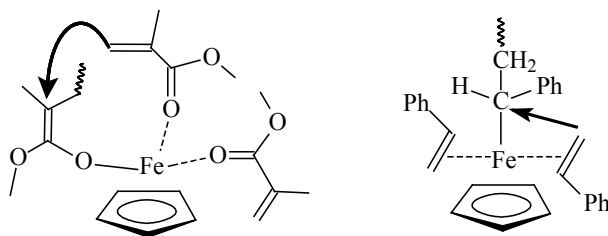


QUANTUM-CHEMICAL STUDY OF THE PROCESS OF COPOLYMERIZATION OF METHYL METHACRYLATE AND STYRENE IN THE PRESENCE OF METALLOCENES

Galimullin R.R., Friesen A.K., Sigaeva N.N., Glukhov E.A., Kolesov S.V.

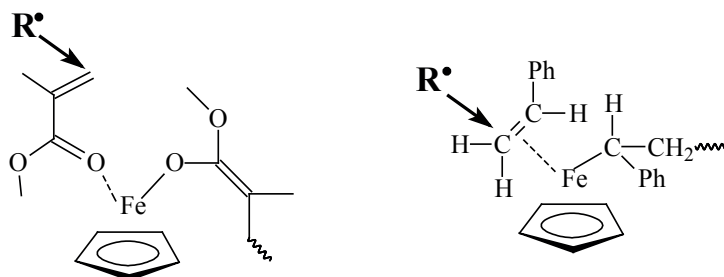
*Ufa Institute of Chemistry UFRC RAS, 450054, Ufa, prospect Oktyabrya 69,
e-mail: gip@anrb.ru*

It was previously shown that metallocenes have a significant influence on the process of radically initiated copolymerization of methyl methacrylate and styrene¹. The presence of metallocenes in the composition of the initiating system influenced the composition, molecular weights and microstructure of the copolymers obtained, as compared with copolymers obtained by initiating only benzoyl peroxide. This was associated with the formation of two types of active centers: free-radical and coordination, by analogy with the homopolymerization of these monomers^{2,3}. In the latter case, using quantum-chemical calculations, the possibility of the formation of coordination centers and their structure was established. In particular, it was shown that the coordination centers formed during the polymerization of styrene have a structure that differs from the structure of the active centers formed during the polymerization of methyl methacrylate⁴⁻⁶ (arrows indicate the direction of reactions of coordination chain growth):



Therefore, the question arose of how these active centers can work in the copolymerization of methyl methacrylate and styrene, provided that there are no homopolymers in the composition of the polymerization mass¹. In this regard, in this work, quantum-chemical calculations were carried out in order to establish the scenario of copolymerization of methyl methacrylate and styrene initiated by benzoyl peroxide in the presence of ferrocene. It was found that as a result of a series of transformations, including the release of the growth radical from the complex, the subsequent coordination of the “foreign” monomer, as well as reactions of the addition of free radicals to the molecules of metal-coordinated monomers, it is possible to rearrange one type of active site to another.

High probability of the formation of copolymers is not in the coordination sphere of the metal, as in the case of coordination growth of the homopolymer chain, but due to the addition of radicals by coordinated monomers, as shown in the diagram below:



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