

NMR STUDY
OF NON-EQUILIBRIUM
STATE OF FULLERENE C₆₀
IN *N*-METHYL-2-PYRROLIDONE

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S u m m a r y

The results of ¹H NMR researches concerning the interaction between fullerene C₆₀ and *N*-methyl-2-pyrrolidone (NMP) molecules in an as-prepared solution are reported. By comparing the spectra for pure NMP and the C₆₀-NMP system, the formation of a complex between fullerene and solvent molecules is revealed, which is responsible for the time-dependent solvatochromic effect discovered earlier. Different magnitudes of chemical shifts for α -, β -, γ -, and α' -protons in the NMP molecules allowed a hypothesis to be put forward that the interaction in the C₆₀-NMP system occurs through the formation of a donor-acceptor bond between the keto-group of an NMP molecule and a fragment of a C₆₀ molecule. The results of quantum chemical simulation for the C₆₀·NMP complex with a stoichiometric composition of 1:1 testify to a redistribution of the electron density over the system of bonds in an NMP molecule induced by a C₆₀ molecule.