a possibility of efficient interaction of $\cdot OO^-$ with GSH, with probable formation of stable complexes (Fig. 1). Under analogous interaction with one •OH, on the contrary, there occurs an increase of electron density on oxygen atom of hydroxyl radical by 0.208e, as a result the bond length S(22) - H(23) increases in glutathione molecule from 0.132 to 0.317 nm that points to the possibility of this atom breaking off GSH molecule and its further attachment to •OH with formation of water molecule (Fig. 2).

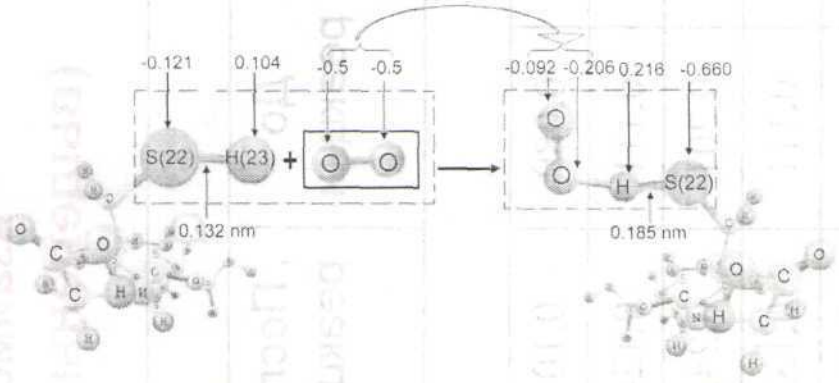

Figure 1 – Scheme of interaction of GSH molecule with $\cdot OO^-$ (arrows point to charges on atoms according to Lyovdin)

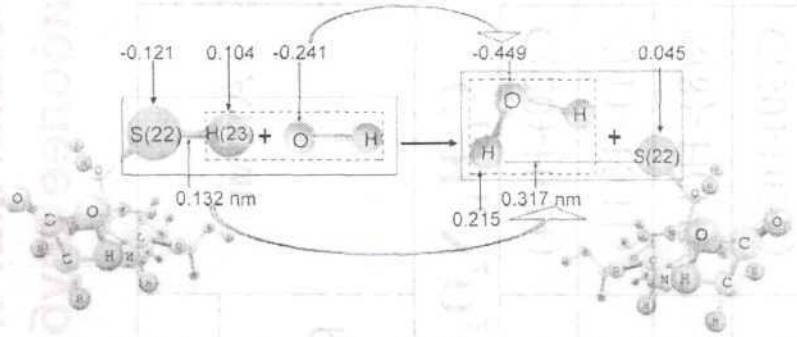

Figure 2 – Scheme of interaction of GSH molecule with •OH (arrows point to charges on atoms according to Lyovdin)

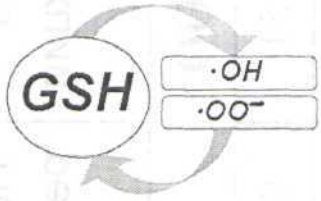

Figure 3 – Scheme of redistribution of electron density of GSH molecule as a result of interaction with radicals

Table 1 – Comparative distribution of charges q according to Lyovdin and activation energies E_a under GSH molecule interaction with free oxygen radicals at a point of global minimum

Interaction			q, a.o.			E_a, kJ/mol
			S(22)	H(23)	O*	
GSH	•OH	Without PCM	0.045	0.215	-0.449	101
		PCM	0.036	0.222	-0.465	100
	$\cdot OO^-$	Without PCM	-0.660	0.216	-0.206	17
		PCM	-0.731	0.211	-0.187	7

*Indicated atom of radical which directly interacts with atom H(23) of GSH molecule.

Thus, the interaction of a molecule of studied antioxidant with free oxygen radicals initiates redistribution of electron density in the glutathione molecule in different directions (Fig. 3) [13].

To bring the results of quantum-chemical modeling closer to real conditions of interaction of the antioxidant molecule with •OH and $\cdot OO^-$ in human organism the authors performed simulation of water medium influence on the mechanism of GSH molecule interaction with free oxygen radicals in terms of Firefly 8 program. An analysis of results obtained has shown that the mechanism of electron density redistribution with allowance for water medium influence with dielectric constant e = 78.355 at T = 298 K within the continual model of the solvent PCM for these interactions remains almost unchanged, that is confirmed by comparison of charges distribution according to Lyovdin, corresponding distances in GSH, •OH, $\cdot OO^-$, as well as the values of activation energy of the reactions of GSH molecule interaction with •OH and $\cdot OO^-$ (Table 1).

Thus, the quantum chemical simulation of glutathione molecule interaction with •OH and $\cdot OO^-$ has shown that, allowance for the influence of water medium do not practically influence redistribution of electron density of glutathione molecule and permit concluding that the studied reaction proceeds following the acid-base mechanism, under these conditions GSH appears as acid in respect of •OH in accordance with the set scheme (Fig. 3).

Thus, the mechanism of glutathione molecule interaction with •OH and $\cdot OO^-$ has been investigated.

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