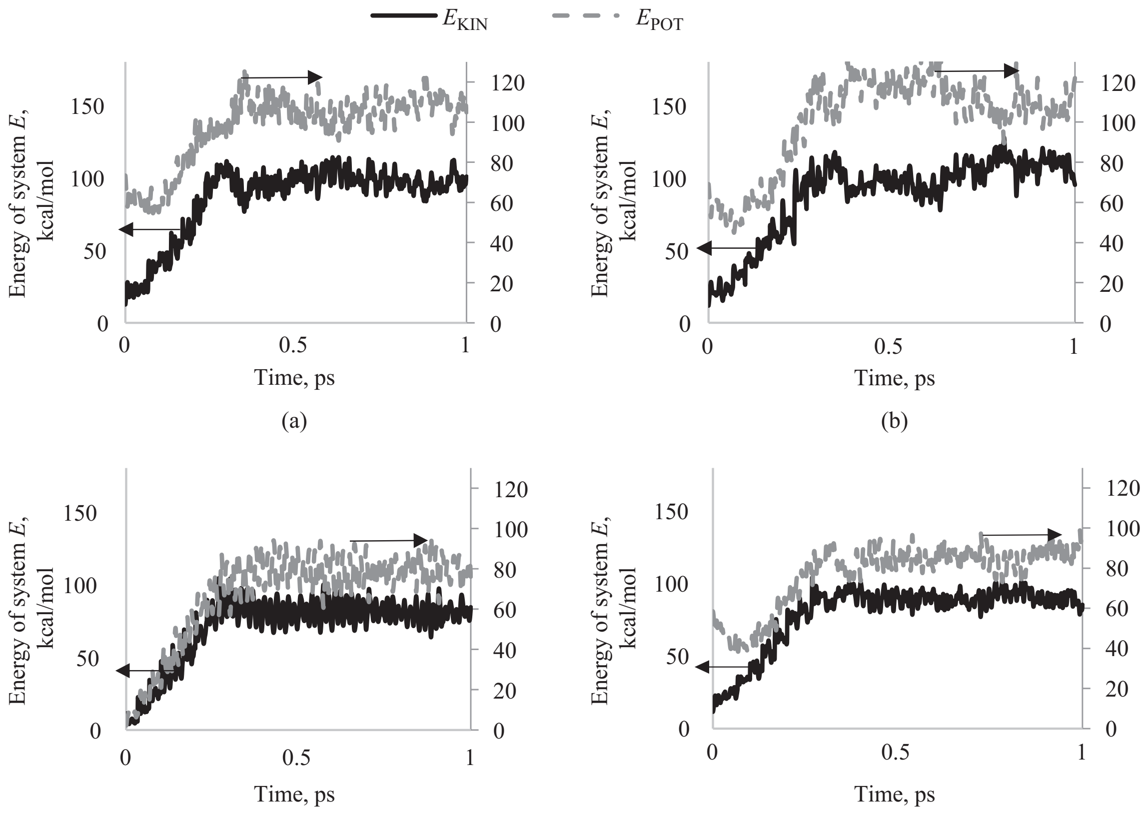
Compound	E, kJ/mol	E_{NBR}, kJ/mol	E_{system}, kJ/mol	ΔE, kJ/mol	Solubility of compound in rubber
O	−226352	−385474	−643961	−32134.8	Soluble
S	−244968	−385474	−633457	−3014.7	Soluble
Se	−257781	−385474	−646345	−3089.71	Soluble
IPPD	−229879	−385474	−618360	−3006.74	Soluble

Note: E are the calculated energies of individual compounds under study, E_{NBR} are the calculated energies of nitrile butadiene rubber, E_{system} are the calculated energies of mixtures of nitrile butadiene rubber with compounds under study in a box simulating the volume of rubber, and $\Delta E = E + E_{\text{NBR}} - E_{\text{system}}$.

not have time to form during the oxidation reaction with oxygen at high temperatures. In this connection, the ***O*** compound can be expected to exhibit antioxidant properties that prevent the thermo-oxidative destruction of macromolecules, but do not prevent the structuring of rubber at nitrile groups.

Changes in the energies of the system and individual substances showed that negative energy values suggest that the polymer–substance system may exhibit self-organization capabilities and consequent compatibility.

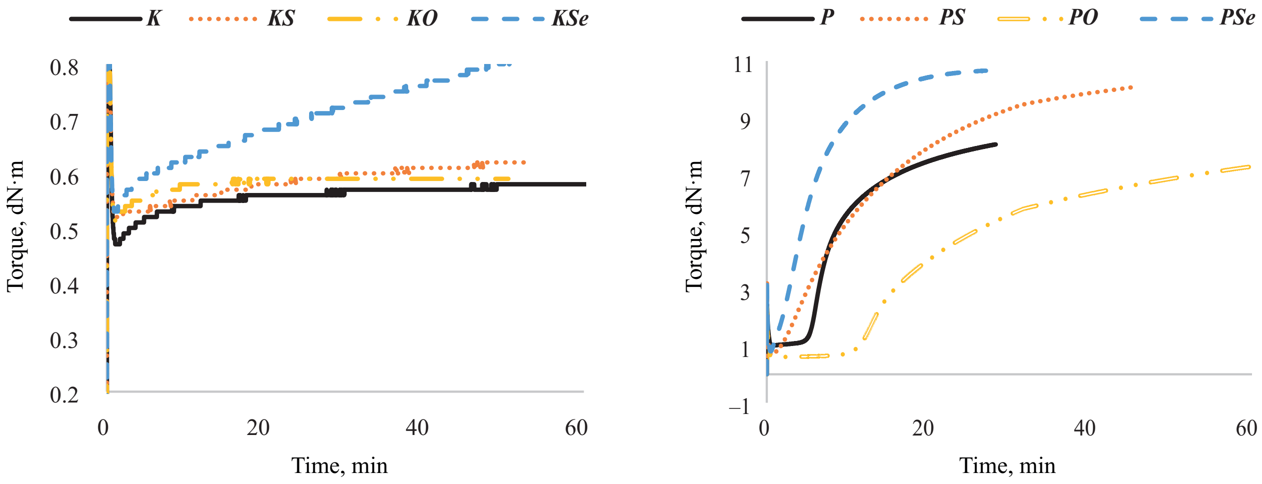
Figure 3 illustrates the effect of ureas and their ***S***- and ***Se***-containing analogs at a temperature of 150°C on the structuring of BNKS-28 AN rubber without a vulcanizing group and for rubber compounds vulcanized with a standard sulfur-containing system.



(a) (b)

(c) (d)

Fig. 2. Calculated minimum values of kinetic energy E_{KIN} and potential energy E_{POT} of (a) the standard antioxidant ***IPPD***, (b) urea ***O***, and (c) ***S***-containing and (d) ***Se***-containing analogs in rubber



(a) (b)

Fig. 3. Torque versus time for BNKS-28 AN rubber with the urea analogs under study (a) without a vulcanizing system and (b) with the ***CBS***–sulfur vulcanizing system

The dependencies in Fig. 3a show that the ***Se*** compound causes structuring of nitrile butadiene rubber (***KSe*** sample) even in the absence of a crosslinking agent. To a somewhat lesser extent, an increase in torque is also observed upon the introduction of a sulfur-containing analog of urea into the rubber.

Since the presence of the vulcanization accelerator ***CBS*** can lead to side reactions during the vulcanization of rubbers containing oligomeric unsaturated polyketone [18], we assessed the effect of urea and its sulfur- and selenium-containing analogs on vulcanization. Upon the introduction of the synthesized products into rubber compounds containing a vulcanizing system (Fig. 3b), it was noted that the ***S***- and ***Se***-containing analogs of urea (in the composition of the ***PS*** and ***PSe*** samples) caused a decrease in the parameter "time to the onset of vulcanization" from 6 to 3 and 2 min, respectively. In addition, the maximum torques of the vulcanizates increased from 8 to 10 daN·m for both additives. In this regard, we note that these compounds act as vulcanization coagents during the formation of the elastomer structure.

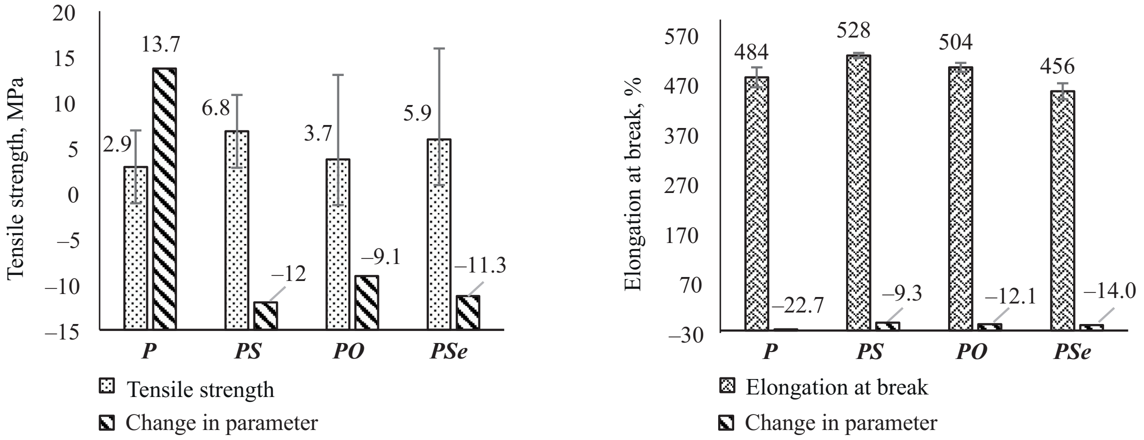
For the ***O*** compound, we noted the opposite effect. The use of this compound together with the ***CBS***–sulfur vulcanizing system led to an increase in the prevulcanization time of rubbers from 6 to 15 min and a subsequent decrease in the torque and total vulcanization rate. The experimental vulcanization data confirm the assumptions based on the results of the quantum-chemical calculation in HyperChem 8.0.

Figure 4 shows the physical and mechanical characteristics of vulcanized rubbers and their change after aging at 100°C for 72 h.

The results of the assessment of the parameters "engineering tensile strength" and "relative elongation at break" (Figs. 4a and 4b) and their changes after aging show that the introduction of the ***S***- and ***Se***-containing analogs of urea increases the tensile strength of rubbers. The introduction of the ***O*** compound has an insignificant effect on this parameter. However, in all cases, the sign of the change in the engineering tensile strength was reversed, and in the case of rubbers containing the ***O*** compound, this parameter changed to a lesser extent. Here it is likely that the introduced additives shift the process toward the destruction of macromolecules, thus preventing crosslinking along the nitrile groups of the rubber. The change in the relative elongation at break after aging somewhat decreased for rubbers containing the compounds under study.

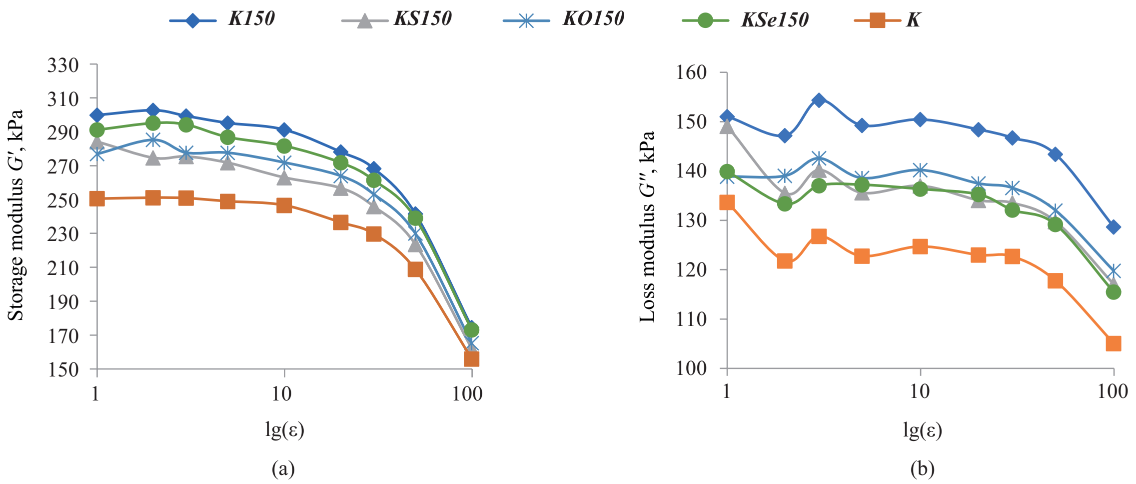
For the obtained mixtures of rubber with urea and its ***S***- and ***Se***-containing analogs, as well as rubbers based on them, the changes in storage modulus G' and loss modulus G'' were estimated. Figure 5 demonstrates the effect of urea and its ***S***- and ***Se***-containing analogs on the change in the storage and loss moduli of rubber (assessed in accordance with ASTM D6601-02) after its exposure in rheometer molds at a temperature of 150°C for 4 h.

It can be seen from Fig. 5 that prolonged exposure of BNKS-28 AN rubber to an elevated temperature (150°C for 4 h) results in a significant increase in the storage modulus and loss modulus due to crosslinking along the nitrile groups of the rubber (see Fig. 6). However, as seen from the slightly reduced values of the storage and loss moduli, the presence of ***S***, ***Se***, or ***O*** in the rubber slows down this process. At the same time, the total crosslink density after exposure to the above temperature changes by 18% for BNKS-28 AN and 8% in the case of using the ***O*** compound (Table 3). Here, it is important to note that the total crosslink density ν_{tot} is the sum of the physical crosslink density ν_{ph} and the chemical crosslink density ν_{ch}, and



(a) (b)

Fig. 4. Effect of the studied urea analogs on (a) engineering tensile strength and (b) relative elongation at break and their changes after thermo-oxidative aging at 100°C for 72 h



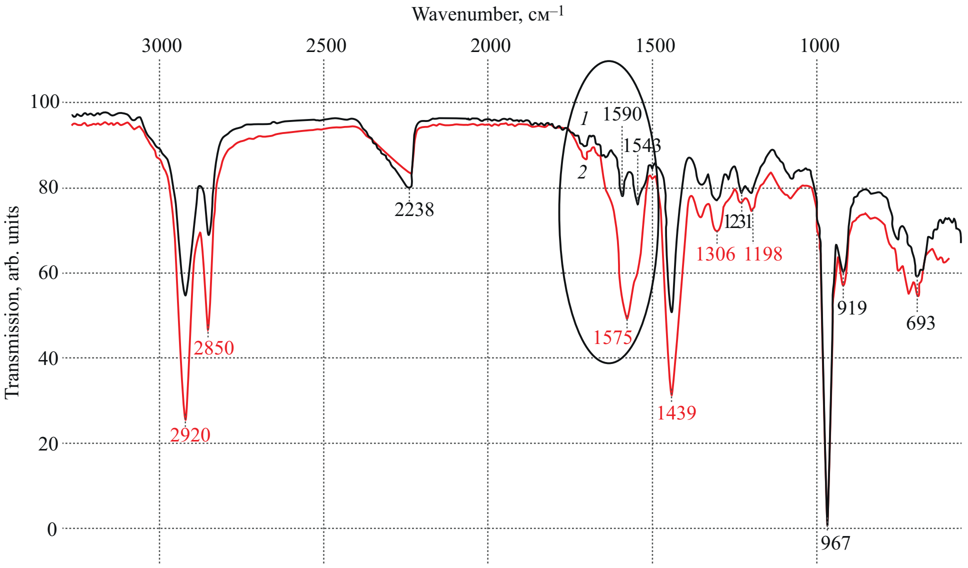
(a) (b)

Fig. 5. (a) Storage modulus G' and (b) loss modulus G'' versus logarithm ε of shear strain

Table 3. Effect of the studied compounds on the total crosslink density ν_{tot} in rubbers and elastomers before and after exposure to elevated temperatures

Exposure of rubber compounds to 150°C for 4 h				
Rubber compound	***K150***	***KO150***	***KS150***	***KSe150***
$\nu_{tot}\cdot10^{-3}$, mol/cm^3	0.33	0.30	0.30	0.32
Rubber	***P***	***PO***	***PS***	***PSe***
$\nu_{tot}\cdot10^{-3}$, mol/cm^3	0.87	0.81	0.95	0.94
Aging of rubbers at 90°C for 72 h				
Rubber	***P90***	***PO90***	***PS90***	***PSe90***
$\nu_{tot}\cdot10^{-3}$, mol/cm^3	1.16	1.02	1.20	1.22

Note: the total crosslink density of rolled BNKS-28 AN rubber is $0.28\cdot10^{-3}$ mol/cm^3.



(a)

Fig. 6. FTIR spectra before (*1*, black) and after (*2*, red) aging of rubbers containing (a) 1-(3-chlorophenyl)-3-phenylurea (***KO*** and ***KO150***), (b) 1-(3-chlorophenyl)-3-phenylthiourea (***KS*** and ***KS150***), and (c) 1-(3-fluorophenyl)-3-phenylselenourea (***KSe*** and ***KSe150***)

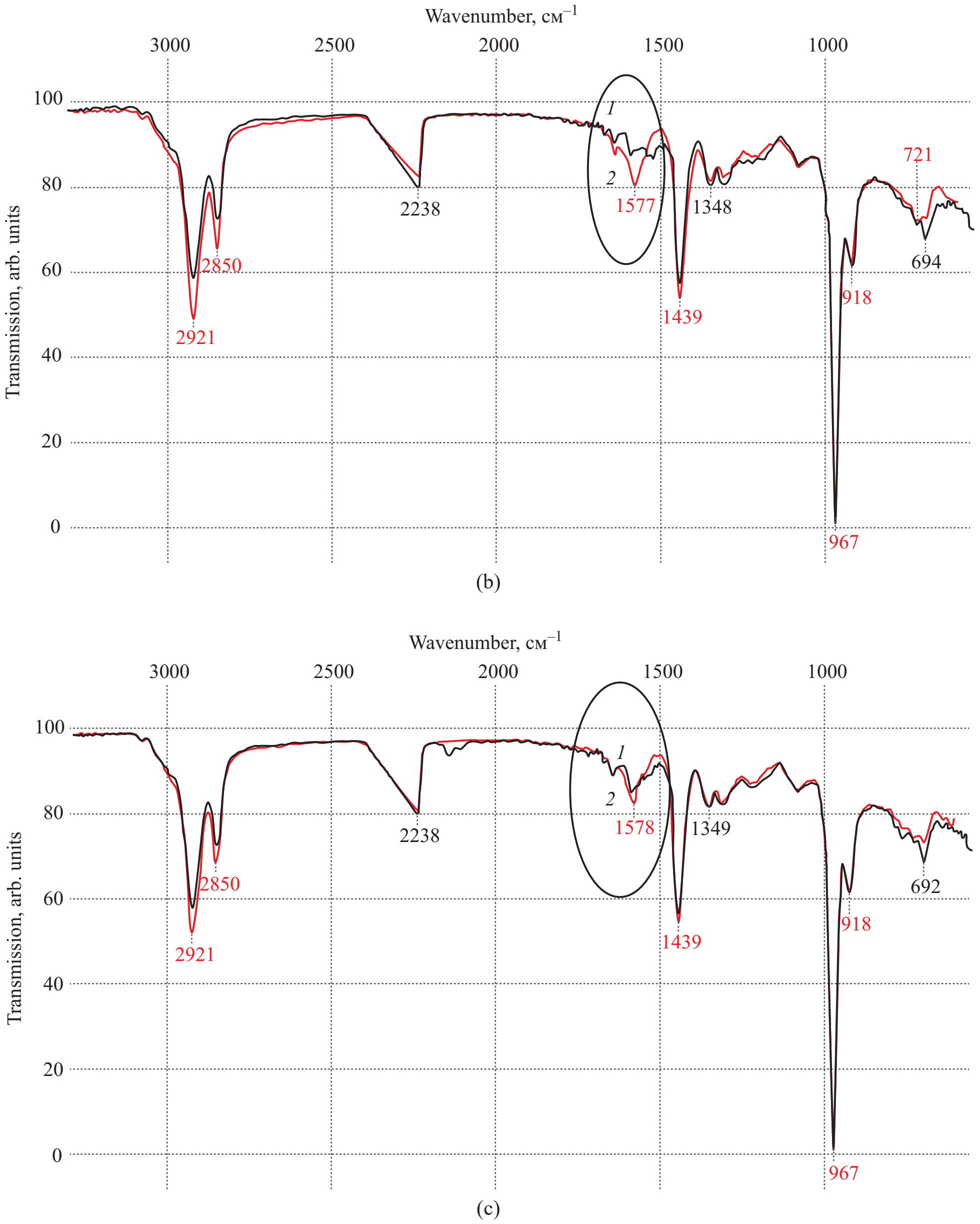
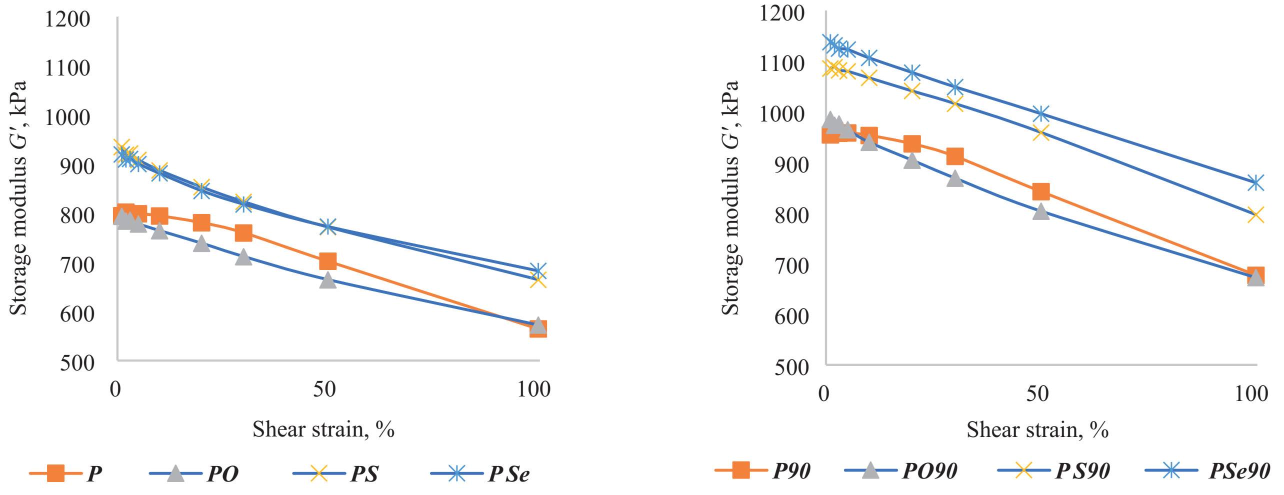


Fig. 6. FTIR spectra before (*1*, black) and after (*2*, red) aging of rubbers containing (a) 1-(3-chlorophenyl)-3-phenylurea (***KO*** and ***KO150***), (b) 1-(3-chlorophenyl)-3-phenylthiourea (***KS*** and ***KS150***), and (c) 1-(3-fluorophenyl)-3-phenylselenourea (***KSe*** and ***KSe150***)

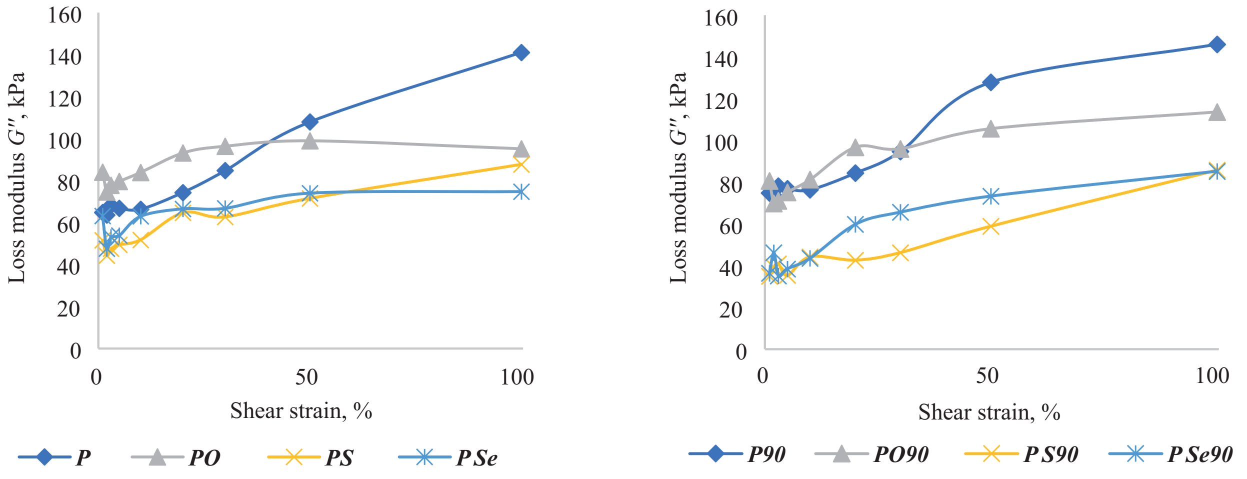
the primary ν_{tot} value estimated for noncrosslinked rubber is determined by the physical intertwining of macromolecules. Exposure of BNKS-28 AN rubber to a temperature of 150°C leads to the processes of destruction of the rubber macromolecules and their crosslinking by nitrile groups, with the latter being predominant. As a result of the structuring of the macromolecules, the rubber lost its ability to dissolve in toluene and chloroform, thus preventing an assessment of the change in the characteristic viscosity. At the same time, the FTIR spectra (Fig. 6) show a significant increase in the spectral band in the region of 1575–1590 cm^{-1}, which characterizes the formation of a C=N–C crosslink.

Despite the insignificant change in the degree of crosslinking for the rubber with urea after exposure to an elevated temperature (***KO150***), the passband at 1592 cm^{-1} (C=N–C group) demonstrated a significant increase. At the same time, there was a decrease in the band of the nitrile group of the rubber at 2250 cm^{-1}. For the ***S***-containing analog of urea, the increase in the passband at 1592 cm^{-1} (C=N–C group) and decrease in the band of the nitrile group of the rubber at 2250 cm^{-1} were exhibited to a lesser extent. In the case of using the ***Se***-analog of urea in the rubbers based on nitrile butadiene rubber, the chemical crosslinking of its macromolecules is probably due to the ability of the above compound to act as a donor of crosslinking agents,



(a) (b)

Fig. 7. Storage moduli G' (a) before and (b) after aging at 90°C for 72 h of the unfilled rubbers (***P*** and ***P90***) and rubbers containing 1-(3-chlorophenyl)-3-phenylurea (***PO*** and ***PO90***), 1-(3-chlorophenyl)-3-phenylthiourea (***PS*** and ***PC90***), and 1-(3-fluorophenyl)-3-phenylselenourea (***PSe*** and ***PSe90***)



(a) (b)

Fig. 8. Loss moduli G'' (a) before and (b) after aging at 90°C for 72 h of the unfilled rubbers (***P*** and ***P90***) and the rubbers containing 1-(3-chlorophenyl)-3-phenylurea (***PO*** and ***PO90***), 1-(3-chlorophenyl)-3-phenylthiourea (***PS*** and ***PC90***), and 1-(3-fluorophenyl)-3-phenylselenourea (***PSe*** and ***PSe90***)

rather than to the formation of C=N–C crosslinking at nitrile groups.

Similarly, the change in dynamic properties before and after aging at 90°C for 72 h was carried out in rubbers containing the ***CBS***–sulfur vulcanizing group (Figs. 7 and 8).

The rubbers containing the ***S***- and ***Se***-containing analogs of ureas demonstrate a significant increase in the storage modulus in comparison with the unfilled rubbers (Fig. 7). For the ***PO*** rubber, the modulus value remained virtually unchanged. After thermo-oxidative aging of the rubbers, an increase in the storage modulus was noted for all rubbers (Fig. 7b). In the presence of the vulcanizing group, the storage moduli of the ***S***- and ***Se***-containing urea analogs significantly increase. The change in the loss modulus due to shear deformation is shown in Fig. 8.

The dependencies in Fig. 8a indicate that the dissipation of mechanical energy into thermal energy is due to an increase in the component of the complex modulus. The introduction of urea and its ***S***- and ***Se***-containing analogs leads to a decrease in the dissipation of mechanical energy into thermal energy due to a higher total crosslink density, which increases

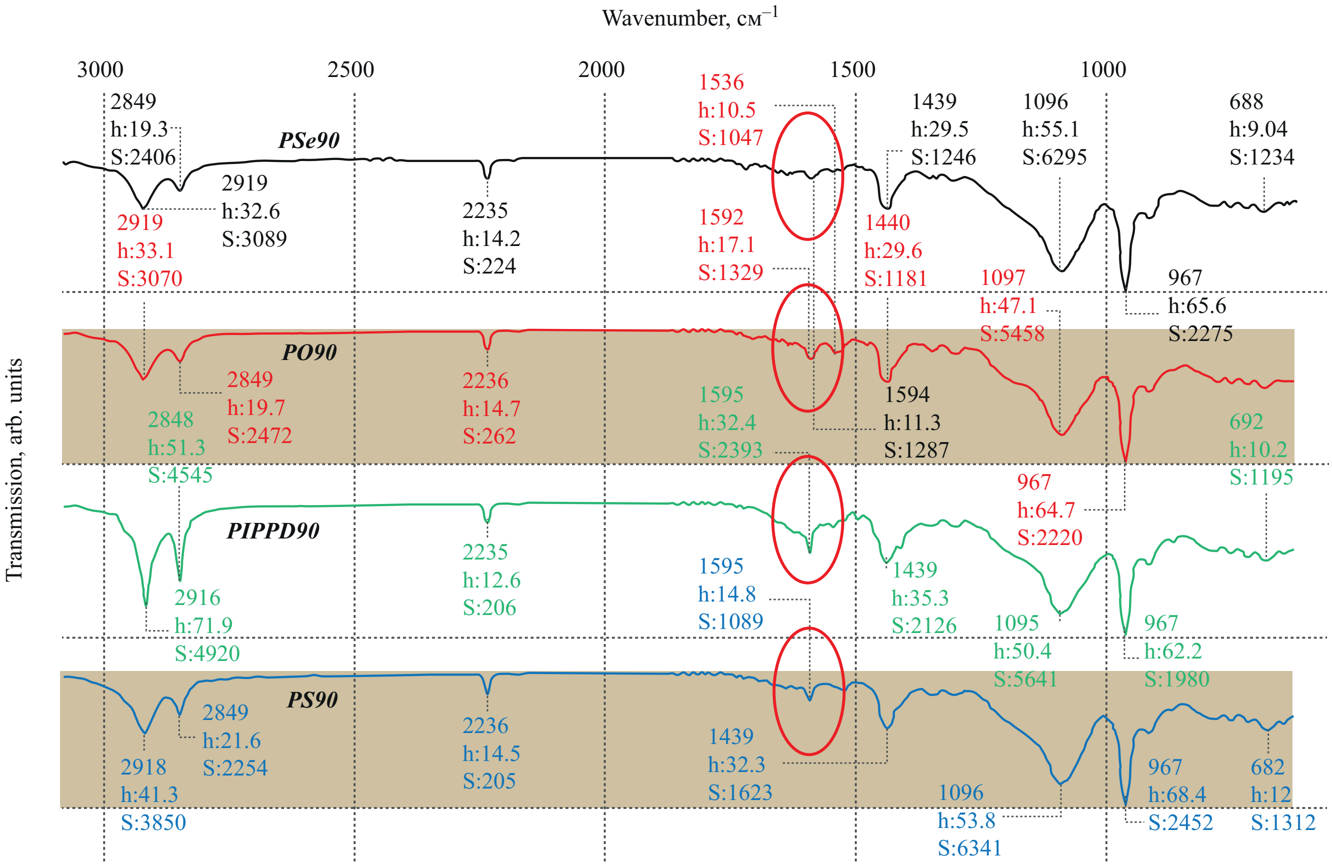


Fig. 9. FTIR spectra of rubber based on BNKS-28 AN after thermo-oxidative aging

from $0.87 \cdot 10^{-3}$ mol/cm^3 for BNKS-28 rubbers without additives to $0.94 \cdot 10^{-3}$ mol/cm^3 for the ***S***- and ***Se***-containing analogs. The loss modulus after thermo-oxidative aging (Fig. 8b) also increases to a greater extent for the ***PO90*** rubbers. In this case, the total crosslink density after thermo-oxidative aging of rubbers changes from 33%, 23%, 25%, and 29% for the rubbers ***P90***, ***PO***, ***PS90***, and ***PSe90***, respectively. This demonstrates a certain stabilizing effect of the used urea compounds. However, as indicated by the FTIR spectra, the protective action mechanisms are of a different nature (Fig. 9).

As in the case with rubber, the FTIR spectra show an increase in the transmission band in the region of 1590–1595 cm^{-1}. However, for the rubbers containing selenium (***PSe90***), no peak in this region is observed after aging, while for the analog containing sulfur, this peak is characterized by a less significant increase.

Comparing the obtained calculated data on the electron affinity energy for urea and its ***S***- and ***Se***-containing analogs (Table 1) with the total crosslink densities of the corresponding rubbers (Table 3), we note their similar trend. Namely, the decrease in the electron affinity energy in the series of the studied compounds from 0.051 and −1.115 to −1.365 eV (for ***O***, ***S***, and ***Se***, respectively) leads to an increase in the total crosslink density of the corresponding rubber samples ***PO***, ***PS***, and ***PSe*** from 23% and 25% to 29%, respectively.

CONCLUSIONS

The study has shown that 1-(3-chlorophenyl)-3-phenylurea, 1-(3-chlorophenyl)-3-phenylthiourea, and 1-(3-fluorophenyl)-3-phenylselenourea exhibit activity as vulcanization accelerators and heat stabilizers of rubbers. The values and sign of electron affinity energy obtained by quantum chemical calculations can be used to predict the possibility of using individual molecules as vulcanization accelerators. At the same time, with increasing magnitude of negative electron affinity energy, the vulcanization rate in the main period increases along with a decrease in the time before the onset of vulcanization. For example, with a change in the electron affinity energy from 0.051 (urea) to −1.115 (thiourea) and −1.365 eV (selenourea), the time before the onset of vulcanization changes from 15 to 3 and 2 min, respectively. In the case of using selenourea, according to the results of IR spectroscopy, no cyclization of nitrile groups of rubber is observed either. As a result of thermo-oxidative aging of rubbers based on BNKS-28 AN rubber without a stabilizer and with 1-(3-chlorophenyl)-3-phenylurea, 1-(3-chlorophenyl)-3-phenylthiourea, and 1-(3-fluorophenyl)-3-phenylselenourea, the total crosslink density changes in the series 33%, 23%, 25%, and 29%, respectively. In turn, the change in tensile strength after thermo-oxidative aging is +13%, −9%, −12%, and −11.3% for the rubber samples ***P***, ***PO***, ***PS***, and ***PSe***, respectively. In this regard, we note that the use of 1-(3-chlorophenyl)-3-phenylurea somewhat improves the stability of rubbers during thermal-oxidative aging, whereas 1-(3-chlorophenyl)-3-phenylthiourea and 1-(3-fluorophenyl)-3-phenylselenourea do not worsen this parameter when introduced into the rubber compound.

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Authors’ contributions

E.S. Bochkarev—design of the research concept, planning and conducting experimental studies, processing the data obtained, preparation of the data obtained for publication.

D.M. Zapravdina—design of the research concept, planning and conducting experimental studies, processing the data obtained, preparation of the data obtained for publication.

Ya.P. Kuznetsov—conducting the experiment, data processing, and analysis of the results.

I.M. Mkrtchian—conducting IR research.

V.V. Burmistrov—design of the research concept, development of the experiment, discussion and analysis of the results, writing the text of the article.

M.A. Vaniev—consultation on conducting individual stages of the study, scientific editing.

The authors declare no conflicts of interest.

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