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BEHAVIOR OF ESTONIAN KUKERSITE KEROGEN IN MOLECULAR MECHANICAL FORCE FIELD

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The MM+ force field efficiency in gaining new insights into the structure, properties and genesis of Estonian kukersite kerogen is elucidated. As an initial structure 2D compositional model is used. Based on the ability of kerogen to form hydrogen bonds realistic conformers are designed. The partition of the energy components in various conformers including solvated ones is analyzed. It is shown that the presence of water molecules facilitates the creation of hydrogen bonds i.e. the formation of non-covalent cross-linking. Further experimental and computational research into the swelling behavior of kerogen is promising.

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