INTERACTIONS IN COMPOSITES OF METHYLENE BLUE DYE WITH MoS_2 AND C60 FULLERENE CHARACTERIZED BY LASER DESORPTION/IONIZATION MASS SPECTROMETRY

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Among a variety of nanocomposites, in the present work, we studied a combination of methylene blue (MB) dye with molybdenum disulfide MoS+2 and fullerene C60. The unification of several biologically active components is currently tested for the combined therapy of cancer with the expectation of a synergistic effect of different mechanisms of action: separately, MB is used for photodynamic therapy, while MoS+2 is promising for photothermal therapy. Biological effects of C60 are also a subject of intense research. This determines the importance of studying molecular processes, possible covalent and noncovalent interactions in composites of these substances.

Two-component (MB + MoS_2), (C60 + MoS_2), (MB + C60), and three-component (MB + MoS_2 + C60) systems were prepared by ultrasound treatment of aqueous mixtures of the components.

A method of choice for studying intermolecular interactions in the multi-component systems is laser desorption/ ionization (LDI) mass spectrometry.

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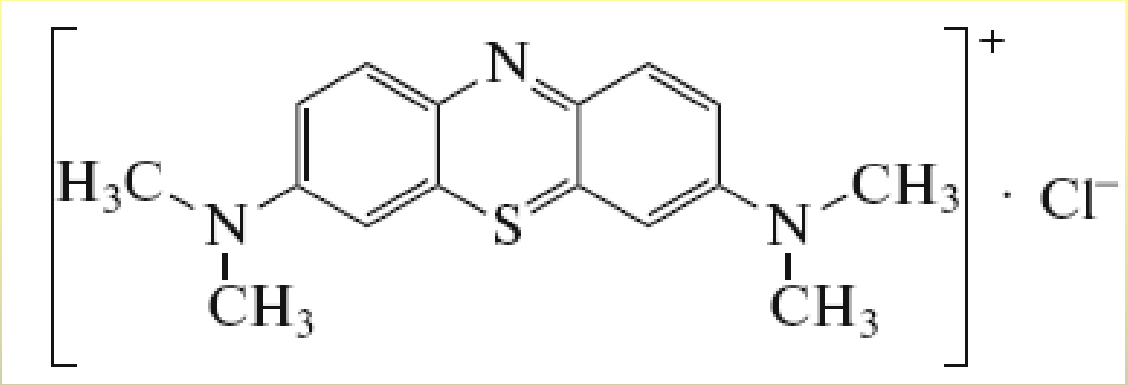
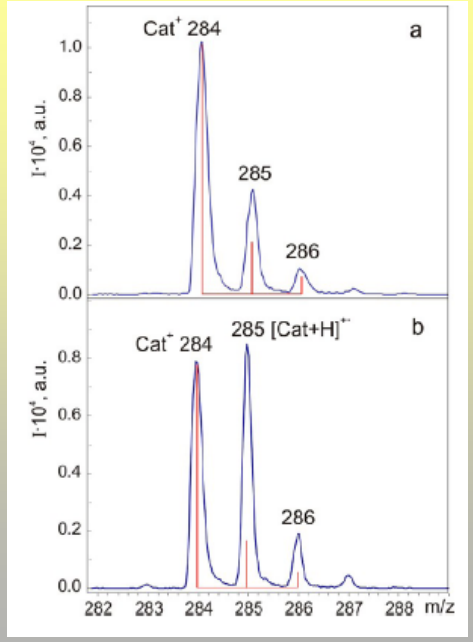
Earlier, we have established correlations between the aggregation state and intermolecular interactions of the MB dye with characteristic features of its mass spectra [1, 2], which we were guided by in our present studies. In brief, it was established that in the case of monomeric adsorption of MB+ cations on inert substrates, such as carbon nanotubes [1], an abundant signal of MB+ cation is recorded in the desorption mass spectra. In the case of MB dimerization or aggregation, a redox reaction occurs, resulting in the formation of the [MB + H]+ reduction product [2], readily detected in the mass spectra.





1. V.V. Chagovets, M.V. Kosevich, S.G. Stepanian, O.A. Boryak, V.S. Shelkovsky, V.S. Leontiev, V.A. Pokrovskiy, V.A. Karachevtsev, J Phys Chem C, **116**(38) 20579 (2012).
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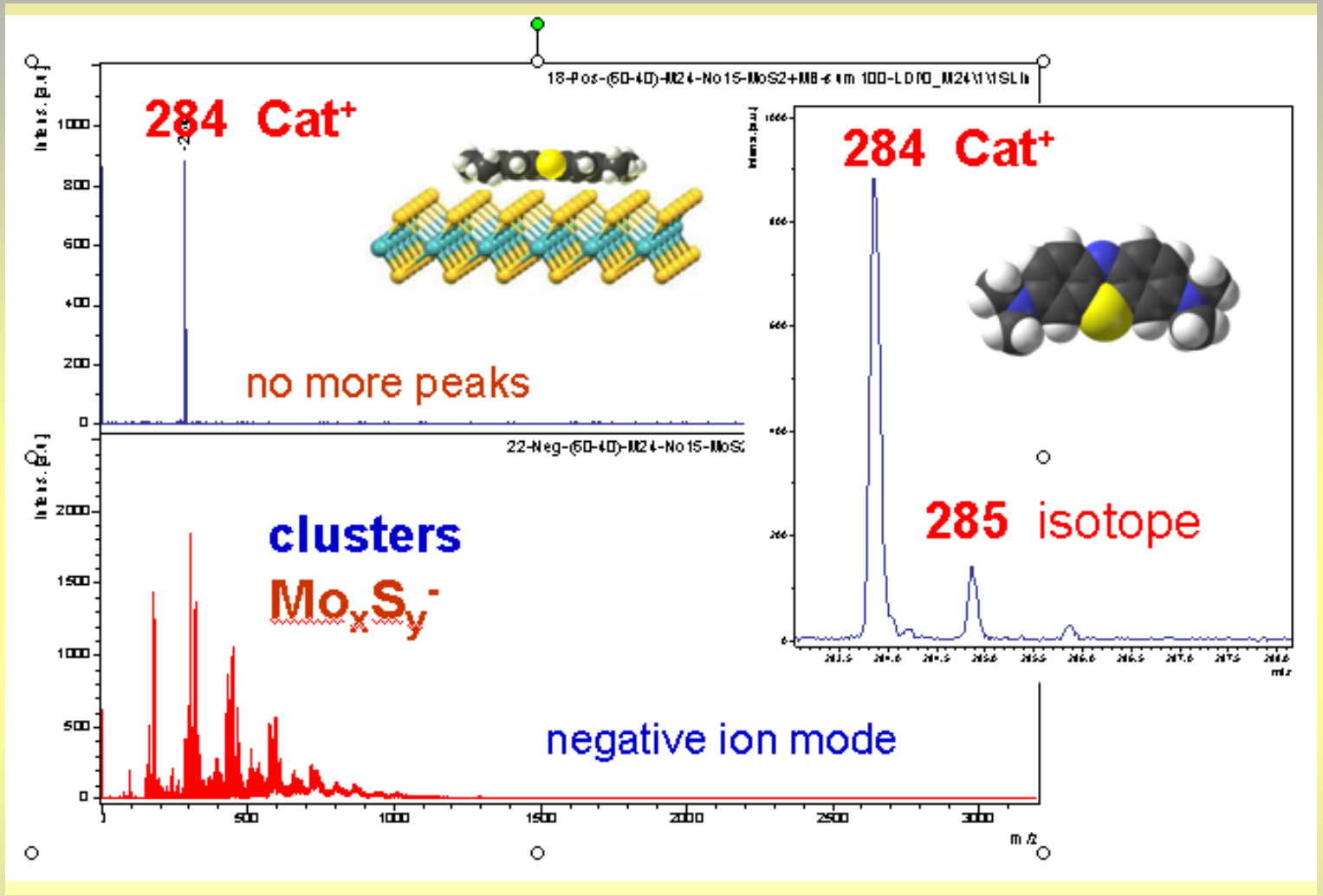
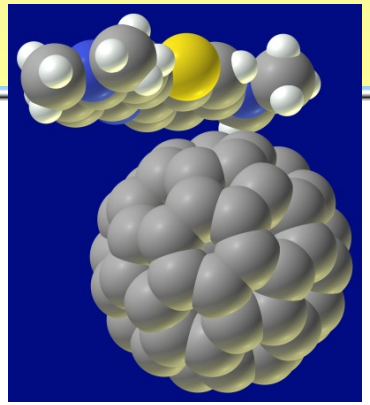


Binary ($MB+MoS_2$) system

In the positive ion LDI mass spectra of binary ($MB + MoS_2$) nanocomposite, an abundant signal of MB^+ cation was recorded, which pointed to monomeric adsorption of the MB^+ cation at the partially negative MoS_2 surface. Similarly to the case with carbon nanotubes, noncovalent electrostatic interactions took place.

In the LDI mass spectra of the binary (MB + C_{60}) system, substantial "damage" of MB^+ was observed: there was a set of peak groups corresponding to sequential loss of four methyl $–CH_3$ groups present in the MB^+ structure. In the higher mass range, there was a set of peak groups which may be tentatively attributed to MB dimer and species related to loss and addition of CH_3 groups. Obviously, these transformations were caused by redox interactions of MB^+ with C_{60}.



This effect of C_{60} was preserved in the triple (MB + MoS_2 + C_{60}) composite: a similar set of MB^+ fragments formed due to $–CH_3$ loss was registered along with the peaks characteristic of C_{60} and MoS_2. The products of MB^+ polymerization, however, were not observed obviously because of the relatively low content of MB^+ at the MoS_2 surface.