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The triplet biradical states of the arenes, as a basis for paramagnetic centers of asphaltenes and a source of soft radical thermolysis in SCF-extraction processes for processing super viscous oil and resin-asphaltene mixtures

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Abstract

For the first time we were able to explain the efficiency of SCF-extraction of asphaltenes from the position of quantum-chemical analysis of elementary reactionary acts is explained. The basis is the property of polynuclear condensed aromatic hydrocarbons to be under normal conditions in the biradical triplet state relatively long time. Thanks to this, numerous radical processes are initiated, leading to a soft destruction of asphaltenes. Decay affects fragments containing ester, ester and carboxyl groups. Proceeding from the obtained energy specifics, we can state that we have described from the new side biradical triplet objects in asphaltenes, which are, in fact, analogues of the triplet form of oxygen. It is shown that the triplet biradicals of condensed polynuclear aromatic compounds show high activity under conditions of propane-butane GFR extraction. Asphalts obtained by this technology contain a considerable amount of free radicals. Concentrations of radical particles are sufficient to completely destroy the structure of the wood at temperatures of 120-140 °C. Under normal conditions, most radicals are deactivated, delocalizing themselves through arena polycycles.

With the example of naphthalene, it has been shown that aromatic condensed polynuclear compounds can exist thermodynamically in the form of biradical triplet states, which react barrierlessly with certain active radicals, for example hydroxyl radical, thus exhibiting the properties of an inhibitor of active radicals.

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