**Name and address of co-authors:**
Shchitova Natalia, docent
Telegina Anna, PhD student
Moscow State University, Russia

**Title:** Amphiphilic and electronic properties of acid dyes and their behaviour in wool dyeing and bioelimination

**Abstract**
Present study is focused on the detailed analysis of the behaviour of acid dyes in wool dyeing and on discussion of quantitative structure-property relationships between amphiphilic properties of dyes and their levelling, migration behaviour, rate of sorption by the fibre. Besides this light fastness of acid dyes and their bioelimination in wastewater are analysed from the point of view of electronic properties of dye molecules.

Basic principal for utilising the parameter of amphiphilicity could be illustrated by correlation of their calculated values with surface properties of several acid dyes (*C.H Giles, 1981*). Several examples of analysis of dye behavour in real dyeing systems show the possibilities of predicting the amphiphilic properties of acid dyes. One of them illustrates a good correlation between the overdyeing effect of series of acid dyes (*J. Kraska et al., 1990*) and hydrophobic properties of pyrazolone derivatives. Sorption of acid pyrazoline dyes by wool and polyamide (*N.E Evans, 1978*) exhibits also good correlation with calculated parameter of hydrophobicity.

A detailed analysis of acid dyes for wool dyeing (*A.L.Byalsky et al., 1971*) demonstrates that levelling and migration properties of dyes goes through maximum *versus* the parameter of hydrophobicity, while the rate of sorption by wool exhibits an opposite behaviour. This observation gives an evidence of dual sorption mechanism through ionic interaction with ionised amino-groups and molecular interaction with hydrophobic regions in wool.

Analysis of data base for acid, active and reactive dyes (*J.H. Churchley et al, 2000*) revealed correlation of HOMO (higher occupied molecular orbital) and LUMO (lower unoccupied molecular orbital) energies, with light fastness as well as chemical and biochemical degradation of dyes in wastewater.

The results of these studies summarise a wide variety of previous research and could be utilised for design of dyes and prediciting their technical properties such as dye affinity to wool, levellness, migration, compatibility, fastness of dyeings and bioelimination in wastewater.